

COMPUTER ARCHITECTURE

① By Newton's eqn.

Quantum Mechanics
Mechanics of a particle can be expressed as:

$$m \frac{d^2x}{dt^2} = F$$

$$\Rightarrow -\frac{\partial V}{\partial x} = m \frac{d^2x}{dt^2}$$

$$F = -\frac{\partial V}{\partial x}$$

② By Maxwell's eqn.

$$\frac{\partial F_x}{\partial x} = \frac{F(x)}{E}$$

→ For Schrodinger's eqⁿ to be derived, assumptions made are

① It must be consistent with de-Broglie-Einstein postulates i.e.

$$\lambda = \frac{h}{P} \quad \text{and} \quad E = h\nu$$

$$\nu = c/\lambda$$

② It must satisfy the non-relativistic energy conservation i.e.

$$E = P^2 + V. \quad [V \text{ is PE}]$$

③ It must be linear in $\psi(x, t)$. That is, if ψ_1 & ψ_2 are the two separate solⁿ, then $\psi = C_1 \psi_1(x, t) + C_2 \psi_2(x, t)$, is also a solⁿ.

(any arbitrary linear combination,

ψ is have some first power
 C_1, C_2 can have any arbitrary values.

→ This assumption assures that we can add number of waves linearly to obtain wave packet

④ The PE V may be a func. of x in conservative cases & may be a func. of time as well.

for free particle, $V=0$ $\therefore F = -\frac{\partial V}{\partial x}$
 $F=0$

Writing ψ in terms of ϕ , part 1,

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

$$\frac{\partial \psi}{\partial t}, \quad E = \hbar \omega \quad \left[\text{from } \text{Q. 2} \right]$$

$$\omega = \frac{2\pi f}{\lambda} = 2\pi c N = \frac{2\pi c}{\lambda}$$

$$\hbar = \frac{e}{\omega} = \frac{h\nu g}{\omega} = \frac{hc}{2\pi c \cdot 2\pi} = \frac{h}{2\pi}.$$

$$\hbar = \frac{e}{\omega} = \frac{h\nu g}{\omega} = \frac{hc}{2\pi c \cdot 2\pi} = \frac{h}{2\pi} \Rightarrow \hbar \omega = \frac{\hbar^2 \cdot \omega^2}{2\pi} + V_0.$$

Time dependent Schrödinger wave eqn ①,

$$\text{A plane wave mechanics wave moving along } x\text{-axis is given by } \psi(x, t) = A e^{i(kx - \omega t)} \quad \text{②}$$

(i) Free particle

$$\nu = 0 \Rightarrow \mu = 0 \Rightarrow \frac{dp}{dt} = 0 \quad (\text{as, } p \text{ is constant})$$

total energy of a non relativistic free particle of mass m moving along x -axis:

$$E = \frac{p^2}{2m} \quad (\text{only KE})$$

$$\text{Now, } \frac{dp}{dt} = -i\hbar \psi \quad \text{where } \psi = \psi(x, t)$$

$$i\hbar \frac{d\psi}{dt} = \hbar \omega \psi$$

$$\text{or } i\hbar \frac{d\psi}{dt} = \frac{e}{\omega} \hbar^2 k^2 \psi$$

$$\text{Now, } \frac{d\psi}{dt} = ik\psi \text{ and } \frac{d^2\psi}{dx^2} = -k^2\psi$$

$$\text{So, } -\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} = \frac{e}{2m} \cdot \frac{d^2\psi}{dx^2}$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = \frac{1}{2m} \cdot \psi \quad \text{--- ③} \quad P = \frac{\hbar k}{2m} \cdot \frac{e}{\lambda} = \frac{e}{2m} \cdot \frac{c}{\lambda}$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = i\hbar \frac{d\psi}{dt}} \quad [\text{from Q. 2}]$$

\hookrightarrow time dependent Schrödinger wave eqn ④ ⑤

free particle of mass m .

Particle under external force

$$\text{Total Energy, } E = \frac{p^2}{2m} + V(x, t)$$

$$\text{Multiplying both sides by wave function } \psi(x, t), \\ \underline{p^2} \cdot \underline{\psi(x, t)} + \underline{V(x, t)} \cdot \underline{\psi(x, t)} = \underline{E \cdot \psi(x, t)}$$

From eqn ②,

$$\frac{p^2}{2m} \cdot \psi(x, t) + V \cdot \psi(x, t) = i\hbar \frac{d\psi}{dt} \quad \text{④}$$

and, from ③,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V \cdot \psi(x, t) = i\hbar \frac{d\psi}{dt} \quad \text{⑤}$$

Time independent Schrödinger wave equation:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V \cdot \psi(x, t) = i\hbar \frac{d\psi}{dt}.$$

0 \checkmark $\psi(x, t) = \phi(x) \cdot f(t) \rightarrow$ method of separation of variables

$$\Rightarrow -\frac{\hbar^2}{2m} f \cdot \frac{d^2\phi}{dx^2} + V(x) \phi \cdot f = i\hbar \phi \cdot \frac{df}{dt}$$

$$\Rightarrow \frac{-\hbar^2}{2m} \cdot \frac{1}{\phi} \frac{d^2\phi}{dx^2} + V = i\hbar \cdot \frac{1}{f} \frac{df}{dt} = E \cdot \phi(x)$$

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

(iii) is analogous to Schrödinger eq':

$$\frac{d^2\psi}{dx^2} + k_0^2 \psi = 0$$

to minimize

$$\text{Now, } i\hbar \frac{1}{i\hbar} \frac{df}{dt} = E \cdot dt$$

$$\Rightarrow i\hbar \frac{df}{dt} = E \cdot dt$$

$$\Rightarrow \ln f = \int_{t_0}^t E \cdot dt + \ln C$$

$$\Rightarrow \ln(f/c) = \frac{-i}{\hbar} E t$$

$$\Rightarrow f(t) = c \cdot e^{-\left(\frac{iE}{\hbar}\right)t}$$

$$\text{Now, } \psi(n, t) = c \cdot \phi(n) \cdot e^{-(iE/\hbar)t}$$

$\phi(n) \rightarrow$ eigen func'
 $\psi(n) \rightarrow$ wave func'

now, energy in case of bound situation are discrete & every possible energy has a corresponding eigen function. In general,

$$\psi(n, t) = \sum_{n=1}^{\infty} c_n \phi_n(x) \cdot e^{-(iE/\hbar)t}$$



e.g.

Particle in an infinite potential well —
 (particle in a box) for $0 < x < L$, $\psi(x) = 0$

in region $L < x < \infty$, $\psi(x) = 0$
 boundary condition i.e. $\phi(x=0) = 0$ & $\phi(x=L) = 0$

on region 2,

$$-\frac{\hbar^2}{2m} \frac{d^2\phi}{dx^2} = E \cdot \phi$$

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

$$\Rightarrow \boxed{\frac{d^2\phi}{dx^2} + \frac{2mE}{\hbar^2} \cdot \phi = 0}$$

Ex:

$$\phi(n) = \text{incident} + \text{reflected}$$

$$f = 0 \text{ at } x=0 \Rightarrow B = 0$$

$$\phi(n) = A \sin(kx)$$

$$\text{Now, } kL = n\pi \quad n = 1, 2, 3, \dots$$

$$\Rightarrow \text{Now, } E_n = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2m L^2} \propto \frac{n^2 \hbar^2}{2m L^2}$$

$$\text{Thus, } \phi(x) = A \sin \frac{n\pi}{L} x$$

E_1, E_2, E_3, \dots are possible energies for a free particle confined in a box.
 ϕ_1, ϕ_2, \dots are possible eigen functions

PROBABILITY DENSITY:

- presence of i in the wave function means that ψ has no physical interpretation.
- But wave function has physical interest. Wave function has all the information of a particle which the uncertainty principle allows.
- Has defined a term called probability density $P(x, t)$ which gives the probability per unit length / volume of finding the particle near x and at time t .
- Relation betw. $\rho(x, t)$ and wave function

$$\rho(x, t) = \psi^*(x, t) \cdot \psi(x, t)$$

$|\psi|^2 = \psi^* \psi$ is always real & positive

$$x_1 + x_2 = R + i\theta$$

$$\frac{\partial P}{\partial t} = \frac{1}{2m} \left[\frac{\partial^2 \psi}{\partial x^2} \left(p^2 \frac{\partial \psi}{\partial x} - p \frac{\partial p}{\partial x} \right) \right]$$

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

$$= -\frac{\partial (S)}{\partial x}$$

$$\frac{\partial P}{\partial t} + \frac{\partial S}{\partial x} = 0$$

$$S = \frac{-i\hbar}{2m} \left[p^2 \frac{\partial \psi}{\partial x} - \psi \frac{\partial p}{\partial x} \right]$$

$$E_1 \quad \psi^* = \psi, \quad S = 0$$

* for the particle,

$$\psi \sim e^{i\hbar t} (A_n e^x - B_n e^{-x})$$

$$\psi^* \sim e^{-i\hbar t} (A_n' e^x - B_n' e^{-x})$$

$$\frac{E}{E_0} = \frac{V}{V_0} = \frac{c}{c_0} = \frac{1}{\epsilon_0}$$

$$\int E \cdot d\vec{s} = \frac{q - q'}{c_0}$$

$$\Rightarrow E \Lambda = \frac{q - q'}{c_0} \cdot \frac{c_0}{c}$$

$$\Rightarrow E = \frac{q}{A_{th}} - \frac{q'}{A_{th}}$$

$$\Rightarrow \frac{E_0}{E_{th}} = \frac{q}{A_{th}} - \frac{q'}{A_{th}}$$

$$\Rightarrow \frac{q}{A_{th}} = \frac{q}{A_{th}} - \frac{q'}{A_{th}}$$

$$\Rightarrow q' = q - q'$$

$$\Rightarrow q' = q \left(1 - \frac{1}{c_0} \right)$$

$$* \quad f \cdot d\vec{s} = \frac{q}{c_0} - \frac{1}{c_0} (q_0 - q)$$

$$= \frac{q_0}{c_0 \epsilon_0} = \frac{q_0}{\epsilon_0 c_0}$$

$$\Rightarrow \frac{q_0}{\epsilon_0 c_0} = \frac{q_0}{\epsilon_0 c_0}$$

θ = flux density
 B = electric field
 P = polarization.

$$\Rightarrow \frac{P}{A} = \frac{B_0 t + P_0}{B_0 t + P_0}$$

$$* \quad \rho_c = \frac{ze \times \text{charge inside the sphere of radius } r}{4\pi \epsilon_0 \cdot r^2}$$

$$\text{charge density, } \rho = \frac{-ze}{4\pi r^3}$$

$$\text{charge inside the sphere of radius } r = \frac{4\pi}{3} \frac{r^3}{\epsilon_0} n^2$$

$$\therefore \rho_c = -ze \times \frac{2e \frac{r^3}{\epsilon_0}}{4\pi r^3} = -\frac{2^2 e^2 r}{4\pi \epsilon_0 \cdot r^3}$$

$$* \quad \text{At equilibrium, } \rho_c = -zeE \quad (\text{Gauss's law})$$

$$\Rightarrow \frac{+2e^2 r}{4\pi \epsilon_0 \cdot r^3} = +zeE$$

$$\Rightarrow \boxed{r = \frac{4\pi \epsilon_0 \cdot z E}{2e}}$$

Therefore, electric dipole moment

$$\mu_e = Z e \alpha$$

$$\mu_e \propto E$$

$\frac{\alpha_e}{\alpha_e = 4\pi e_0 \cdot R^3}$

Gelijke massa per unit elektrische lading

\rightarrow if no. of open seats α unit volume in N , then
classification is given as

$$P_c = 10^{10} \text{ erg/s}$$

$$f_i = \lambda \alpha_i E$$

$$f = N^{4\pi G \rho / c^4}$$

$$f_e = \frac{N}{m \cdot v}$$

Susceptibility

$$\Delta = \text{def} \in \tau$$

$$= \overline{P} + \overline{E}$$

$$\Rightarrow \vec{p} = \vec{E}(e - e_0)$$

$$= \overline{E} (e_x - e_c)$$

$$= \overrightarrow{g_0} f_{\epsilon_k - 1}$$

$$\Rightarrow \ell_{\alpha-1} = \frac{P}{\ell_\alpha E} = \kappa \quad (\text{defines how easily } g \text{ can be carried out})$$

(defines how easily ^{to} in what
context a desire can
be pacified with the
help of electric jolt.)

$$\begin{aligned}
 X &= \frac{\rho}{\epsilon_0 c} = \frac{N \mu e}{\epsilon_0 c} \\
 &= \frac{N \alpha \epsilon_0}{\epsilon_0 c} = \frac{N \alpha \epsilon}{c} \\
 \alpha &= \frac{X \epsilon_0}{N} = \frac{N \mu e V}{N c \epsilon_0} = \frac{\mu e V}{c \epsilon_0} \\
 &\text{freq of } CO_2 = 6.023 \times 10^{13} \text{ Hz} \\
 &\text{freq of } CO_2 = 6.023 \times 10^{13} \text{ Hz} \\
 &\text{freq of } CO_2 = \frac{6.023 \times 10^{13}}{94} \\
 &\text{freq of } CO_2 = 6.4 \times 10^{12} \text{ Hz} \\
 &Y = \frac{M}{V} \\
 1.447 &= \frac{44 \times 10^{-3}}{N_0 \times V} \\
 &= \frac{44 \times 10^{-3}}{6.023 \times 10^{23} \times V} \\
 V &= \frac{44 \times 10^{-3}}{6.023 \times 10^{23} \times 1.447} \\
 \alpha_e &= 4 \pi \epsilon_0 \cdot R^3 \\
 &= 4 \pi \epsilon_0 \times (2 \times 10)^3 \\
 \text{Given } R &= ? \quad \epsilon = ? \quad N = 2.4 \times 10^{25} \\
 \alpha_e &= 4 \pi \epsilon_0 \cdot R^3 \\
 \Rightarrow R &= \left(\frac{\alpha_e}{4 \pi \epsilon_0} \right)^{1/3} = 5.42 \times 10^{-11} \text{ m} \\
 \text{Given } \alpha_e &= 1 - \chi \quad \text{A/c to Langmuir's theory of polarization} \\
 &= 1 - \chi \quad \text{theory of polarization} \\
 \chi &= N_0 \epsilon_0 \left[e^{4 \pi \epsilon_0} - \frac{1}{a} \right]
 \end{aligned}$$

* classical mechanics

$$\text{Given: } x\dot{x} + y\dot{y} + z\dot{z} = R^2 \sin \omega t \\ \frac{\partial}{\partial t} (x\dot{x} + y\dot{y} + z\dot{z}) = R^2 \sin \omega t$$

$$x\ddot{x} + y\ddot{y} + z\ddot{z} = R^2 \sin \omega t \cdot \omega^2 \\ \frac{x^2}{2} + \frac{y^2}{2} + \frac{z^2}{2} = -\frac{R^2 \cos \omega t + C}{\omega^2}$$

$$\Rightarrow x^2 + y^2 + z^2 - 2c + \frac{2R^2 \cos \omega t}{\omega^2} = 0$$

$$f(x, y, z, t) = 0$$

$$\frac{df}{dt} = -2a^2 \sin \omega t \neq 0$$

So, homogeneous & non-linear

$$\text{dof} = 3N - 1 = 3 \cdot 2 - 1 = 2 = \text{dimension of config. space}$$

$$T = \frac{1}{2} m \dot{\theta}_1^2 + \kappa \dot{\theta}_2 \dot{\theta}_2 + \frac{1}{2} \beta \dot{\theta}_2^2 \quad \text{dof} = 2$$

$$P = \frac{1}{2} \kappa \dot{\theta}_2^2$$

$$\textcircled{1} \quad L = T - V = \frac{1}{2} m \dot{\theta}_1^2 + \kappa \dot{\theta}_2 \dot{\theta}_2 + \frac{1}{2} \beta \dot{\theta}_2^2 - \frac{1}{2} \kappa \dot{\theta}_2^2$$

$$\textcircled{2} \quad P_1 = \frac{\partial L}{\partial \dot{\theta}_1}$$

$$P_1 = \frac{\partial L}{\partial \dot{\theta}_1} = m \dot{\theta}_1^2$$

$$\textcircled{3} \quad P_2 = \frac{\partial L}{\partial \dot{\theta}_2} = \kappa \dot{\theta}_2 + \beta \dot{\theta}_2^2$$

$$\textcircled{4} \quad \dot{P}_1 = -\frac{\partial V}{\partial \theta_1}$$

$$\textcircled{5} \quad \dot{P}_2 = -\frac{\partial V}{\partial \theta_2} - \kappa \theta_2 - \beta \theta_2^2 = 0$$

$$\textcircled{6} \quad \frac{\partial L}{\partial \theta_1} = \alpha \dot{\theta}_2 - \kappa \theta_2 - \beta \theta_2^2 = 0$$

α, β is the cyclic component of P_2 .

$$\textcircled{5} \quad \dot{\theta}_2 \rightarrow \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}_2} \right) - \frac{\partial L}{\partial \theta_2} = 0$$

$$\therefore \frac{d}{dt} (m \dot{\theta}_2) - (\kappa \dot{\theta}_2 - \beta \theta_2) = 0$$

$$\Rightarrow m \ddot{\theta}_2 - \kappa \dot{\theta}_2 + \beta \theta_2 = 0$$

$$\dot{\theta}_2 \rightarrow \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}_1} \right) - \frac{\partial L}{\partial \theta_1}$$

$$\therefore \frac{d}{dt} (m \dot{\theta}_1) - (\alpha \dot{\theta}_2 - \beta \theta_2) = 0$$

$$\Rightarrow \alpha \dot{\theta}_2 + \beta \dot{\theta}_2 = 0 \quad / \quad \alpha \dot{\theta}_2 + \beta \dot{\theta}_2 = \text{constant}$$

Physics

#Maxwell-Boltzmann stat.

$$W = \prod_{i=1}^n \frac{n!}{m_i!} \left(\beta_i\right)^{m_i} \quad \text{probabilities}$$

#No. way.

$$N = T! \frac{\theta_1!}{m_1!} \frac{\theta_2!}{m_2!} \dots \frac{\theta_n!}{m_n!}$$

#B.E. stat.

$$(g_i + n_{i-1}) C_{n_i}$$

#Pipelining

Component Arrangement

Number of jobs = n_k
Time taken by each job
each job is divided into k subjobs

$$\begin{matrix} P_1 \\ P_2 \\ P_3 \\ \vdots \\ P_k \end{matrix}$$

Time taken by one pipeline process = $\eta_k t$

$$\# \text{ Efficiency, } \eta_k = \frac{n_k t}{n} = \frac{n_k}{k + (n-1)}$$

#Efficiency, $\eta_k = \frac{n_k}{k + (n-1)} \rightarrow$ Part delay.

#Pipelining is a technique of decomposing a certain sequential task into subtasks, with each subtask being executed in a special dedicated stage that

operates concurrently with all other stages.

Speed up (S_k)

$T \rightarrow$ total period
pipelined \rightarrow total time required = $[k + (n-1)]T$

Non-pipelined \rightarrow $T_k = n_k T$

$$S_k = \frac{T_k}{T} = \frac{n_k T}{[k + (n-1)]T} = \frac{n_k}{[k + (n-1)]}$$

$\max n_k \rightarrow k$. as $n \rightarrow \infty$

#Efficiency, E_k

$$\frac{E_k}{K} = \frac{S_k}{K} = \frac{n_k}{[k + (n-1)]}$$

#throughput, H_k : Number of jobs completed in single unit time

$$H_k = \frac{E_k}{T} = \frac{n_k}{T[k + (n-1)]} = \frac{n_k}{[k + (n-1)]T}$$

$\max n_k H_k = \frac{1}{T} = f$ when $E_k \rightarrow 1$ as $n \rightarrow \infty$

$$\boxed{H_k = E_k \cdot f = \frac{E_k}{T} = \frac{S_k}{K T}}$$

#Classification of Pipelining

Pipelining

① Static or linear
Pipelining

→ everything is decided
prior to the process

② Dynamic or Next-line pipelining
→ configuration may change as of when
required
→ more useful
→ much more complex & expensive

- * Types:
- ① Arithmetic Pipelining
 - ② Instruction Pipelining
 - ③ Processor Pipelining

Processor Pipeline

$$\text{① } \begin{array}{|c|c|c|c|c|c|c|} \hline S_1 & 1 & 2 & 3 & 4 \\ \hline X & X & X & X & X \\ \hline \end{array} \quad \text{Evaluation since } d = 1.$$

$$\begin{array}{|c|c|c|c|c|c|c|} \hline S_1 & 1 & 2 & 3 & 4 \\ \hline X & X & X & X & X \\ \hline \end{array}$$

$$\text{Forbidden gaps} = 2 - 1 = 1, \quad 2 - 6 = 4, \quad 6 - 1 = 5,$$

$$4 - 2 = 2, \quad 5 - 3 = 2, \quad 7 - 5 = 2$$

$$\therefore 7 - 3 = 4$$

$$\rho_L = 1, 3, 6, 8^+$$

Initial collision vector

$$\begin{array}{ccccccc} 2 & 7 & 6 & 3 & 4 & 3 & 2 & 1 \\ 0 & 1 & 0 & 1 & 2 & 0 & 1 & 0 \end{array}$$

$$\therefore \text{ev} = \underline{\underline{1011010}} \longrightarrow \textcircled{state 1}$$

→ right shift size by 1 of register or

$$\begin{array}{ccccccc} 1 & 0 & 1 & 4 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 \end{array}$$

$$\underline{\underline{1111111}} \quad (\text{state 2})$$

$$\rho_L = 8^+$$

→ right shift size by 3 of register or

$$\begin{array}{ccccccc} 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 \end{array}$$

$$\underline{\underline{1011011}} \quad (\text{state 3}) \quad \rho_L = 3, 6, 8^+$$

→ right shift size by 6 of register or

$$\begin{array}{ccccccc} 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{array}$$

$$\underline{\underline{1011011}} \quad (\text{final write})$$

$$\begin{array}{|c|c|c|c|c|c|c|} \hline S_1 & 1 & 2 & 3 & 4 \\ \hline X & X & X & X & X \\ \hline \end{array}$$

$$\rightarrow \text{right shift by 1},$$

$$100$$

$$\begin{array}{c} 0 \\ 1 \\ 1 \\ 1 \end{array} \quad (\text{S1})$$

$$\rightarrow \text{right shift by 2},$$

$$100$$

$$\begin{array}{c} 0 \\ 0 \\ 1 \\ 1 \end{array} \quad (\text{S2})$$

$$\begin{array}{c} 1 \\ 0 \\ 0 \\ 1 \end{array} \quad (\text{S3})$$

$$\begin{array}{c} 1 \\ 0 \\ 0 \\ 0 \end{array} \quad (\text{S4})$$

Simple queue:

$$(1, 4), (2, 4),$$

$$(1, 1, 4), (2, 2, 4)$$

$$(1, 1, 1, 4), (1, 2, 2, 4)$$

$$(1, 1, 1, 1, 4), (1, 2, 2, 1, 4)$$

$$(1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 4)$$

$$(1, 1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 1, 4)$$

$$(1, 1, 1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 1, 1, 4)$$

$$(1, 1, 1, 1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 1, 1, 1, 4)$$

$$(1, 1, 1, 1, 1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 1, 1, 1, 1, 4)$$

$$(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 1, 1, 1, 1, 1, 4)$$

$$(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 4), (1, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 4)$$

$$\text{Graded queue: } \underline{\underline{1234}}$$

STATISTICAL MECHANICS

o Statistical mechanics is the branch of physics which studies macroscopic system from a microscopic or molecular point of view.

→ Its goal is to understand & predict macroscopic phenomena, i.e. to calculate macroscopic properties from the properties of the individual molecules making up the system.

→ Thus, the aim of statistical mechanics is to derive the general laws of thermodynamics by all thermodynamic relations for a given system.

→ The main object of S.M. "To establish the laws governing the behavior of macroscopic quantity of a system by using the laws governing the behavior of the particles of that system in thermal equilibrium."

CLASSIFICATION

statistical
mechanics

quantum
mechanics

classical
statistical
mechanics

(ideal with classical particle)
→ classical mechanics
→ classical statistics
Eg: ideal gas molecules

PHYSICS LAB

Expt 1: Verification of Stefan's law & determination of Stefan's constant.

o Total energy of all wavelengths radiated from a black body depends upon its Temp. only.

→ If we consider law, total radiant energy E (radiated uniformly) emitted, radiated per second from unit surface area of black body is proportional to fourth power of its absolute temp.

$$E \propto T^4$$

$$\Rightarrow E = \sigma T^4$$

→ If body is not perfectly black & has relative emittance ϵ then $E = \epsilon \sigma T^4$

$$\therefore T = \sqrt[4]{\frac{E}{\epsilon \sigma}}$$

→ Stefan's law is true for both emission & absorption of radiant energy. Stefan's theory of heat exchange,

→ $\frac{1}{2} \epsilon \sigma T^4$ to a black body at absolute temp T_1 passes σT_1^4 per secnd black body B at absolute temp T_2 , passes σT_2^4 per secnd per unit area each of gains σT_1^4 & σT_2^4 per unit area per secnd respectively. Hence, net loss of energy per secnd per unit area is given by, $E = \sigma (T_1^4 - T_2^4)$ the black body is given by,

→ For a non-black body, total emitted energy per secnd per unit area, $E = \sigma \epsilon (T_1^4 - T_0^4)$

* Apparatus: Metal filament inside electrode (made of nickel) is made of tungsten → The temp coefficient of the resistance goes up to 10^4 K per $1^\circ C$. remain constant upto very high temperature of the filament;

$$\left(\frac{R_2}{R_{273}} \right) = \left(\frac{T_2}{273} \right)^{1.2}$$

$$(A) \sin(\omega t + \phi) = \alpha e^{j\omega t}$$

$$(B) \alpha = BN - K$$

$$= g(x) - L$$

$$= 2$$

\Rightarrow Holonomic = integrable

Integrability $\Rightarrow f'(x_1, x_2) = 0$

Exogeneity $\Rightarrow f'(y_1, y_2) = 0$

Order = No. of independent variable

Required to specify a classical mechanical system is called dof.

(C) dimension = dof = 2

$$(D) \frac{dx}{dt} + b \cdot \frac{dy}{dt} + c \cdot \frac{dz}{dt} = \alpha t^2$$

$$\Rightarrow x \dot{x} + y \dot{y} + z \dot{z} = \alpha t^2 dt$$

$$\Rightarrow \frac{x^2}{2} + \frac{y^2}{2} + \frac{z^2}{2} = \frac{\alpha}{3} t^3 + C \quad \rightarrow \text{Holonomic}$$

$$\Rightarrow x^2 + y^2 + z^2 = \frac{2\alpha}{3} t^3 + 2C$$

$$\Rightarrow x^2 + y^2 + z^2 - q_0 - \frac{2}{3} \alpha t^3 = 0$$

$$f(x_1, y_1, z_1, t) = 0$$

$$\Rightarrow \frac{\partial f}{\partial t} = -2at^2 \neq 0 \rightarrow \text{Nonholonomic}$$

$$(E) \quad T = \alpha g_1 g_1 + \beta g_2 g_2 \quad V = \text{free}(g_2)$$

$$(F) \quad L = p_1 \dot{v}_1 - \alpha g_1 g_1 - \beta g_2 g_2 - V_{\text{ext}}(g_1)$$

$$L = p_1 \dot{v}_1$$

$$\Rightarrow \text{gen. mech. } T$$

$$p_1 = \frac{\partial L}{\partial \dot{v}_1}$$

$$\text{gen. func. } \{g_1\}$$

$$g_1 = \frac{\partial L}{\partial v_1}$$

$$\text{gen. func. } \{g_2\}$$

$$g_2 = \frac{\partial L}{\partial \dot{v}_2}$$

$$\text{gen. func. } \{g_3\}$$

$$g_3 = \frac{\partial L}{\partial \ddot{v}_3}$$

$$\text{gen. func. } \{g_4\}$$

$$g_4 = \frac{\partial L}{\partial \dot{v}_4}$$

$$\text{gen. func. } \{g_5\}$$

$$g_5 = \frac{\partial L}{\partial \dot{v}_5}$$

$$\text{gen. func. } \{g_6\}$$

$$g_6 = \frac{\partial L}{\partial \dot{v}_6}$$

$$\text{gen. func. } \{g_7\}$$

$$g_7 = \frac{\partial L}{\partial \dot{v}_7}$$

$$\text{gen. func. } \{g_8\}$$

$$g_8 = \frac{\partial L}{\partial \dot{v}_8}$$

$$\text{gen. func. } \{g_9\}$$

$$g_9 = \frac{\partial L}{\partial \dot{v}_9}$$

$$\text{gen. func. } \{g_{10}\}$$

$$g_{10} = \frac{\partial L}{\partial \dot{v}_{10}}$$

$$\text{gen. func. } \{g_{11}\}$$

$$g_{11} = \frac{\partial L}{\partial \dot{v}_{11}}$$

$$\text{gen. func. } \{g_{12}\}$$

$$g_{12} = \frac{\partial L}{\partial \dot{v}_{12}}$$

$$\text{gen. func. } \{g_{13}\}$$

$$g_{13} = \frac{\partial L}{\partial \dot{v}_{13}}$$

$$\text{gen. func. } \{g_{14}\}$$

$$g_{14} = \frac{\partial L}{\partial \dot{v}_{14}}$$

$$\text{gen. func. } \{g_{15}\}$$

$$g_{15} = \frac{\partial L}{\partial \dot{v}_{15}}$$

$$\text{gen. func. } \{g_{16}\}$$

$$g_{16} = \frac{\partial L}{\partial \dot{v}_{16}}$$

$$\text{gen. func. } \{g_{17}\}$$

$$g_{17} = \frac{\partial L}{\partial \dot{v}_{17}}$$

$$\text{gen. func. } \{g_{18}\}$$

$$g_{18} = \frac{\partial L}{\partial \dot{v}_{18}}$$

$$\text{gen. func. } \{g_{19}\}$$

$$g_{19} = \frac{\partial L}{\partial \dot{v}_{19}}$$

$$\text{gen. func. } \{g_{20}\}$$

$$g_{20} = \frac{\partial L}{\partial \dot{v}_{20}}$$

$$\text{gen. func. } \{g_{21}\}$$

$$g_{21} = \frac{\partial L}{\partial \dot{v}_{21}}$$

$$\text{gen. func. } \{g_{22}\}$$

$$g_{22} = \frac{\partial L}{\partial \dot{v}_{22}}$$

$$\text{gen. func. } \{g_{23}\}$$

$$g_{23} = \frac{\partial L}{\partial \dot{v}_{23}}$$

$$\text{gen. func. } \{g_{24}\}$$

$$g_{24} = \frac{\partial L}{\partial \dot{v}_{24}}$$

$$q(t, x, v) = e^{-i(Kx - \omega t)}$$

$$S = -\frac{i\hbar}{2m} \int [v^* \frac{\partial \psi}{\partial x} - v \frac{\partial \psi^*}{\partial x}]$$

$$+ \frac{e}{2m} \int [e^{-i(Kx - \omega t)} \cdot A e^{i(Kx - \omega t)} \cdot (\frac{\hbar}{i} \nabla) +$$

$$e^{-i(Kx - \omega t)} \cdot (\frac{\hbar}{i} \nabla) \cdot A e^{i(Kx - \omega t)}]$$

$$= -\frac{e\hbar}{2m} \int [A(k) \psi \psi^*]$$

$$= \frac{e\hbar}{2m} \int [A(k) \psi^* \psi]$$

At equilibrium, resultant = zero at

$$\Rightarrow \frac{1}{2} \rho_0 E + \frac{1}{4\pi \epsilon_0} \frac{\rho_0}{r}$$

$$\Rightarrow r = 4\pi \epsilon_0 \cdot \frac{R^3 \cdot E}{2\rho}$$

o. Electric dipole moment,

$$\mu_E = Ze \cdot r$$

$$\mu_E = 4\pi \epsilon_0 \cdot \rho^3 \cdot E$$

$$\text{So, } \mu_E \propto E.$$

$$\boxed{\alpha = \frac{\mu_E}{E}}$$

↳ electric susceptibility

$$\rho_E = \alpha E$$

$$\rho_E = N \alpha \epsilon_0 \cdot R^3 \cdot E$$

$$\rho_E = N \alpha \epsilon_0 \cdot E$$

$$\overrightarrow{P} = \frac{\rho_E}{\epsilon_0 E}$$

$$\overrightarrow{P} = \frac{\rho_E}{\epsilon_0 E} \cdot \overrightarrow{E} = \overrightarrow{E} - \overrightarrow{P}$$

$$\overrightarrow{P} = \overrightarrow{E} - \overrightarrow{P}$$

Numerical methods

→ iterative method for first order ODE:

• Euler's

→ If x_n is calculated, then there is no need to calculate previous values x_{n-1}, x_{n-2}, \dots . Only one value is needed for the calculation of x_n .

→ Examples of this type: • Euler's
• Runge-Kutta RK4.

→ these methods choose the step size Δx where $x_n = x_0 + n\Delta x$, $n=1, 2, \dots$

so that the stepsize is controlled by a specified tolerance.

→ It should be kept small so that higher accuracy is achieved and hence these methods can be applied for the value of the independent variable in a limited range only.

↳ these methods are called single step methods as they compute the value of $f(x)$ from x_n only.

Statistical Mechanics

Classical Statistical Mechanics

Nucleus with classical particle

→ Objects Maxwell-Boltzmann

Eq: ideal gas molecules

Particles with half integral spin.

→ Objects Fermi-Dirac

Eq: electron, proton, neutron, He⁺ atom,

deuteron, π-

nucleon

He⁺ atom etc.

Eq: photon,

photon,

etc.

→ Objects Bose-Einstein statistics

Eq: electron, proton, neutron, He⁺ atom etc.

π-

deuteron, π-

nucleon

He⁺ atom etc.

N

Statistical Mechanics

Classical Statistical
Mechanics
(classical mechanics
particle)

→ object Maxwell-Boltzmann
eq: ideal gas molecules

Particle with half integer spin

→ object Fermi-Dirac

Particle with integer spin
↑
electron, proton,
neutron,
He⁺ atom,
muon,
tau-lepton,
Higgs boson etc.

SUMMATION STATES (ENERGY STATES), ENERGY LEVELS AND DEGENERACY:

→ For a particle of mass m in a cubic box of side L ,
the $\frac{1}{L}$ to momentum mechanics, a stationary wave is

completely equivalent to such a particle.
y. wavelength, λ , of the stationary wave
 $\lambda_i = \frac{1}{n_i L}$ [where n_i is an integer equal to
the number of antinodes].

6) A stationary wave is related to the momentum
 p of the particle through the relation,

$$p = \frac{\hbar k}{\lambda}$$

so, $p_i = n_i \frac{\hbar k}{L}$
i.e., $p_i = m_i \frac{\hbar}{L}$
if a particle is free to move in any dirⁿ within
a cubic box of side L , where sides are
parallel to the x, y, z axes of a rectangular
coordinate system, the x, y, z components of the
momentum have the values:

$$p_x = m_1 \frac{\hbar}{L}, \quad p_y = m_2 \frac{\hbar}{L}, \quad p_z = m_3 \frac{\hbar}{L}$$

Quantum Statistics
Mechanics
(classical with quantum particle)

→ object quantum numbers n_x, n_y and n_z .

$$\rightarrow \text{For particle of mass } m, \text{ speed } v \text{ of momentum, } p = mv, \text{ kinetic energy is } E.$$

$$\rightarrow E_i = \frac{p_i^2}{2m} = \left(n_x^2 + n_y^2 + n_z^2 \right) \frac{\hbar^2}{8mL^2}$$

$$\text{where, } n_x^2 + n_y^2 + n_z^2 = n_i^2$$

* The values of n_x, n_y, n_z are said to define the state of a particle, and the energies corresponding to the different possible values of n_i are the possible energy levels.

* The energy levels depend only on the values of n_i and not on the individual values of n_x, n_y and n_z .
The same energy levels will have the same energy.

* In general, a number of different states is often said to be degenerate. The symbol ρ_i is used to designate the degeneracy of level i , i.e., the number of states having the same energy E_i .

STATISTICAL MECHANICS

- * Statistical mechanics develops a relation b/w the macroscopic behaviours (i.e. bulk properties) of system in terms of microscopic behaviours (individual property) using the law of probability of distribution function of two types:
 - A. Classical Statistics: Properties of motion of individual micro-particles can be explained by classical mechanics
 - Maxwell-Boltzmann statistics
 - B. Quantum Statistics: Properties of motion of individual micro-particles can be explained by quantum mechanics
 - Fermi-Dirac & Bose-Einstein statistics
- * (A) explains many physical phenomena like temp., pressure, energy etc. However, fails to explain phenomena like black body radiation or specific heat. (B) explains these.
- * All three statistics i.e. NB, FD, BE give the same result at high temp. & low pressure.
- # ENERGY LEVELS & ENERGY STATES
- * A thermodynamic system is always associated with some discrete energy levels in which a large no. of particles can be accommodated.
- the principal quantum number (n) gives energy level of a system
- * Every energy level is associated with a large number of particles of all the quantum numbers (m_1, m_2, \dots) for any two particles are not the same.
- Thus, there are several states corresponding to an energy level & they are called energy states.
- no. of quantum states for a given energy level is called degeneracy of the level:

MACROSTATE & MICROSTATE

- o MACROSTATE: An isolated system consisting of a fixed number (N) of non-interacting identical particles having a fixed internal energy (E) occupying a fixed space of volume (V) is said to be macrostate.
 - o MICROSTATE: The number of different meaningful ways (of the various particles in the macrostate) in which the total energy (E) of the system can be distributed among its constituent particles are called microstate.
- ↳ Thus, a large number of microstates may lead to the same macrostate.
- Ex: Number of distinguishable particle = 2 allowed energy states, $E, 2E, 3E$
- Part Energy = $1E$
- Possible combinations:

C	2E	3E
No. of particles in each state	1	1
Energy	0	2

that total energy = $3E$.

Here, total no. of macrostates = possible no. of combination of particles

$$= 2$$

(sol 8/20)

Now, let the particles be a.g.b.

Macrostate	E	2E	3E	No. of microstates
1 0 1	all	0	6/12	2
0 2 0	0	a g b	0	1

So, total no. of microstates = ≈ 3

- # THE THERMODYNAMIC PROBABILITY: the ratio no. of possible microstates of a system corresponding to a given macrostate (also called thermodynamic frequency) is called thermodynamic probability for it (m_1, m_2, \dots, m_k)

- For n particles, the no. of microstates for it (m_1, m_2, \dots, m_k) macrostate is :

$$N_{m_1, m_2, \dots, m_n} = \frac{n!}{m_1! (m_2! \dots m_n!)}$$

Ex: For n distinguishable particles, for its $(3, 1)$ microstate
see no. of microstates (i.e., N)

$$N_{3,1} = \frac{4!}{3! \cdot 1!} = 4$$

Note: In equilibrium, all the microstates are equally probable. Hence, all the microstates i.e., the energy states of arrangement (ω) of atoms in the energy states of the system should also come to a maximum.

PHASE SPACE: To describe both the position & state of motion of the particle, it is required to set up a six dimensional space in which a point has 6 coordinates x, y, z (position) & p_x, p_y, p_z (momentum coordinates) along 6 mutually L -axes. This combined position & momentum specifies a single particle is called a phase space.

NUMBER OF EQUIVOLNT STATES (OF UNIT CELLS) WITHIN ENERGY RANGE E AND $E+dE$, IN THE PHASE SPACE,
OR, DENSITY OF STATES:

Let us consider a phase space of volume containing a system of particles. A small volume element in phase space is given by

$$d\Omega = dx dy dz dp_x dp_y dp_z$$

[where, x, y, z, p_x, p_y, p_z are the coordinates of a pair in phase space]

So, finite volume of the phase space available for a particle is:

$$\tau = \iiint \iiint dx dy dz dp_x dp_y dp_z$$

$$\Rightarrow \tau = \iiint \iiint dx dy dz \iiint dp_x dp_y dp_z.$$

→ It is possible to divide the phase space into a large number of elementary cells of equal volume (i.e., $d\Omega$).

→ Using Planck's uncertainty principle, $dx \cdot dp_x \approx h$, where h is constant.

→ So, minimum size of volume for a quantum mech. system $dt = dx dy dz dp_x dp_y dp_z \cong h^3$

Now, the number of cells in phase space corresponding to momentum p and $p+dp$ is

$$d(p) dp = \text{Volume in phase space corresponding to momentum } p \text{ to } p+dp$$

A_3

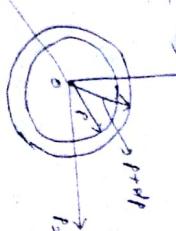
$$\Rightarrow d(p) dp = \iiint dx dy dz \iiint dp_x dp_y dp_z$$

Now, volume of system of particles,

$$V = \iiint dx dy dz$$

$$\therefore d(p) dp = \frac{V \iiint dp_x dp_y dp_z}{h^3} \quad (1)$$

→ We evaluate the volume of the system ($= \iiint dp_x dp_y dp_z$) in momentum space corresponding to momentum interval p and $p+dp$, we take a sphere of radius $p+dp$, such that all the points lying on the sphere have a momentum $p \leq p' \leq p+dp$.



The "v" of sphere in momentum space is

$$\sqrt{p^2 = p_x^2 + p_y^2 + p_z^2} = 2\pi E$$

E is energy of particle of mass m

Taking another concentric sphere of radius $p+dp$, the volume of the spherical shell enclosed between the two spheres of radius p & $p+dp$ is given by

$$\iiint dp_x dp_y dp_z = \text{surface area of the sphere of radius } p \times \text{thickness of the cell}$$

$$\Rightarrow \iiint dp_x dp_y dp_z = 4\pi p^2 \cdot dp$$

Putting this in (1),

$$\boxed{\theta(1) \cdot dp = \frac{V}{h^3} 4\pi p^2 \cdot dp} \quad (2)$$

For particles having two allowed values of the spin quantum number ($m_s = \pm \frac{1}{2}$) ? the no. of available quantum states (i.e., cells) is twice of (2),

$$\theta(n) \cdot dP = \frac{2V}{h^3} \cdot n \rho^2 \cdot dP$$

$$\Rightarrow \boxed{\frac{\partial P}{\partial \rho} \cdot d\rho = \frac{2V}{h^3} \cdot n \rho^2 \cdot dP} \quad (3)$$

Again, $\rho^2 = 2mE$

$$\Rightarrow \frac{\partial P}{\partial \rho} \cdot d\rho = 2m \cdot dE \quad (4)$$

Substituting in (3), we get the number of quantum states available in the phase space corresponding to energy E and dE ,

$$g(E) \cdot dE = \frac{8\pi V \sqrt{2mE}}{h^3} \cdot m \cdot dE$$

$$\Rightarrow \boxed{g(E) \cdot dE = \frac{8\pi^2 n V \cdot m^{3/2} E^{1/2}}{h^3} \cdot dE} \quad (5)$$

MAXWELL-BOLTZMANN STATISTICS:

Maxwell Boltzmann statistics gives the statistical

- ① behaviour of identical spinless particles obeying Pauli's exclusion principle.
- ② these particles do not obey Pauli's exclusion principle and no. of particles.

- ③ If N = total no. of particles, then energies E_1, E_2, E_3, \dots respectively.
- N_1, N_2, N_3, \dots particles have quantum states E_1, E_2, E_3, \dots respectively, corresponding to degeneracy, according to given distribution,

the total probability for given distribution

$$W = N! \prod_i \frac{(g_i)^{N_i}}{N_i!} \quad (1) \text{ possible states}$$

→ gives no. of microstates

→ for most probable distribution, $d\ln W = 0$

$$\text{Thus, } \sum_i \ln \left(\frac{N_i}{g_i} \right) dN_i = 0 \quad (2)$$

now if (2) is subjected to condition,

$$\sum_i N_i e^i = \text{constant} \Rightarrow \sum_i e^i dN_i = 0$$

$$\sum_i N_i = \text{constant} \Rightarrow \sum_i dN_i = 0$$

New, $\boxed{N_i = e^{-\beta E_i}}$

$$\text{where, } \boxed{\frac{1}{Z} = \sum_i g_i e^{-\beta E_i}}$$

is called partition function

Thus, eq (2) becomes

$$\boxed{N_i = \left(\frac{N}{Z} \right) g_i e^{-\beta E_i}}$$

Maxwell-Boltzmann distribution function?

$$\boxed{\frac{N_i}{g_i} = \frac{1}{e^{\beta E_i}}} \text{ gives the probability of a particle to occupy an energy state } E_i$$

Disadvantages of MB:

→ can't explain the energy distribution of the molecules of ideal gas to a fair degree of accuracy.

However, fails to explain the energy distribution of indistinguishable particles like electrons or photons.

Note: The ratio N_i/g_i is called occupation index.

- ① $N_i/g_i \ll 1 \rightarrow$ the system is called non-degenerate
- ② $N_i/g_i > 1 \rightarrow$ the system is called degenerate.
- ③ $N_i/g_i \gg 1 \rightarrow$ strongly degenerate. It is seen for Bosons particles.

Quantum statistics:

→ Many particles like obey Pauli's exclusion principle which states that each quantum state can accommodate only one particle.

→ Also, quantum statistics particles that are indistinguishable & identical.

$$\boxed{N_i = \frac{1}{h^3} \cdot \frac{V}{(2\pi m E_i)^{3/2}} \cdot e^{-\beta E_i}} \quad (3)$$

$\propto \rho^2$ are constant depending upon the physical property of the system

A. PERIODIC STATISTICS:

Postulates: (1) Particles are indistinguishable & identical energy state can accommodate either no particle or only one particle.

- (2) Only Pauli's exclusion principle, i.e. each angular momentum, $m_s \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ since $m_s = \pm \frac{1}{2}$ in H_1)
- (3) Particles have $\pm \frac{1}{2}$ angular spin (i.e. spin $\frac{1}{2}$)

* EQUATIONS: The particles there are indistinguishable, canonical having $\frac{1}{2}$ integral spin and obey the statistics are called fermions.

i.e., position, neutrons, protons, β^- decay no. of nucleons is odd (${}^1\text{H}^3, {}^3\text{Li}^7, {}^6\text{C}^{13}$).

* Probability of the entire distribution,

$$W = \prod_i N_i! = \prod_i \frac{\theta_i!}{N_i!(\theta_i - N_i)!}$$

* For most probable distribution, $d(\ln W) = 0$

$$\sum_i \ln \left(\frac{N_i}{\theta_i - N_i} \right) dN_i = 0$$

Also, the system must satisfy conservation of total no. of particles i.e. $\sum dN_i = 0$ of conservation of total energy i.e. $\sum E_i dN_i = 0$

* As distribution law:

$$N_i = \frac{\theta_i}{e^{\alpha + \beta E_i} + 1}$$

α, β are Lagrange's undetermined multipliers

* For fermions in statistical equilibrium at temp. T ,

$$\alpha = -E_f/k_B T$$

$$\beta = \frac{1}{k_B T}, \quad \text{where } E_f = \text{Free energy of the system}$$

$$k_B = \text{Boltzmann constant}$$

$$= 1.38 \times 10^{-23} \text{ J.K}^{-1}$$

i.e. all energy states having $E_i < E_f$ are occupied

i.e. all energy states having $E_i > E_f$ are occupied by a single fermion (i.e. electron)

$$(2) \text{ If } n = 0 \text{ & } E_i > E_f \Rightarrow f(E) = \frac{1}{1 + e^{-\infty}} = 0$$

i.e. all energy states having $E_i > E_f$ are unoccupied.

$$N_i = \frac{\theta_i}{e^{(E_i - E_f)/k_B T} + 1}$$

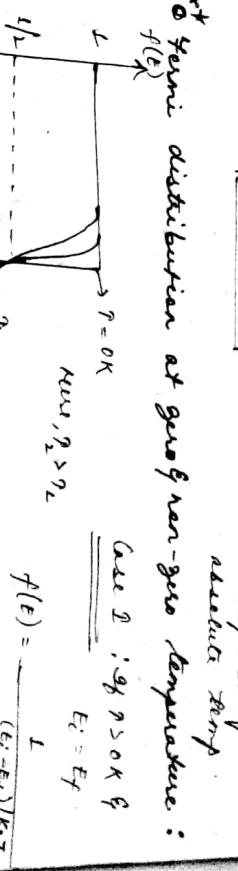
as distribution law.

* Fermi distribution function:

$$f(E) = \frac{1}{1 + e^{(E_i - E_f)/k_B T}}$$

$E_f = \text{Fermi energy at absolute zero}$
 $T = \text{corresponding absolute temp.}$

* Fermi distribution at zero & non-zero temperature:



$$f(E) = \frac{1}{1 + e^{(E_i - E_f)/k_B T}}$$

Case 1: $\theta_i \gg k_B T$

Fermi distribution function

Temp. $\theta_i > E_f$
Temp. $> 0K$.

$$f(E) = \frac{1}{1 + e^{-\infty}} = 0$$

case 2: $\theta_i \ll k_B T$

$$f(E) = \frac{1}{1 + e^{(E_i - E_f)/k_B T}} = \frac{1}{2}$$

thus, free Fermi energy and the probability of occupation of a Fermion is $\frac{1}{2}$ for any

Temp. $> 0K$.

* As distribution law:

$$N_i = \frac{\theta_i}{e^{(E_i - E_f)/k_B T} + 1}$$

i.e. all energy states having $E_i < E_f$ are occupied

by a single fermion (i.e. electron)

$$(2) \text{ If } n = 0 \text{ & } E_i > E_f \Rightarrow f(E) = \frac{1}{1 + e^{\infty}} = 0$$

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as distribution law.

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At $T = 0K$, Fermi energy ($E_F = E_F(0)$) is that energy level upto which all the energy states are filled up by fermions & all the energy states above it are empty. The Fermi energy E_F is the highest occupied energy level of fermions at $T = 0K$. We know, Fermi energy is the max. energy that can be occupied by a fermion (i.e., electron) at $0K$.

o Electron gas in metal:

→ Metals have a large no. of free e^- because of which they are good conductors.

Electrons free e^- move freely in the metal & continuously collide with the atoms. So, they behave like a gas called electron gas.

→ e^- are elementary particles with $\frac{1}{2}$ integral spin.

In a metal e^- have their quantified energy levels and obey Pauli's exclusion principle. So, they are called fermions & not obey Po. statistics.

→ If we consider a continuous distribution of energy among 'N' number of free electrons in electron gas, then for electrons with their energy range E and $E + dE$, $\theta(E)$ is replaced by $\theta(E)dE$ & $\theta(E)$ is replaced by $n(E)dE$ in its distribution law.

$$n(E)dE = \frac{\theta(E)dE}{e^{(E-E_F)/kT}}$$

o Fermi - Dirac law of energy distribution for free e^-

in metal : $\theta(E) = \frac{1}{e^{(E-E_F)/kT} + 1}$

where $\theta(E)dE$ is the number of e^- within the energy range E and $E + dE$, taken from eq. ④,
or $n(E)dE = \frac{\theta(E)dE}{e^{(E-E_F)/kT} + 1}$.

∴ Fermi weight, E_F in metal : $N(E_F) = \text{no. of } e^- \text{ within the energy range } E_F \text{ and } E_F + dE$.

→ If $N(E_F)$ is the total number of e^- within the energy range E_F and $E_F + dE$, then from eq. ④,

$N(E_F) = \frac{1}{e^{(E_F-E_F)/kT} + 1}$.

∴ Fermi weight, E_F of a metal : $E_F = \frac{1}{N} \int_{-\infty}^{\infty} \frac{e^{(E-E_F)/kT}}{e^{(E-E_F)/kT} + 1} dE$

$$\theta(E)dE = \frac{2\pi V \rho^2 dE}{h^3} = \frac{8\pi k \rho (T)dE}{h^3} \quad \text{⑤}$$

Now, $\rho = \text{mass} / \text{volume}$ (for non-relativistic case)

$$\Rightarrow \rho dE = m dE$$

$$\Rightarrow \rho dE = m dE$$

$$\theta(E)dE = \frac{8\pi V}{h^3} T \cdot m dE$$

Substituting value in ⑤,

$$N(E_F)dE = \frac{8\pi V \sqrt{2}}{h^3} \cdot m^{1/2} \cdot E^{1/2} \cdot dE$$

Or law of energy distribution for free e^- in metals.

o Value of Fermi energy (Fermi energy) & total no. of electrons in metal as absolute zero.

→ At absolute temp ($T = 0K$), the total no. of isolated numbers of energy states occupied by the e^- from the lowest range up to E_F (Fermi energy).

→ Electrons are fermions. Thus, each energy state has only one electron. So, taking no. of e^- ,

$$N = \int_0^{\infty} \theta(E)dE = \frac{8\pi V m}{h^3} \int_0^{\infty} E^{1/2} dE$$

$$= \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} E_F^{9/2} \times \frac{1}{3}$$

$$N = \frac{16\sqrt{2}\pi V m^{9/2}}{3 \cdot h^3} E_F^{9/2} \quad \text{→ Expression of total no. of } e^- \text{ in a metal at } 0K.$$

NOTE : $\frac{N}{V} = \frac{\text{Atomic no.} \times \text{Density}}{\text{Atomic weight}}$

→ When given $\frac{N}{V}$ find E_F and find N/V .

- mean internal energy (\bar{E}) of free \bar{e} of a system at absolute zero.

$$\bar{E} = \frac{1}{N} \int_{-\infty}^{\infty} E f(E) dE$$

N : total no. of
free \bar{e} is a
total of volume

$$\bar{E} = \frac{1}{N} \int_{-\infty}^{\infty} E [f(E) \theta(E) \cdot dE] - P \cdot n(E) dE + f(E) \theta(E) dE \quad \text{--- (1)}$$

$$\text{or, } \bar{E} = \frac{1}{N} \int_{-\infty}^{\infty} E f(E) \theta(E) \cdot dE + \frac{1}{N} \int_{-\infty}^{\infty} E f(E) \theta(E) \cdot dE \quad \text{--- (2)}$$

if $\theta = 0$ $\Rightarrow E < Ef$, $f(E) = 1$

as, at $\theta = 0$, $E \geq Ef$, $f(E) = 0$
so, and part of (1) is 0.

$$\bar{E} = \frac{1}{N} \int_{Ef}^{\infty} E f(E) \cdot dE \quad \text{--- (2)}$$

$$\text{Now, } \int_{Ef}^{\infty} \theta(E) dE = 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} E^{1/2} \cdot dE$$

$$\therefore \bar{E} = \frac{1}{N} \int_{Ef}^{\infty} E \cdot 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} E^{1/2} \cdot dE$$

$$= \frac{4\pi V}{N} \left(\frac{2m}{h^2}\right)^{3/2} \int_{Ef}^{\infty} E^{3/2} \cdot dE$$

$$\text{So, } \bar{E} = \frac{4\pi V}{N} \left(\frac{2m}{h^2}\right)^{3/2} \frac{2}{3} Ef^{5/2} = \left[\frac{8\pi V}{N} \left(\frac{2m}{h^2}\right)^{3/2} Ef^{3/2} \right]_{Ef}^{\infty}$$

--- (3).

for absolute zero,

$$Ef = \frac{hf}{2m} \left(\frac{3N}{8\pi V}\right)^{1/2}$$

$$\Rightarrow Ef^{3/2} = \left(\frac{hf}{2m}\right)^{3/2} \frac{3N}{8\pi V}$$

$$\text{Thus, } \bar{E} = \left[\frac{3\pi V}{5N} \left(\frac{2m}{h^2}\right)^{3/2} \left(\frac{hf}{2m}\right)^{3/2} \frac{3N}{8\pi V} \right] Ef$$

$$\Rightarrow \bar{E} = \frac{3}{5} Ef \quad \begin{matrix} \text{Mean val of } e \\ \text{involving } q=0 \end{matrix}$$

BOSON: SPIN 0 PARTICLES

- Since the statistical treatment of indistinguishable identical particles involving spin ($m_S = 0, \pm \frac{1}{2}, \dots$)
- So not every Pauli's exclusion principle is valid, can accommodate any no. of particles.
- Have symmetric wave function.

BOSONS: particles that are indistinguishable identical, have integral spin & obey SCF.

Ex: photons, photons, π -meson, α -particle, β -meson.
 \rightarrow if total no. of nucleons is even, no. of possible distinguishable θ distinct arrangements of N_i particles with $(g_i - 1)$ partitions

W = \prod_{i=1}^n \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!}

\rightarrow most probable θ distribution, $d(\ln W) = 0$

$$\sum [\ln N_i - \ln (\beta_i + N_i)] dN_i = 0 \quad \frac{dN_i}{\sum L_i dN_i} = 0$$

Distribution law:

$$N_i = \frac{e^{-\beta_i}}{e^{\alpha + \beta_i} - 1}$$

In thermal equilibrium yet because at temp T , $\mu \rightarrow$ chemical potential of the system

$$\alpha = -\frac{f\epsilon}{k_B T}, \quad \beta = \frac{1}{k_B T}$$

$$\text{So, } N_i = \frac{e^{(\epsilon_i - \mu)/k_B T}}{e^{(\epsilon_i - \mu)/k_B T} - 1}$$

Distribution func:

$$f(E) = \frac{N_i}{e^{(E - \mu)/k_B T} - 1} \quad \begin{matrix} \text{for } \epsilon_i > \mu \\ \text{G. gets reduced to } N_B \end{matrix}$$

DERIVATION OF PLANCK'S LAW OF RADIATION

A/c to Planck's radiation law the amount of energy radiation per unit volume by a black body lying betw. the freq. range $\nu \& (\nu + d\nu)$ is given by:

$$t(\nu) d\nu = \frac{8\pi h \nu^3}{c^3} \frac{e^{-h\nu/kT}}{e^{h\nu/kT} - 1}$$

Similarly,

Electrons are scarce.

- In black body radiation, photons of diff. energies are absorbed or emitted by the atoms of the walls of the enclosure. So, $\sum n_i = \text{constant}$ even though total energy remains constant. Here, multiplying $\Delta = \hbar$.
- From S.E. distribution law,

$$n_i = \frac{\theta_i^2}{e^{\theta_i kT} - 1} = \frac{f_i}{e^{\theta_i kT} - 1}$$

Thus, the no. of photons in freq. range $\nu \& (\nu + d\nu)$ obtained by multiplying n_i by $t(\nu) d\nu$ is given by:

$$\text{on } t(\nu) d\nu = \frac{\theta(\nu) d\nu}{e^{\theta(\nu) kT} - 1}$$

Here, $\theta(\nu) d\nu$ is the no. of quantum states betw. ν and $(\nu + d\nu)$.

If V is volume of given place space, the no. of quantum states corresponding to momentum in the range betw. p and $(p + dp)$ is

$$g(p) dp = \frac{8\pi V}{\hbar^3} p^2 dp$$

$$\text{Now, } p = \sqrt{\frac{E}{m}}$$

$$\text{Thus, } g(p) dp = \frac{8\pi V}{\hbar^3 m^{3/2}} E^{1/2} f(E) dE$$

$$\text{Now, } t = m v^2 = \frac{\theta(\nu)}{A^2}$$

$$g(p) = \frac{\theta(\nu)}{A^2}$$

$$dp = \frac{C}{v} \cdot d\nu$$

$$\text{So, } g(\nu) d\nu = \frac{8\pi V}{\hbar^3} \cdot \frac{p^2 d\nu}{c^2} \cdot \frac{1}{e^{\theta(\nu) kT} - 1}$$

$$= \left(\frac{8\pi V}{c^3} \right) \nu^2 d\nu$$

$$\text{Thus, } n(\nu) d\nu = \left(\frac{8\pi V}{c^3} \right) \nu^2 d\nu \cdot \frac{1}{e^{\theta(\nu) kT} - 1}$$

$$t = \theta(\nu)$$

Now, amount of energy per unit volume of the enclosure betw. the freq. range ν and $\nu + d\nu$ is given by,

$$E = \left(\frac{\theta(\nu)}{\nu} \right) \cdot n(\nu) d\nu = \frac{8\pi h \nu^3}{c^3} \cdot \frac{1}{e^{\theta(\nu) kT} - 1}$$

$$\text{For } \nu = \frac{v \lambda = c}{\nu = \left(\frac{c}{\lambda} \right)}$$

CARRIER CONCENTRATIONS OR SEMICONDUCTOR

$n_e \rightarrow$ "no." of free e^- in conduction band

$n_h \rightarrow$ " " holes in valence "

$f(E)$ can be used to calculate "no."

" E_{cut} " in conduction band!

$$n(E) dE = f(E) dE \cdot f(E)$$

↑
conduction band
distribution

density of free
electrons
↓
valence band

↑
no. of free
electrons

$$n_e = \int_E^{\infty} f(E) \cdot f(E) \cdot dE$$

E_C
 $E_F =$ highest occupied level in conduction band
 $E_V =$ lowest " in valence band

$$E_C = \frac{E_F - E_V}{k_B T}$$

$$n_e = n_{e0} e^{-\frac{E_C}{k_B T}}$$

$$n_{e0} = \frac{1}{V_2} \left(\frac{m_e^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

"one" of holes in n_A , $n_{A0} = n_A - \frac{1}{V_2} n_e e^{-\frac{(E_F - E_V)}{k_B T}}$

$$n_{A0} = \frac{1}{V_2} \left(\frac{m_A^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

intrinsic one of charge carriers:

$$n_i^2 = n_e n_A = \left(n_{e0} e^{\frac{(E_F - E_C)}{k_B T}} \right) \cdot \left(n_{A0} e^{-\frac{(E_F - E_V)}{k_B T}} \right)$$

$$= n_{e0} n_{A0} e^{\frac{(E_F - E_C)}{k_B T}}$$

$$= \frac{1}{V_2} \left(\frac{m_e^* m_A^*}{\pi \hbar^2} \right)^{3/2} (k_B T)^3 e^{-\frac{(E_F + E_V)}{2 k_B T}}$$

$$= \frac{3 \pi k_B T}{4} (m_e^* m_A^*)^{3/2} k_B T^3 e^{-\frac{(E_F + E_V)}{2 k_B T}}$$

$$\left(\frac{k_B T}{4 \pi \hbar^2} \right)^3 = A' T^3 e^{-\frac{E_F + E_V}{2 k_B T}} \quad A' = \frac{3 \pi k_B T}{4 \pi} (m_e^* m_A^*)^{3/2} k_B T^3$$

$$= A' T^{3/2} e^{-\frac{E_F + E_V}{2 k_B T}}$$

$$n_i^2 = A' T^{3/2} e^{-\frac{E_F + E_V}{2 k_B T}}$$

↳ independent of Fermi level but depends upon E_F .

ni ↑ for ΔE_F fermi level of its position for intrinsic semiconductors

In an "intrinsic" semiconductor, $n_e = n_A$

$$n_{e0} = n_{A0} e^{-\frac{(E_F - E_C)}{k_B T}}$$

$$\Rightarrow \frac{1}{V_2} \left(\frac{m_e^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{\frac{(E_F - E_C)}{k_B T}} = \frac{1}{V_2} \left(\frac{m_A^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{-\frac{(E_F - E_V)}{k_B T}}$$

$$\Rightarrow m_e^* T^{3/2} e^{\frac{(E_F - E_C)}{k_B T}} = m_A^* T^{3/2} e^{-\frac{(E_F - E_V)}{k_B T}}$$

$$\Rightarrow e^{\frac{(E_F - E_C - E_V)}{k_B T}} = \left(\frac{m_A^*}{m_e^*} \right)^{3/2}$$

$$\Rightarrow \frac{E_F - E_C - E_V}{k_B T} = \frac{3(E_F - E_V)}{2 k_B T}$$

$$E_F = \frac{3}{2} E_F - \frac{3}{2} E_V$$

gives the partition of energy band in intrinsic semi.

Fermi level & its position in extrinsic semi
 $n_e + n_A = n_D + n_H$
and for N type, $n_D > n_H$, $n_D \gg n_H$.
 $n_D = n_{D0} e^{\frac{(E_F - E_C)}{k_B T}}$

$$n_e = n_{D0} e^{\frac{(E_F - E_C)}{k_B T}}$$

$$\Rightarrow n_D = n_{D0} e^{\frac{(E_F - E_C)}{k_B T}} = n_D e^{\frac{(E_F - E_C)}{k_B T}}$$

$$\Rightarrow E_F = E_C - k_B T \ln \frac{n_D}{n_{D0}} = \frac{E_C}{1 - \frac{E_C}{k_B T}}$$

$$n_D > n_H \text{ so, } E_F > E_C$$

so, E_F shifted in direction of Fermi level.

$$n_D = \frac{1}{V_2} \left(\frac{m_D^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$n_H = \frac{1}{V_2} \left(\frac{m_H^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

J. Par. & Spec.

卷之三

$$n_A = n_{A0} e^{-\frac{E_F - E}{k_B T}}$$

$$= \frac{f_1 - f_2}{f_1 + f_2} = \frac{\alpha_1 - \alpha_2}{\alpha_1 + \alpha_2}$$

$$\frac{m}{m+1} \sin x + 1 = f_3(x)$$

$\mu \sqrt{\rho}$

فیض

$$\sum_{k=2}^{\infty} \frac{1}{k^2} (n+1)^{k-2}$$

$$= n(n-1) + c(n-1) + c(n)$$

Jan
100°
100°

$$c(0) + c(1) + \dots + c(n)$$

$$\text{Therefore } \sum_{k=0}^n a_k x^k = \frac{1}{(1-x)^2} \left[\frac{1}{x} + \frac{(n+1)x^n}{(1-x)} + \sum_{k=1}^{n-1} a_k (n-k+1)x^{n-k} \right].$$

$$\frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$$

卷之二

10

$n \leftarrow \text{length}(\beta)$

$$\frac{N}{\mu} = \frac{N}{\mu} = \frac{N}{\mu}$$

~~for $i \leftarrow l$ to n~~
~~for $j \leftarrow i+1$ to $n-1$~~
~~$\text{if } A[i] > A[j]$~~
~~$\text{swap } A[i] \leftrightarrow A[j]$~~

$$g \leftarrow m[x, y] + m[k+i] + \rho_{k-1}, \rho_k, \rho_i$$

if $\theta \in m[i,j]$
 $m[i',j] \leftarrow \theta$
 $L[i',j] \leftarrow k$

for each $a \in \mathbb{Z}$

repeat
until
(θ)

~~return~~

SUMMARY OF THE STATEMENTS

- the explanation of natural or physical phenomena in terms of quantum physics necessitates the transition from deterministic classical physics to a probabilistic quantum physics.
- the probabilistic description of the motion of micro-particle can be expressed by a function, called wave function.
- # THE WAVE FUNCTION: represents a pure quantum state of a system; specifies a pure stationary system.
- W.H.: describes the spacetime of each exactly moving quantum mechanical particle.
- denoted by $\psi(\vec{r}, t)$ & measures the probability of finding a particle about a position.
- is single valued, continuous & finite.
- is a square integrable function.
- magnitude of $|\psi(\vec{r}, t)|^2$ is large in the regions where the probability of finding the particle is high & is small in the regions where the probability of finding it is low.
- # PROBABILITY DENSITY:
- the probability density of a particle is the probability of finding the particle per unit volume of a given space at a particular time.
- * NORMALISED WAVE FUNCTIONS: the condition of an expressible wave function is that the integral of $|\psi|^2$ over all space is $\int_{-\infty}^{+\infty} \psi^* \psi dV$ (dV is small volume element surrounding a point) must be finite.
- Then, $\int_{-\infty}^{+\infty} |\psi|^2 dV = \int_{-\infty}^{+\infty} |\psi|^2 dV$ indicates the particle must be somewhere in space. At all times, the above condition must be satisfied that every the function ψ is a wave function.
- It is known as normalising.
- * For a wave function represented by complex function we can write $\psi = A + iB$, then,
- $\psi^* \psi = (A - iB)(A + iB) = A^2 + B^2$
- Since, A & B are real quantity, so $A^2 + B^2$ is always a positive real quantity.
- As A & B are two

~~Now, probability density is expressed as the product of normalized wave function & its complex conjugate.~~

$$y = \psi^*(x, t) \cdot \psi(x, t) = |\psi(x, t)|^2$$

PROBABILITY:

→ The probability that the particle will be found in the volume element dV at x, t is $y dV = |\psi d\mathbf{r}|^2$.

→ Since, the particle must be somewhere in space, the total probability P , to find the particle in space should be equal to 1.

$$P = \int_{-\infty}^{+\infty} y dV = 1$$

→ In 2D case, the probability of locating the particle within a distance dx is given by

$$P dx = y dx$$

Since, the particle must be somewhere along the x -axis, the total probability for the one dimensional motion over all values of x must be 1.

$$\int_{-\infty}^{+\infty} y^2 dx = 1$$

→ Dimension of 1D wave func. is $L^{-1/2}$. Dimension of 3D wave func. is $L^{-3/2}$.

SUPERPOSITION PRINCIPLE:

→ A system can have different possible allowed states.

→ The wave function (ψ) represents the actual state of the system.

• The superposition principle states that if any system, Schrödinger differential eq. (linear), has several sets of wave functions, then the linear combination of these sets with different coefficients is also a set of sets with different coefficients. Thus,

$$\psi = a_1 \psi_1 + a_2 \psi_2 + \dots = \sum a_n \psi_n$$

a_n = coeff. of state ψ_n .

→ This implies that the actual state of the system is a linear combination of three allowed states with different coefficients.

→ Here, the wave func. are normalized & are orthogonal to each other.

• The probability of finding the system in a particular state (say ψ_2) depends on its corresponding coefficient (a_2).

Thus, P (finding particle in state ψ_2) = $|a_2|^2$.

* Orthonormal wave func.: ψ_1, ψ_2, ψ_3 are orthonormal if their inner product is zero.

* OBSERVABLE: Observables are quantities associated with a physical system that can be measured or observed.

OPERATORS IN QUANTUM MECHANICS:

→ An operator is a mathematical rule that changes a given function into a new function.

If A is an operator, it is represented by \hat{A} .

Op: If $\hat{A} = \frac{d}{dx}$, then when it operates on $f(x)$,

$$\frac{d(f(x))}{dx} = \hat{A}f$$

Linear Operators: If \hat{A} is a linear operator, it satisfies the

① $\hat{A}(cf) = c\hat{A}f$, c is constant

② $\hat{A}(f+g) = \hat{A}f + \hat{A}g$, f, g are two

→ In quantum mech., each dynamical variable such as position, momentum, energy etc. is represented by a linear operator.

COMPUTATION: Commutator of two operators α and β is represented by $[\alpha, \beta]$ and is defined as

$$[\alpha, \beta] = \hat{\alpha}\hat{\beta} - \hat{\beta}\hat{\alpha}$$

If $[\alpha, \beta] = 0$, the two operators are called commutative. Else, if $[\alpha, \beta] \neq 0$, the two operators are called non-commutative.

Momentum operator

Let us do angular's op[†] of matter wave,

$$\hat{A} = \frac{\partial}{\partial t}$$

$$\text{Now, } \hat{A} = \frac{\partial}{\partial t} \text{ and } \hat{P} = \frac{\partial}{\partial x}$$

Now, suppose the wave function has a free particle in the position & dis[†] i.e.
 $\psi(x,t) = A e^{i(kx - \omega t)}$

$$\text{or, } \hat{A} \frac{\partial \psi}{\partial t} = \hat{A} \hbar \psi = \rho_1 \psi$$

$$\text{or, } \frac{\partial}{\partial t} \frac{\partial \psi}{\partial t} = \hat{A}^2 \hbar^2 \psi = \rho_2 \psi$$

thus, operator \hat{P}_1 is given by

$$\hat{P}_1 = \frac{i\hbar}{\partial} \frac{\partial}{\partial x} \quad \text{as } \hat{P}_1 = -i\hbar \frac{d}{dx}$$

Similarly,

$$\hat{P}_2 = \frac{i\hbar}{\partial} \frac{\partial}{\partial t} \quad \text{and } \hat{P}_2 = \frac{i\hbar}{\partial} \frac{\partial}{\partial t}$$

thus, in so, the operator \hat{P} can be represented by

$$\hat{P} = \frac{i\hbar}{\partial} \vec{v} = -i\hbar \vec{v}$$

* \hat{P} is gradient, which is a generalization of the usual concept of derivative of a func. in 1D to a func. in several dimensions. in so, cartesian coordinate system,
 $\vec{v} = \frac{\partial}{\partial t} \vec{r} + \frac{\partial}{\partial t} \vec{r}^1 + \frac{\partial}{\partial t} \vec{r}^2 + \dots$

ENERGY OPERATOR :

$$\left[E = \hat{H} \psi = \hbar \omega \right]$$

$$= \frac{\hbar}{i} \frac{\partial}{\partial t} \psi = \frac{\hbar \omega}{i} \psi$$

Suppose the wave func. of a particle in position

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

$$\Rightarrow \frac{\partial \psi}{\partial t} = -i\hbar A e^{i(kx - \omega t)}$$

$$\Rightarrow \frac{d\psi}{dt} = -i\hbar \psi$$

$$\Rightarrow i\hbar \frac{d\psi}{dt} = \hbar \omega \psi = E \psi$$

$$\Rightarrow \boxed{E = i\hbar \frac{d}{dt}}$$

* Proof. $\left[\hat{x}, \hat{p}_x \right] = i\hbar$
 let $f(n)$ be the func. in which these two operators

$$[\hat{x}, \hat{p}_x] f(n) = [\hat{x} \hat{p}_x - \hat{p}_x \hat{x}] f(n)$$

$$= (\hat{p}_x \hat{x} f(n)) - (\hat{p}_x \hat{x} f(n))$$

$$= \hat{x} \frac{\partial}{\partial t} \hat{p}_x f(n) - \hat{p}_x \frac{\partial}{\partial t} \hat{x} f(n)$$

$$= i\hbar \frac{\partial}{\partial t} f(n) - \frac{\partial}{\partial t} i\hbar \frac{\partial}{\partial x} f(n) - f(n) \frac{\partial}{\partial x} \frac{\partial}{\partial t}$$

$$= -i\hbar \frac{\partial}{\partial t} f(n) = f(n)i\hbar$$

$$\Rightarrow [\hat{x}, \hat{p}_x] = i\hbar$$

Physical significance: This eq[†] implies that any position operator do not commute. Thus, it is impossible to measure position & momentum simultaneously along same direction with the same accuracy. This supports Heisenberg's position-momentum principle.

EIGEN (or proper or characteristic) FUNCTION AND EIGEN VALUE:

- If an operator acting on a function will always produce the same function multiplied by a constant factor, the function is called an eigen function of the operator. The constant is known as eigen value of the given operator. Thus if \hat{A} is an operator that operates on a given function $f(x)$, then

$$\boxed{\hat{A} \cdot f(x) = c f(x)} \quad \text{--- (1)}$$

where, c is constant

Eq. ① is known as eigen value eq.

Note: All operators in quantum mechanics have eigen values of eigen values.

(ψ is said to have a free particle as well as free bound particle).

kinetic energy operator (\hat{T})

$$\hat{T} = \frac{p^2}{2m}$$

New, $\hat{T}\psi = (kE)\psi$

New, kE is the eigen value of KE operator.

$$\psi = A e^{ikx/\hbar}$$

$$\frac{\hbar}{i} \frac{d\psi}{dx} = \hat{P}_n \psi \cdot \frac{\hbar}{i} = P_n \cdot \psi$$

$$\Rightarrow \frac{d\psi}{dx} = i P_n \cdot \psi$$

$$\frac{d^2\psi}{dx^2} = \left(\frac{i P_n}{\hbar} \right)^2 \psi$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = \left(\frac{P_n^2}{\hbar^2} \right) \psi$$

$$\text{So, } \frac{1}{2m} \frac{d^2}{dx^2} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$$

* heat energy operator (H)

$$H\psi = E\psi$$

$$H\psi = (\hat{T} + \hat{V})\psi = \hat{T}\psi + \hat{V}\psi$$

$$= -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi$$

New, from Schrodinger's wave independent eq.,

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

$$\text{So, } \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \hat{V}$$

* Angular momentum operator:

$$\hat{L} = \vec{r} \times \vec{p} = \begin{vmatrix} i & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & i \end{vmatrix}$$

$$= i(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y) + j(\hat{x}\hat{p}_z - \hat{z}\hat{p}_x) +$$

* In quantum mech., each operator is associated with an operator which acts on ψ to give ψ' .

$$\text{So, } \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar \left[\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial y^2} \right]$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -i\hbar \left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial z^2} \right]$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar \left[\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} \right]$$

Applications of operators: I. Commutator operator in Q.M.

$$[\hat{x}_1, \hat{p}_1] = i\hbar$$

so, eigen value of \hat{x}_1 : $[\hat{x}_1, \hat{p}_1]\psi = i\hbar \psi$

$$[\hat{x}_1, \hat{p}_1]\psi = [\hat{x}_1 \hat{p}_1 - \hat{p}_1 \hat{x}_1]\psi$$

$$= \frac{i\hbar}{i} \frac{d\psi}{dx} - \frac{i\hbar}{i} \frac{d(x\psi)}{dx}$$

$$= \cancel{\frac{i\hbar}{i} \frac{d\psi}{dx}} - \frac{i\hbar}{i} \frac{d^2\psi}{dx^2} - \frac{4\hbar^2}{2} \frac{d\psi}{dx} = 0$$

$$\text{So, } [\hat{x}_1, \hat{p}_1] = 0$$

↳ commutation

Rule for commutation operator:

$$\text{① } [\hat{A}, \hat{B}] = 0$$

$$\text{② } [\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$$

$$\text{③ } [\hat{A}^a, \hat{B}^b] = \hat{A}^a [\hat{B}^b, \hat{C}] + [\hat{A}^a, \hat{C}] \hat{B}^b$$

$$\text{④ } [\hat{A}^a, \hat{B}^b \hat{C}] = [\hat{A}^a, \hat{B}] \hat{C} + \hat{B} [\hat{A}^a, \hat{C}]$$

$$* [\hat{A}^m, \hat{B}^n]$$

$$\text{Using } n = 2, [\hat{A}^m, \hat{B}^2] = \hat{A}^m [\hat{B}^2, \hat{B}] + [\hat{B}^2, \hat{A}^m]$$

$$[\hat{A}^m, \hat{B}^2] = \hat{A}^m [\hat{B}^2, \hat{B}] + i\hbar \hat{A}^m = 2i\hbar \hat{A}^m$$

$$\text{Taking } n=3, [\hat{x}^3, \hat{p}_n] = [\hat{x}^2, \hat{x}],$$

$$[\hat{x}^2, \hat{p}_n] + [\hat{x}^0, \hat{p}_n] \hat{x}$$

$$= \hat{x} \cdot i\hbar \hat{t} + i\hbar \hat{x}^2 \hat{x}$$

$$= i\hbar \hat{x}^3$$

$$\begin{aligned} &= \int_{-\infty}^{+\infty} \psi^*(n, x) \left(-i\hbar \frac{d}{dx} \right) \psi(n, x) dx \\ &= \int_{-\infty}^{+\infty} \psi^*(n, x) \left(-i\hbar \frac{d}{dx} \right)^2 \psi(n, x) dx \end{aligned}$$

$$\text{Thus, } [\hat{x}^m, \hat{p}_n] = m i\hbar \hat{x}^{m-2}$$

$$* [\hat{p}_n^m, \hat{x}] = -[\hat{x}, \hat{p}_n^m] =$$

$$\text{taking } m=2, -[\hat{x}, \hat{p}_n^2] = -[\hat{x}, \hat{p}_n \hat{p}_n]$$

$$= -\{[\hat{x}, \hat{p}_n] \hat{p}_n + \hat{p}_n [\hat{x}, \hat{p}_n]\}$$

$$= -[\hat{x} i\hbar \hat{p}_n + i\hbar \hat{p}_n]$$

$$= -2 i\hbar \hat{p}_n^2$$

$$\text{using } n=2, -[\hat{x}, \hat{p}_2^2] = -[\hat{x}, \hat{p}_2 \hat{p}_2]$$

$$= -\{[\hat{x}, \hat{p}_2] \hat{p}_2 + \hat{p}_2 [\hat{x}, \hat{p}_2]\}$$

$$= -\hat{p}_2 i\hbar \hat{p}_2 - \hat{p}_2^2 i\hbar = -3 i\hbar \hat{p}_2^2$$

$$\text{Thus, } [\hat{p}_n^m, \hat{x}] = -m i\hbar \hat{p}_n^{m-2}$$

EXPECTATION VALUE OF DYNAMICAL VARIABLES:

The quantity that depends upon the coordinates (x, y, z, t)

of a particle is called dynamical variable.

E.g: position, momentum, energy etc.

* The expectation value (or average value) of a dynamical quantity is the mathematical expectation [in the sense of probability theory] of the result of a single measurement.

In other words, it is an average of the results of a large number of measurements on independent identical system.

* The expectation value of any function $f(x)$ is given by:

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} \psi^*(x, t) f(x) \psi(x, t) dx$$

subjected to the normalization condition $\int_{-\infty}^{+\infty} |\psi(x, t)|^2 dx = 1$

* Expectation value of momentum:

$$\langle \hat{p}_x \rangle = \int_{-\infty}^{+\infty} \psi^*(n, x) \hat{p}_x \psi(n, x) dx$$

$$= \int_{-\infty}^{+\infty} \psi^*(n, x) \left(-i\hbar \frac{d}{dx} \right) \psi(n, x) dx$$

$$\langle \hat{p}_x \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi^*(n, x) \frac{d}{dx} \psi(n, x) dx$$

* Expectation value of energy:

$$\langle E \rangle = \int_{-\infty}^{+\infty} \psi^*(n, x) \left(i\hbar \frac{d}{dx} \right) \psi(n, x) dx$$

$$\Rightarrow \langle E \rangle = i\hbar \int_{-\infty}^{+\infty} \psi^*(n, x) \frac{d}{dx} \psi(n, x) dx$$

Note: If energy of particle is E_n , its momentum is ~~presently~~ $p_n = \pm \sqrt{2mE_n}$. It is expected that p_n would be non-zero. The \pm sign indicates that the particle is in such a potential, so that it will move back & forth.

As a result, its average momentum

$$\langle p_x \rangle = \sqrt{2mE_n} + (-\sqrt{2mE_n}) = 0$$

BASIC POSTULATES OF QUANTUM (OR WAVE) MECHANICS:

• The wave eq' of a particle can be described on the basis of the wave nature of particle and by applying quantum concepts to various classical equations of mechanics.

→ Quantum mechanics can be understood with the help of the following postulates:

① The space time behaviour of a particle is given by function $\psi(x, y, z, t)$. This function & its space derivative $\left(\frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial y} + \frac{\partial \psi}{\partial z} \right)$ are continuous, single valued & finite.

② In quantum mechanics, each quantum (physical parameter) is associated with quantum mechanics operator. e.g:

Variable

Symbol

Quantum mech. operator

- (a) Position $\vec{r}_n, \psi_n, \hat{r}_n, \hat{\psi}_n$
- (b) Momentum p_n, \hat{p}_n

$$E = -i\hbar \frac{d}{dt}$$

(c) Energy $E = -i\hbar \frac{d}{dt} \psi_n$

- (d) The probability that the particle with wave function ψ will be found in the volume element dV is $|\psi|^2 dV$

(e) The total probability of finding the particle somewhere in the space must be equal to 1, since probability $P = \int |\psi|^2 dV = 1$

(f) The expectation value of any dynamical quantity (say A) corresponding to its operator \hat{A} is given by

$$\langle A \rangle = \int \psi^* \hat{A} \psi dV$$

- (g) The only possible value of measurement of a dynamical variable A , whose operator is \hat{A} , is given by $\langle A \rangle$:

$$\langle A \rangle = \text{const}$$

(h) Schrödinger's wave equation: ψ is called eigen value of \hat{p}_x to the eigen values of eigen function of quantum state n .

(i) Schrödinger's wave equation:

Schrödinger's wave equation describes the behaviour of wave function (i.e. space-time behaviour of the moving particle) associated with matter waves under different physical situations.

1. Time dependent wave equation
Here, the potential V depends on time, so, the wave ψ describes the change of position of the particle with time.

Let a plane monochromatic wave moving along x -direction be given by $\psi(x, t) = A e^{i(kx - \omega t)}$

$$\psi(x, t) = A e^{i(kx - \omega t)} \quad [\text{here, } k = \frac{2\pi n}{\lambda}]$$

$$\text{Also, } E = \hbar \omega = \frac{p^2}{2m} = \frac{p^2}{2m} = \hbar k$$

$$\text{From } \text{Eqn } (2)$$

$$i\hbar \frac{d\psi}{dt} = -\hbar k \frac{d^2\psi}{dx^2} \quad \rightarrow \text{This is a sine dependent wave Eqn for a free particle of mass } m$$

$$\text{Now, } \frac{i\hbar}{\partial t} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

$$\frac{i\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi$$

$$\text{From Eqn } (2)$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\hbar k^2 \frac{\partial^2 \psi}{\partial x^2} \quad \rightarrow \text{This is a sine dependent wave Eqn for a free particle of mass } m$$

- (i) For free particle

• no external force acting on the particle

• Since, no potential energy of the particle (i.e. $V=0$)

• Has constant momentum as $P=0 \Rightarrow \frac{dp}{dt}=0$

$\Rightarrow P = \text{constant}$

• Total energy of a non-relativistic free particle of mass m moving along x -dir. (only k_x)

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

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

$$\Rightarrow \frac{d\psi}{dt} = -i\hbar \omega \psi$$

$$\Rightarrow i\hbar \frac{d\psi}{dt} = \hbar \omega \psi = E \psi$$

$$\text{Again, } \frac{d^2\psi}{dx^2} \quad (A) \text{ not } \propto$$

$$\frac{\partial^2 \psi}{\partial x^2} = i\hbar \omega \psi$$

$$\Rightarrow \frac{\hbar}{i} \frac{\partial \psi}{\partial x} = \frac{\hbar \omega}{i} \psi$$

$$\Rightarrow \frac{\hbar^2 \psi}{2m} = \left(\frac{\hbar \omega}{i} \right)^2 \psi$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \frac{\hbar \omega^2}{2m} \psi \quad (3)$$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi \quad (2)$$

$$\text{For } \psi = A e^{i(k_x x - \omega t)}, \psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

where, \vec{R} = position of particle

$$\vec{v}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

(1) Particle under an external force

$$\text{Total energy}, E = \frac{p_x^2}{2m} + V(x, t) \quad \text{--- (1)}$$

Multiplying both sides by $\psi(x, t)$

$$E \psi(x, t) = \frac{\hbar^2}{2m} \psi''(x, t) + V(x, t) \psi(x, t)$$

$$\text{From eqn (1)} \quad \frac{i\hbar}{2m} \frac{d\psi}{dt} = \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x, t) \psi(x, t)$$

$$\frac{i\hbar}{2m} \frac{d\psi}{dt} = \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x, t) \psi(x, t)$$

Since $\psi(x, t)$ is time dependent Schrödinger's wave eqn has particle under an external force is

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

For 1D motion,

$$\frac{-\hbar^2}{2m} \frac{\partial^2\psi}{\partial x^2} + V(x, t) \psi = i\hbar \frac{\partial\psi}{\partial t} \quad \text{--- (2)}$$

where, $\psi = \text{Kanninenian wave function}$ so motion

$$= -\frac{\hbar^2}{2m} \frac{\partial^2\psi}{\partial x^2} + V(x, t) \psi$$

B. Time independent Schrödinger's wave equation & its sol'n for Eigen Value eqn.

→ In this case, the potential energy (or, the force that acts on the particle) is a function of position (\vec{x}) only i.e. $V = V(\vec{x})$

* In this case, probability density of the particle is independent of time & the state is called stationary state)

→ Now, 1D time dependent Schrödinger's wave eqn is

$$\frac{-\hbar^2}{2m} \frac{\partial^2\psi}{\partial x^2} + V(\vec{x}) \psi(x, t) = i\hbar \frac{\partial\psi}{\partial t} \quad \text{--- (1)}$$

Given ψ is partial differential eqn of two variables (\vec{x}, t). When the pt. 't' is a func. of position only & not of time, the eqn is separable into the energy E is constant, the eqn is separable into the time independent part, so, we can write

$$[\psi(\vec{x}, t) = \phi(\vec{x}) f(t)] \quad \text{--- (2)}$$

→ Substituting this in (1), we can method of separation of variables.

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

dividing by $\phi \cdot f$,

$$\frac{-\hbar^2}{2m} \frac{1}{\phi} \frac{\partial^2\phi}{\partial x^2} + V(\vec{x}) = i\hbar \frac{1}{f} \frac{\partial f}{\partial t}$$

func. of position

func. of time

→ Possible when cons. (which is E) constant = E_{HC}

So, we can write,
 $\frac{-\hbar^2}{2m} \frac{1}{\phi} \frac{\partial^2\phi}{\partial x^2} + V(\vec{x}) = E$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{\partial^2\phi}{\partial x^2} + V(\vec{x}) \phi = E \phi$$

solution for Eigen value eqn:

We have, $i\hbar \frac{1}{f} \frac{\partial f}{\partial t} = E$

$$\Rightarrow i\hbar \frac{df}{dt} = Ef$$

$$\Rightarrow \frac{df}{dt} = -\frac{ie}{\hbar} f$$

$$\Rightarrow \ln f(t) = -\frac{ie}{\hbar} t$$

integrating both sides, we have
 $\ln f(t) = -\frac{ie}{\hbar} t + \ln c$

$$\Rightarrow \ln \frac{f(t)}{c} = -\frac{ie}{\hbar} t$$

$$\Rightarrow f(t) = C e^{-\frac{ie}{\hbar} t}$$

Now, $\psi(\vec{x}, t) = \phi(\vec{x}) \cdot C e^{-\frac{ie}{\hbar} t}$ [since, $\phi(\vec{x})$ is a function].

which gives the sol'n of eigen value eqn.

each set of wave independent wavefunction "g" corresponding to a definite energy "E" are written, $\psi = \psi_n(x)$ as the soln for $E = E_n$, the particular soln is $\psi(\vec{r}, t) = \psi_n(\vec{r}) e^{-iEt/\hbar}$.

and it belongs to a definite energy E_n .

The probability of finding a particle doesn't depend upon time:

$$\text{Prob.} / |\psi_n(\vec{r}, t)|^2 = |\psi_n(\vec{r}, t) \cdot \psi_n(\vec{r}, t)|$$

$$= |\psi_n(\vec{r})|^2 - (\bar{\psi}_n(\vec{r}))^* \cdot \psi_n(\vec{r}) \cdot \bar{\psi}_n(\vec{r}) \cdot \psi_n(\vec{r})$$

$$= 1.0 * \psi_n(\vec{r}) \cdot \psi_n^*(\vec{r}), \text{ etc.}$$

$$\left[\text{Now, } \psi \psi^* = 1 \int \psi_n(\vec{r}) \cdot \psi_n^*(\vec{r}) \right]$$

$$\text{so, } \left| \int \psi_n(\vec{r}, t) \right|^2 = \left| \int \psi_n(\vec{r}) \right|^2$$

*: Probability is same as in terms of momentum

Energy of particle of mass m ,

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

Now, since independent wavefunctions & wave eq's are:

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \cdot \psi(x) = E \cdot \psi(x)$$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \psi(x) [E - V]$$

$$= \psi(x) \cdot \frac{p^2}{2m}$$

$$\Rightarrow -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} = p^2 \psi(x)$$

$$\Rightarrow \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{E^2}{\hbar^2} \psi(x) = 0 \right] \text{ is wave eqn of a particle of mass } m \text{ if momentum } p.$$

$$\text{In } 3b, \boxed{\nabla^2 \psi + \frac{E^2}{\hbar^2} \psi(x) = 0}$$

PHYSICAL SIGNIFICANCE OF WAVE FUNCTIONS:

The wave function $\psi(x, t, y, z)$ gives the space-time distribution of each moving quantum

- measures the probability of finding a particle always at a position.
- the quantity $|\psi|^2$ gives the probability of finding a particle per unit volume in the space (i.e. probability density in the space).
- probability of finding a particle between x_1 & x_2 is $P = \int |\psi|^2 dx$

$$P = \int |\psi|^2 dx$$

* The magnitude is larger in regions where the probability of finding the particle is high & is zero in regions where the probability of finding the particle is low.

- The wave function & its space derivative ($\frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}, \dots$) should be continuous, single valued & finite everywhere.
- Conservation of ψ for a meaningful set of wavefunctions:

① It should be a sum of space & time, $\psi = \psi(x, t, y, z, \vec{r}, \vec{k})$

② The wave function & its space derivatives $\frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}, \dots$ must be continuous, single valued & finite everywhere.

③ The wave function ψ must be continuous in all regions except those regions where $E, V(x, y, z) = \infty$

④ Must be normalizable i.e. ψ approaches 0 as $x \rightarrow \infty$

Reason: If ψ has finite value as $x \rightarrow \infty$, then the $\int |\psi|^2 dx$ will blow off; hence, ψ

becomes non-normalizable.

Eq. of Physics ψ : $\psi(x, t) = e^{-iEt/\hbar}$

$$\rightarrow e^{-ikx}$$

$$\rightarrow \sin kx, \cos kx$$

$$\rightarrow e^{i(kx-\omega t)}$$

limit, for some given

$$\text{Wavelength } \lambda : \rightarrow e^{i k \lambda}$$

$$\rightarrow \sin k\lambda, \cos k\lambda$$

DIMENSION OF WAVE FUNCTIONS $\psi(x, y, z, t)$

We know Probability density, $J = |\psi|^2$

so, $[\psi(x, y, z, t)]^2 = \text{probability density}$

$$\Rightarrow [\psi(x, y, z, t)]^2 = \rho^2 \psi^2 \cdot V^{-1/2}$$

$$[\text{Volume}] = l^3 \quad \& \quad 1 \text{ is dimensionless}$$

$$\text{so, } [\psi(x, y, z, t)]^2 = \frac{l^{-3/2}}{2m} \cdot \rho \cdot \psi^2$$

Schrödinger's wave equation for a free particle ϕ , it is solution:

for free particle, $V=0$

$$4\psi''_{xx}(x, y, z, t) = \rho \psi_{yy}(x, y, z, t)$$

$$\rho = \text{constant}$$

$$V=0$$

$$V=0$$

$$\rho = \text{constant}$$

$$V=0$$

$$V=0$$

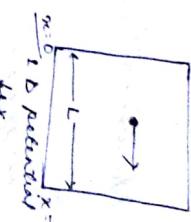
$$\rho = \text{constant}$$

$$V=0$$

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

APPLICATIONS OF SCHRÖDINGER WAVE EQUATION

I. Particle in a 1D box i.e. in an infinitely deep 1D potential well:



St curve for the particle is bounded to move along straight line, say x-axis.

As the potential well is infinitely deep, a particle cannot exist outside the well & is reflected back whenever it reaches the end

Since PE is independent of time, so sine independent of the range. Since ψ is independent of time, so sine independent of the range.

$$\frac{-\hbar^2 d^2 \phi}{2m dx^2} + V(x) \cdot \phi = E \cdot \phi$$

In region where $V(x) = 0$,

$$\frac{-\hbar^2 d^2 \phi}{2m dx^2} = E \phi$$

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

$$[K^2 = 2mE/\hbar^2]$$

$$\Rightarrow \left| \frac{d^2 \phi}{dx^2} + K^2 \phi = 0 \right|$$

General soln of (1) is, $\phi(x) = A \sin kx + B \cos kx$

Now, from boundary conditions

(1) at $x=0$, $\phi(x) = 0$

(2) at $x=L$, $\phi(x) = 0$

thus, for $x=0 \Rightarrow \phi(x) = 0 \Rightarrow B = 0$

so, (2) becomes,

$$\phi(x) = A \sin kx$$

Again at $x=L \Rightarrow \phi(x) = 0$

$$\Rightarrow A \sin kL = 0 \quad (\sin 0 \text{ iff } A=0)$$

$$\Rightarrow kL = n\pi$$

$\Rightarrow \boxed{A = \lambda x}$ where $\lambda x = 2, 2, 3, \dots$ are

your, possible, name pronounced for your adoption here;

EIGEN HAVENS OF ENERGY

$$g_*(\alpha) = \text{Bose gas E.E.}$$

$$P(R = 1) \approx 10^{-24} J_{-5}$$

SHELDON AND ALEXANDER

$$E_R = \frac{A}{2\pi} + \frac{n_X}{L_X}$$

habits are in excess
and a disorder so like
a square of vicious, of vice,
perverted, well.

$$T = \sqrt{\frac{2}{\pi}} \left(\frac{1}{\sqrt{1 - \frac{4}{\pi} \sin^2 k_0}} \right)^{\frac{1}{2}}$$

He also claims that alluvium which it carries on board upon the upper reaches of the river probably has distinct marks of weathering.

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(2) $\frac{d\theta}{dt} = \frac{\partial \theta}{\partial x} \frac{dx}{dt} + \frac{\partial \theta}{\partial y} \frac{dy}{dt}$

② ~~the~~
The young ones
are running around
of their mother.

John (John) Medi

empty land surrounding no
habitat name here yet
Please advise if other details
with it.

NORMALISATION OF PROTEIN LEVELS (i.e. EIGEN FUNCTIONS)

$$P_n(x) = \frac{B \sin(n\pi x)}{\pi}$$

Probability that particle is located in string α is given by mean normalization condition

$$T = \text{up to } 4$$

Scanned by CamScanner

$\Rightarrow K = \frac{n\pi}{L}$ where $n = 1, 2, 3, \dots$ etc.

thus, permissible wave functions for this motion are:

$$\phi_n(x) = B_n \sin \frac{n\pi x}{L}$$

Eigen values of energy:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m} K^2$$

$$\text{Hence, } E_n = \frac{\hbar^2 K^2}{2m}$$

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

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m L^2}$$

Hence, except eigen values are in reality proportional to the square of width of the potential well.

It is also clear that allowed values of energy E_n

depend upon the different values of n . i.e.

so, the particle has discrete values of energy.

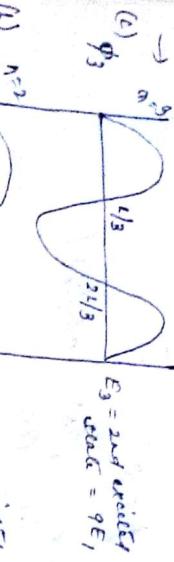
Energy is quantized (discrete).

The different values of E_n are called eigen values of the corresponding values of ϕ_n are called eigen functions.

$\rightarrow E_1 = 0 \Rightarrow \phi_1 = 0$ & $E_2 = 0$. Indicates that particle cannot

exist in a box if its energy is zero.

$$\rightarrow \text{Now, } E_1 = \frac{\hbar^2}{2m L^2}, E_2 = 4E_1, E_3 = 9E_1$$



$$(a) \quad \phi_1 \quad \phi_2 \quad \phi_3$$

$E_1 = 1^{\text{st}}$ excited state = $9E_1$



$$(b) \quad \phi_2 \quad E_2 = 2^{\text{nd}} \text{ excited state} = 9E_1$$

$E_2 = 2^{\text{nd}}$ excited state = $9E_1$



$$(c) \quad \phi_3 \quad E_3 = 3^{\text{rd}} \text{ excited state} = 9E_1$$

$E_3 = 3^{\text{rd}}$ excited state = $9E_1$

Energy band corresponding to normalized wave function for present state is excited

Energy band corresponding to normalized wave function for present state is excited

$$\phi_n(x) \text{ will reduce}$$

NORMALIZED WAVE FUNCTIONS (i.e. EIGEN FUNCTIONS)

$$\phi_n(x) = B_n \sin \frac{n\pi x}{L}$$

Probability that particle is located in length dx is $g(x) dx$. Then normalization condition is

$$\int g(x) dx = 1$$

Since ϕ is $\neq 0$ outside box

$$\int f(x)^2 dx = 1 \Rightarrow \int \sin^2 \frac{n\pi x}{L} dx = 1$$

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

$$\Rightarrow \frac{B_n^2 L}{2} - \frac{B_n^2}{2} \left[\sin \frac{n\pi x}{L} \right]_0^L = 1$$

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

$$\text{So, normalized wave func. / eigen func. for particle inside a well of width } L \text{ is}$$

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

NOTE: ① Expectation value of position of particle is at the middle of the box in all quantum states. i.e.

$$\langle x \rangle = \int \phi_n(x) x \phi_n(x) dx = \frac{L}{2}$$

→ This value is independent of n & doesn't give any info. about the quantum state of the particle.

② If the allowed values of energy are quantized with probability $P_1, P_2, P_3, \dots, P_n$ with expectation in system are $E_1, E_2, E_3, \dots, E_n$ then the expectation value of energy for the system is

$$\text{Expect} = P_1 E_1 + P_2 E_2 + \dots + P_n E_n$$

PROBABILITY CURRENT DENSITY.

→ If a particle moves along the x-axis, the probability of finding the particle in the region $x_1 \rightarrow x_2$.

\rightarrow $\psi(x, t)$ represents the particle's position function of the region.

\rightarrow Probability of finding the particle within the region:

$$\int_{x_1}^{x_2} |\psi(x, t)|^2 dx = \int_{x_1}^{x_2} |\psi^* \psi| dx$$

\rightarrow As the particle moves along the x-axis, the probability of finding the particle in the region decreases with time.

The rate of decrease of probability in the region from x_1 to x_2 per unit time is called the probability current density of the region.

$$P_i = \psi^* \psi \cdot \frac{\partial \psi}{\partial t}$$

$\frac{\partial \psi}{\partial t} = i\hbar \frac{\partial^2 \psi}{\partial x^2} - \frac{eV}{\hbar} \psi \quad \text{--- (1)}$

From which it can be dependent on,

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

$$\Rightarrow \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{eV}{\hbar} \psi \quad \text{--- (2)}$$

$$\text{Now, } \frac{\partial \psi}{\partial t}^* = -\frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2}^* + \frac{eV}{\hbar} \psi^* \quad \text{--- (3)}$$

Putting values in (4)

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

$$= \frac{i\hbar}{2m} \left[\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{e^2 V^2}{\hbar^2} \psi \right] \quad \text{--- (4)}$$

$$= \frac{i\hbar}{2m} \left[\frac{\psi^2}{2m} \left(\frac{\partial \psi}{\partial x} \right)^2 - \frac{\partial \psi}{\partial x} \left(\frac{\partial \psi}{\partial x} \right)^* \right] \quad \text{--- (5)}$$

$$\Rightarrow \frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left[\frac{i\hbar}{2m} \left\{ \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi}{\partial x} \psi^* \right\} \right]$$

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

$$\Rightarrow \frac{\partial P}{\partial x} = -\frac{\partial S}{\partial x}$$

$$\Rightarrow \frac{\partial P}{\partial x} + \frac{\partial S}{\partial x} = 0$$

∴ Probability current density (S) at x is

$$\Rightarrow S = - \int_{x_1}^{x_2} \frac{\partial}{\partial x} |141|^2 dx$$

None: 0 for particle in a box, $S = 0$

→ Since there is no particle within the box, the rate of decrease of probability within the box is zero. The particle is confined within the box.

For free particle, $S = \text{product of its probability density and its speed}$.

$$\text{For free particle, } i(\hbar k - Et) \quad \text{--- (6)}$$

$$\psi(x, t) = A e^{i(\hbar k x - Et)} \quad \text{--- (7)}$$

$$\frac{\partial \psi}{\partial x} = i\hbar k \psi \quad \text{--- (8)}$$

$$\frac{\partial \psi}{\partial x} = \frac{i\hbar k}{m} \frac{\partial \psi}{\partial t} = \frac{-i\hbar k}{m} P_x \psi \quad \text{--- (9)}$$

$$\frac{\partial P}{\partial x} = -i\hbar \frac{\partial \psi}{\partial x} = P_x \psi \quad \text{--- (10)}$$

$$\text{Now, } S = -\frac{i\hbar}{2m} \left[\frac{\psi^2}{2m} \left(\frac{\partial \psi}{\partial x} \right)^2 - \frac{\partial \psi}{\partial x} \left(\frac{\partial \psi}{\partial x} \right)^* \right] \quad \text{--- (11)}$$

$$= -\frac{i\hbar}{2m} \left[\frac{\psi^2}{2m} \left(\frac{\partial \psi}{\partial x} \right)^2 + \frac{\partial \psi}{\partial x} \left(\frac{\partial \psi}{\partial x} \right)^* \right] \quad \text{--- (12)}$$

$$= \frac{e^2 V^2}{\hbar^2 m} \left[\frac{\psi^2}{2m} \left(\frac{\partial \psi}{\partial x} \right)^2 \right] \quad \text{--- (13)}$$

$$\Rightarrow S = \frac{e^2 V^2}{\hbar^2 m} P_x = 141^2 V_a \quad \text{--- (14)}$$

NORMALIZATION OF EIGEN FUNCTIONS

$$\psi(x, t) = \sum_{n=1}^{\infty} c_n \phi_n(x) e^{i(E_n t)/\hbar}$$

We know that, $\int_{-\infty}^{\infty} \psi^* \psi dx = 1 \Rightarrow \left| \sum_{n=1}^{\infty} c_n \phi_n^* \phi_n dx \right|^2 = 1$

$$\Rightarrow \left| \sum_{n=1}^{\infty} c_n \right|^2 = 1$$

In plane orthogonality of eigenfunction :-

Since independent Schrödinger's wave eqn :-

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_m}{\partial x^2} + V(x) \phi_m = E_m \phi_m \quad \text{--- (1)}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_n}{\partial x^2} + V(x) \phi_n = E_n \phi_n \quad \text{--- (2)}$$

As conjugate of ϕ_m ,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_m^*}{\partial x^2} + V(x) \phi_m^* = E_m \phi_m^* \quad \text{--- (3)}$$

(1) $\times \phi_m^*$ and (3) $\times \phi_n$

$$-\frac{\hbar^2}{2m} \phi_m^* \frac{\partial^2 \phi_n}{\partial x^2} + V(x) \phi_m^* \phi_n = E_m \phi_n \phi_m^* \quad \text{--- (4)}$$

$$-\frac{\hbar^2}{2m} \phi_m^* \frac{\partial^2 \phi_m}{\partial x^2} + V(x) \phi_m^* \phi_m = E_m \phi_m^* \phi_m \quad \text{--- (5)}$$

(5) - (4),

$$+\frac{\hbar^2}{2m} \left[\phi_m^* \frac{\partial^2 \phi_n}{\partial x^2} - \phi_n \frac{\partial^2 \phi_m^*}{\partial x^2} \right] = \phi_m^* \phi_n [E_m - E_n]$$

$$\Rightarrow \frac{\hbar^2}{2m} \left[\frac{\partial}{\partial n} \left(\phi_n^* \frac{\partial \phi_n}{\partial n} \right) - \frac{\partial}{\partial n} \left(\phi_n \frac{\partial \phi_n^*}{\partial n} \right) \right] = \phi_m^* \phi_n [E_m - E_n]$$

$$\Rightarrow \frac{\partial}{\partial n} \left[\phi_n^* \frac{\partial \phi_n}{\partial n} - \phi_n \frac{\partial \phi_n^*}{\partial n} \right] = \frac{\partial m}{\partial n} [E_m - E_n] \phi_m^* \phi_n$$

$$\text{On } \int_{-\infty}^{\infty} \phi_n^* \frac{\partial \phi_n}{\partial n} - \phi_n \frac{\partial \phi_n^*}{\partial n} = \frac{m}{\hbar^2} [E_m - E_n] \int_{-\infty}^{\infty} \phi_m^* \phi_n \, dx$$

$$(At \infty, \phi \rightarrow 0)$$

$$\text{So, } \int_{-\infty}^{\infty} \phi_m^* \phi_n \, dx = \begin{cases} 1, & \text{if } m=n \\ 0, & \text{if } m \neq n \end{cases}$$

(orthogonal set of basis function)

- * It means that sum of square of coefficients is sum of $\phi_1, \phi_2, \dots, \phi_n$ is 1 for a superposed state, while $\psi(x) = c_1 \phi_1 + c_2 \phi_2 + \dots + c_n \phi_n$

Now, $\int \psi * \psi \, dx = 1$

$$\Rightarrow \int \left[C_1 \phi_1^* + C_2 \phi_2^* + \dots + C_n \phi_n^* \right] \left[C_1 \phi_1 + C_2 \phi_2 + \dots + C_n \phi_n \right] \, dx = 1$$

$$\Rightarrow C_1^* C_1 \int \phi_1^* \phi_1 \, dx + C_2^* C_2 \int \phi_2^* \phi_2 \, dx + \dots +$$

$C_n^* C_n \int \phi_n^* \phi_n \, dx = 1$
Since $\phi_1, \phi_2, \dots, \phi_n$ are orthogonal and each other, their inner products are zero

$$C_1^* C_1 + C_2^* C_2 + \dots + C_n^* C_n = 1$$

$$\Rightarrow (C_1, C_2, \dots, C_n)^T \cdot (C_1, C_2, \dots, C_n)^T = 1$$

$(C_1^* C_1 = |C_1|^2 \text{ since } C_1 \text{ is constant and similarly for rest})$

LAGRANGIAN & HAMILTONIAN MECHANICS

CONSTRAINT & CONSTRAINT FORCE:

- The restriction on the movement of a body is called constraint and the force which impose these restriction on the motion of the system of particles of the body are called constraint forces or forces of constraint.
- The corresponding equation which describes the motion of the system of particles of the body is known as constraint equation.
- Ex:

(i) In a simple pendulum, independent term of tension, T , is not known. Its value is determined with the help of known quantity of the system.

(ii) In a rigid body, the conservative force acting over any two particles to which keeps the distance constant.

TYPES OF CONSTRAINT:

I ① Mechanistic / Integrable: The constraint relation is independent of velocity and can be expressed in the form of an algebraic

equation $f(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_n, t) = 0$
Also, called geometric constraint.

② Non-Mechanistic / Non-Integrable: depends on velocity. Cannot be expressed in the form $f(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_n, t) = 0$

II ① holonomic (or stationary): Constraint relation does not explicitly depend on time.

$$f(x, y, z, t) = 0 \quad ; \quad \frac{df}{dt} = 0$$

② Rheonomic: Constraint relation is time dependent

$$f(x, y, z, t) = 0 \quad ; \quad \frac{df}{dt} \neq 0$$

SCLERONOMIC

RHEONOMIC

$$\begin{aligned} f(x, y, z) &= 0 \\ \text{Hence, } \frac{\partial f}{\partial t} &= \frac{\partial f}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial t} \\ \text{So, } 0 &= \left(\frac{\partial f}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial t} \right) f \left(\frac{\partial x}{\partial t} + \frac{\partial y}{\partial t} + \frac{\partial z}{\partial t} \right) \end{aligned}$$

$$\Rightarrow 0 = \overline{V} f \cdot \overrightarrow{d\vec{r}} \quad \overline{V} f \perp d\vec{r}$$

$$\Rightarrow \theta = \overline{V} f \cdot d\vec{r}$$

considering another displacement $\Delta \vec{x}'$ within the same time interval $d\tau$, eq. (4) becomes,

$$\nabla f \cdot d\vec{x}' = 0 \quad \text{--- (4)' } \quad \nabla f \cdot d\vec{x} + \frac{\partial f}{\partial t} \cdot dt = 0 \quad \text{--- (4)' }$$

(4)' yields

$$\nabla f \cdot (d\vec{x}' - d\vec{x}') = 0$$

EXAMPLES:

(1) rigid body

$$|\vec{x}_i - \vec{x}_j|^2 = c^2 = 0$$

Mechanics:衙公的

(2) motion of a body on an inclined plane under gravity

$$\theta - x \tan \theta = 0 \quad \text{--- (4), 5}$$

simple pendulum

$$x^2 + y^2 = l^2 \quad \text{--- (4), 5}$$

(3) any deformable body

$$|\vec{x}_i - \vec{x}_j| = f(t) \quad \text{--- (4), 5}$$

(4) a pendulum with variable length $\mu(t)^2 = l^2(t)$ (4), 5

(5) motion of gas molecules in a spherical container

$$|\vec{x}_i| \leq a \quad (\text{WH}, 5)$$

(6) A disc rolling down without slipping on a plane

$$dx - ad\sin\theta = 0 \quad \text{--- (4), 5}$$

In case of disc, if cylinder/spherical ball $\rightarrow N$.

NOTE: ideal constraint : if the sum of work done by constraint forces on the particle of a dynamical system is zero, then the constraint is called the ideal constraint. In that case, $\sum_i \vec{F}_{ij} \cdot \Delta \vec{x}_j = 0$ where x_i is constant place.

e.g.: A particle having circular motion or a sphere rolling down through a plane without slipping

DEGREES OF FREEDOM:

\rightarrow defined as the minimum number of independent coordinates which can specify the position of the system.

\rightarrow the constrained system,

$$\{ \text{dof} = \text{DN} - R \}$$

$N = \text{number of free particles}$

$R = \text{no. of constraints}$

eg. _____.

it works done by constraint force

if we consider a rigid body having two point masses m_1 and m_2 with position vector \vec{x}_1 and \vec{x}_2 from an arbitrary origin respectively.

The total work done by all the i^{th} particles in a rigid body will be $N_i = \sum_j \vec{F}_{ij} \cdot \Delta \vec{x}_j \quad \text{--- (4)}$ where \vec{F}_{ij} is the self force of a equal to zero. We have many done (N). For all the particles in the rigid body becomes,

$$\sum_i \sum_j \vec{F}_{ij} \cdot \Delta \vec{x}_j = \sum_i \sum_j \vec{F}_{ij} \cdot \vec{x}_j = N \quad \text{--- (4)}$$

$$\text{For a rigid body, the eq. of constraint is } |\vec{x}_i - \vec{x}_j|^2 = \text{constant} \quad \text{--- (4), 5}$$

$$\frac{\partial}{\partial t} (\vec{x}_i - \vec{x}_j) \cdot \Delta (\vec{x}_i - \vec{x}_j) = 0 \quad \text{--- (5)}$$

\rightarrow internal force \vec{F}_{ij} between any two particles is directed along the line joining them i.e., \vec{F}_{ij} is always and symmetric in \vec{x}_i and \vec{x}_j .

$$\text{Substituting } \vec{F}_{ij} \text{ in (5), } N = \frac{1}{2} \sum_i \sum_j \vec{F}_{ij} \cdot (\vec{x}_i - \vec{x}_j) \cdot \Delta (\vec{x}_i - \vec{x}_j) = 0 \quad \text{using (5)}$$

hence, the work done by the constraint force will be zero, i.e., an infinitesimally small displacement that occurs without any real change of time (i.e. independence) as is given by $\dot{x}_i = dx_i/dt = 0$.

NORMAL DISPLACEMENT?

It is an infinitesimally small displacement that occurs

Considering another displacement $\Delta \vec{x}_i$ within the same time interval dt , eq. (a) & (b) become,

$$\nabla f \cdot d\vec{x}_i = 0 \quad \text{--- (a)'}$$

$(x_i - x_i')$ fixed

$$\nabla f \cdot (\Delta \vec{x}_i - d\vec{x}_i) = 0$$

\rightarrow

$$\nabla f \cdot (\Delta \vec{x}_i - d\vec{x}_i) = 0 \quad \text{--- (b)'}$$

Examples:

(i) rigid body

(ii) motion of a body in an inclined plane under gravity

$$\theta - \theta_{\text{fixed}} = 0$$

kinematics / kinematic

(iii) motion of a body in an inclined plane under gravity

$$\theta - \theta_{\text{fixed}} = 0 \quad \text{--- (c)}$$

where \vec{F}_{ij} is the self force of i th particle due to a face j and may done (W). See all the particles in the rigid body becomes,

$$\sum_i \sum_j \vec{F}_{ij} \cdot \Delta \vec{x}_i = \sum_i \sum_j \vec{F}_{ij} \Delta x_j = W \quad \text{--- (2)}$$

$$\text{Any deformable body } \sum_i \vec{x}_i - \vec{x}_j \mid = f(x) \quad \text{--- (H, R)}$$

$$\text{A pendulum with variable length } R(t) \stackrel{2}{=} L^2(t) \quad \text{--- (H, R)}$$

$$\text{Motion of gas molecules in a spherical container} \quad (NH, S)$$

$$r_i / R \leq 1$$

(iv) A disc rolling down without slipping on a plane

$$q_x - \theta \sin \theta = 0$$

$$d\theta + \omega d\phi = 0$$

In case of disc, if cylinder / spherical ball $\rightarrow N$.

NOTE: Total constraint : or the sum of work done by constraint forces on the particle of a granular system is zero, then the constraint is called the ideal constraint. In that case, $\sum_i \vec{F}_i \cdot \delta \vec{x}_i = 0$ where F_i is

constraint force.

Eg: A particle having n particles moving on a sphere rolling down through a plane without slipping.

DEGREES OF FREEDOM:

→ defined as the min. no. of independent coordinates, which can specify the position of the system.

→ for a constrained system,

$$[dof = DN - R]$$

$N = \text{number of free particles}$

$R = \text{no. of constraints}$

constraint eqns.

Ex:

$$W = \frac{1}{2} \sum_i \sum_j c_{ij} (\vec{x}_i - \vec{x}_j) \cdot \Delta (\vec{x}_i - \vec{x}_j) = 0$$

$$\sum_i \vec{x}_i - \vec{x}_j \mid = \text{constant} \quad (b)$$

using differentials

$$d(\vec{x}_i - \vec{x}_j) \cdot \Delta (\vec{x}_i - \vec{x}_j) = 0 \quad \text{--- (5)}$$

→ internal force \vec{F}_{ij} betw. any two particles is directed along the line joining them i.e. \vec{F}_{ij} is along $(\vec{x}_i - \vec{x}_j)$. So, $\vec{F}_{ij} = c_{ij} (\vec{x}_i - \vec{x}_j)$, where c_{ij} = real constant and symmetric in i and j .

Substituting \vec{F}_{ij} in (5),

$$W = \frac{1}{2} \sum_i \sum_j c_{ij} (\vec{x}_i - \vec{x}_j) \cdot \Delta (\vec{x}_i - \vec{x}_j) = 0 \quad (\text{using 5})$$

Hence, the work done by the constraint forces vanish.

VIRTUAL DISPLACEMENT?

It is an infinitesimally small displacement that occurs without any real change of time (i.e. instantaneously).

Ex:

Principle of Virtual work:

→ For a system in equilibrium, the resultant force \vec{F}_i acting on each particle must be zero i.e. $\vec{F}_i = 0$.

→ Hence, for any arbitrary virtual displacement $\delta\vec{x}_i$ of a particle in equilibrium, virtual work done is zero.

So, for all the particles of the system, virtual work done is,

$$\left[\sum_i \vec{F}_i \cdot \delta\vec{x}_i = 0 \right] \quad (2)$$

Splitting the total force \vec{F}_i into applied force $\vec{F}_i(a)$ and

force of constraint $\vec{F}_i(c)$,

$$\sum_i (\vec{F}_i(a) + \vec{F}_i(c)) \cdot \delta\vec{x}_i = 0 \Rightarrow \left[\sum_i \vec{F}_i(a) \cdot \delta\vec{x}_i + \sum_i \vec{F}_i(c) \cdot \delta\vec{x}_i = 0 \right] \quad (3)$$

Since work done by constraint force handled i.e.

$$\left[\sum_i \vec{F}_i(c) \cdot \delta\vec{x}_i = 0 \right] \quad (4)$$

then, the principle of virtual work done states that the virtual work done by all the applied forces acting on a system in equilibrium is zero, provided that the total virtual work done by all the constraint forces is equal to zero.

D'ALEMBERT'S PRINCIPLE

For a dynamical system of particles, the equation of motion of any i-th particle of momentum \vec{p}_i due to the applied force \vec{F}_i can be written as,

$$\vec{F}_i = \frac{d}{dt} \vec{p}_i = m \frac{d\vec{x}_i}{dt} \quad (5) \quad (\vec{x}_i \text{ is the position vector of } i\text{-th particle})$$

$$\Rightarrow (\vec{F}_i - m \ddot{\vec{x}}_i) = 0 \quad (2)$$

It implies that under the combined application of reaction force ($-m \ddot{\vec{x}}_i$) & applied force \vec{F}_i , the system is in equilibrium.

→ Applying the principle of virtual work done on the dynamics system,

$$\left[\sum_i (\vec{F}_i - m \ddot{\vec{x}}_i) \cdot \delta\vec{x}_i = 0 \right] \quad (\delta\vec{x}_i \text{ is the virtual displacement})$$

Now, shear force on i-th particle,

$$\vec{F}_i = \vec{F}_i(a) + \vec{F}_i(c)$$

$$\begin{aligned} \text{or, } \delta\vec{x}^1 \text{ becomes,} \\ \sum_i (\vec{F}_i(a) - m \ddot{\vec{x}}_i) \cdot \delta\vec{x}_i + \sum_i \vec{F}_i(c) \cdot \delta\vec{x}_i = 0 \end{aligned} \quad (4)$$

As the virtual work done by constraint forces is zero,

$$\left[\sum_i (\vec{F}_i(a) - m \ddot{\vec{x}}_i) \cdot \delta\vec{x}_i = 0 \right] \quad (4)$$

This is known as D'Alembert's principle.

* If we consider D'Alembert's principle, for the actual motion of any system of particles subjected to constraint forces motion, the sum of work done due to applied forces and due to the forces of inertia in any virtual displacement of the system for each given instant of time, is equal to zero.

Application of D'Alembert's Principle:

→ Let us consider a simple pendulum of mass m & effective length l in $x-y$ plane.

→ Eqn of constraint for the system

$$x^2 + y^2 = l^2 \quad (1)$$

Differentiating (1),

$$2x \cdot dx + 2y \cdot dy = 0$$



$$\Rightarrow x \cdot da + y \cdot dy = 0 \quad (2)$$

Using D'Alembert's principle, we can write 'g' of motion as

$$\sum_i (m \ddot{\vec{x}}_i - \vec{F}_i(a)) \cdot \delta\vec{x}_i = 0 \quad (3)$$

In terms of x & y , (3) can be written as,

$$(m \ddot{x} - F_x) dx + (m \ddot{y} - F_y) dy = 0 \quad (4)$$

F_x & F_y are components of applied force along x & y axes respectively.

Since the applied forces do not include tension (i.e. here, the applied forces do not include tension force of constraint), force of constraint, force (mg) acting on the bob is along

Since the only force (mg) acting on the bob is along y -axis, $F_y = -mg$

$$\therefore F_y = 0$$

Eqn (4) becomes,

$$m \ddot{x} + (m \dot{y} + mg) dy = 0$$

$$\Rightarrow \ddot{x} da + (\dot{y} + g) dy = 0 \quad (5)$$

$$\text{From (2), } dy = -\frac{x \, da}{y}$$

$$\text{Putting in (5), } \ddot{x} da + (\dot{y} + g) \left(-\frac{x \, da}{y} \right) = 0$$

Principle of Virtual work:

- For a system in equilibrium, the resultant force $\vec{F}_i = 0$
- Acting on each particle must be zero i.e. $\vec{F}_i = 0$.
- Hence, for any arbitrary virtual displacement \vec{dx}_i of a particle in equilibrium, virtual work done is zero.

So, for all the particles of the system, virtual work done is,

$$\sum_i \vec{F}_i \cdot \vec{dx}_i = 0 \quad (2)$$

Splitting the total force \vec{F}_i into applied force $\vec{F}_i(a)$ and force of constraint $\vec{F}_i(c)$,

$$\sum_i (\vec{F}_i(a) + \vec{F}_i(c)) \cdot \vec{dx}_i = 0 \Rightarrow \sum_i \vec{F}_i(a) \cdot \vec{dx}_i + \sum_i \vec{F}_i(c) \cdot \vec{dx}_i = 0 \quad (3)$$

Since work done by constraint force vanishes i.e.

$$\sum_i \vec{F}_i(c) \cdot \vec{dx}_i = 0, \text{ we have}$$

$$\sum_i \vec{F}_i(a) \cdot \vec{dx}_i = 0 \quad (4)$$

Thus, the principle of virtual work done states that the virtual work done by all the applied forces acting on a system in equilibrium is zero, provided that the total virtual work done by all the constraint forces is equal to zero.

STELLER'S PRINCIPLE

For a dynamical system of particles, the equation of motion of any i th particle of momentum \vec{p}_i due to the applied force \vec{F}_i can be written as,

$$\frac{\vec{p}_i}{\vec{F}_i} = \frac{\dot{\vec{r}}_i}{m_i} = m_i \ddot{\vec{r}}_i \quad (i) \quad (\vec{r}_i \text{ is the position vector of } i\text{th particle})$$

$$\Rightarrow (\vec{F}_i - m_i \ddot{\vec{r}}_i) = 0 \quad (2)$$

It this implies that under the combined application of reaction effective force $(-\vec{m}_i \ddot{\vec{r}}_i)$ & applied force \vec{F}_i , the system is in equilibrium.

→ Applying the principle of virtual work done on the dynamical system,

$$\sum_i (\vec{F}_i - m_i \ddot{\vec{r}}_i) \cdot \vec{dx}_i = 0 \quad (\vec{dx}_i \text{ is the virtual displacement})$$

Now, work done on i th particle,

$$\vec{F}_i = \vec{F}_i(a) + \vec{F}_i(c)$$

So, eqn (2) becomes,

$$\sum_i (\vec{F}_i(a) - m_i \ddot{\vec{r}}_i) \cdot \vec{dx}_i + \sum_i \vec{F}_i(c) \cdot \vec{dx}_i = 0 \quad (4)$$

 As the virtual work done by constraint force is zero,

$$C \boxed{\sum_i (\vec{F}_i(a) - m_i \ddot{\vec{r}}_i) \cdot \vec{dx}_i = 0}$$

This known as Steller's principle.

* If θ is Steller's principle, for the actual motion of any system of particles subjected to constraint motion, the sum of work done due to applied forces and due to the forces of inertia in any virtual displacement of the system for each given instant of time, is equal to zero.

Application of Steller's Principle:

SIMPLE PENDULUM: Consider a simple pendulum of mass m of effective length l



→ Eqn of constraint for the system
 $x^2 + y^2 = l^2 \quad (1)$

Differentiating (1),

$$2x \cdot dx + 2y \cdot dy = 0$$

→ Using Steller's principle, we can write eqn of motion as

$$\sum_i (m_i \ddot{\vec{r}}_i - \vec{F}_i(a)) \cdot \vec{dx}_i = 0 \quad (3)$$

On basis of eqn (3) can be written as,

$$(m_x - F_x) dx + (m_y - F_y) dy = 0 \quad (4)$$

F_x & F_y are components of applied force along x & y axes respectively.

→ Here, the applied forces do not include tension (the force of constraint). Since the only force (mg) acting on the bob is along

$$y\text{-axis}, F_x = 0 \quad \therefore F_y = -mg$$

Eqn (4) becomes,

$$m_x dx + (m_y + mg) dy = 0 \quad (5)$$

$$\Rightarrow \dot{x} dx + (\dot{y} + g) dy = 0 \quad (5)$$

$$\text{From (2), } \dot{dy} = -\frac{\dot{x} dx}{\dot{y} + g}$$

$$\text{Putting in (5), } \dot{x} dx + (\dot{y} + g)(-\frac{\dot{x} dx}{\dot{y} + g}) = 0$$

$$\Rightarrow \ddot{x}^2 dx - x(\dot{q}^i + p) dx = 0$$

$$\Rightarrow \ddot{q}_2^i - n(\dot{q}_i^i + p) = 0 \quad (6)$$

If amplitude of acceleration is small enough, then

$$q = 0$$

$$\text{so, } (6) \text{ becomes, } -\ddot{q}_2^i - xg = 0$$

$$\Rightarrow \ddot{x}^2 + \omega^2 x = 0 \quad (7)$$

and, since period of oscillations,

$$T = \frac{2\pi}{\omega} = 2\pi \sqrt{\frac{m}{g}}$$

GENERALISED COORDINATES:

→ the generalized coordinates are defined as a set of independent coordinates that completely specify the configuration of a dynamical system.

→ represented by n independent variables q_1, q_2, \dots, q_n , where $m = \text{dof} = 3n - k$.

Analogous of generalized coordinate:

① Definition: the dependence on coordinate system for describing the configuration of a dynamical system.

② Generalized coordinates are independent to each other so that this individual variations (i.e. δq_i) can be considered.

NOTE: for holonomic system, $m(GC) = \text{dof}$
As non holonomic system $m(GC) > \text{dof}$

CONCEPT OF GENERALISED FORCE:

The position vector r_i of a holonomic system of N particles with k constraints can be written as;

$$\vec{r}_i = \vec{r}_i(q_1, q_2, \dots, q_n, t) \approx \vec{r}_i(q_j, t)$$

$$\text{where } m = \text{dof} = n(GC)$$

$$\text{Now, } \delta \vec{r}_i = \frac{\partial \vec{r}_i}{\partial q_1} \delta q_1 + \frac{\partial \vec{r}_i}{\partial q_2} \delta q_2 + \dots + \frac{\partial \vec{r}_i}{\partial q_t} \delta t$$

Per virtual displacement, $\delta \vec{r}_i = dx_i/dt = 0$

Since, virtual displacement is considered at a particular instant,

$$\boxed{\delta \vec{r}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j} \quad (1)$$

Here, δq_j is called generalized displacement or vertical arbitrary displacement.

θ_j = angle coordinate, $\delta \theta_j$ = angular displacement

Hence, in terms of q_{GC} , the virtual work need done due to applied force F_i is,

$$\boxed{\sum_i F_i \cdot \delta q_i = \sum_i F_i \left(\sum_j q_j \frac{\partial r_i}{\partial q_j} \right) \delta q_j = \sum_i F_i \cdot \dot{q}_j \delta q_j} \quad (2)$$

here, \dot{q}_j is the j th component of the generalized force ($= \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j}$)

Generalised force for conservative system:

For a conservative system where its total energy is conserved, the conservative force F_i can be expressed in terms of potential function $V = V(q_i)$ as

$$\vec{F}_i = -\vec{V}_i' \quad (1)$$

$$\text{we know, } \vec{F}_i = \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_i} = -\sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_i}$$

$$\therefore \boxed{\vec{F}_i = -\sum_i \frac{\partial V}{\partial q_i} \cdot \frac{\partial \vec{r}_i}{\partial q_i}} \quad (2)$$

Now, for a conservative system, scalar potential V is function of position only $\therefore \boxed{\vec{F}_i = -\frac{\partial V}{\partial q_i}}$

Generalised potential:

• Velocity dependent potential gives rise to conservative generalized force.

→ when the system is not conservative, potential depends on the generalized velocity \dot{q}_j also.

$$\boxed{\vec{F}_i = -\frac{\partial V}{\partial q_i} + \frac{d}{dt} \left(\frac{\partial V}{\partial \dot{q}_i} \right)} \quad \text{where, } V = V(q_j, \dot{q}_j)$$

is called velocity dependent potential or generalized potential.

GENERALISED MOMENTUM:

• Partial derivatives of energy of a system w.r.t. generalized velocities (\dot{q}_i) are called generalized momentum.

$$\begin{aligned} p_j &= \frac{\partial E}{\partial \dot{q}_j} \\ &= \frac{\partial (T+V)}{\partial \dot{q}_j} = \frac{\partial T}{\partial \dot{q}_j} \end{aligned}$$

[P.T., V , depends only on \dot{q}_j & not on \dot{q}_i , so, $\partial V / \partial \dot{q}_j = 0$]

$$\boxed{p_j = \frac{\partial T}{\partial \dot{q}_j}}$$

LAGRANGIAN FORMULATION

Lagrange's equation of motion are given by,

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_i} \right) - \frac{\partial T}{\partial q_i} = S_i \quad (1)$$

- (a) is applicable to both conservative & non-conservative systems.
- For a "conservative" system, $S_i = -\frac{\partial V}{\partial q_i}$

S_i for "conservative" system, $S_i = -\frac{\partial V}{\partial q_i}$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = -\frac{\partial V}{\partial q_i}$$

$$\Rightarrow \frac{d}{dt} \left[\frac{\partial}{\partial \dot{q}_i} \left(T - V \right) \right] - \frac{\partial}{\partial q_i} \left(T - V \right) = 0 \quad \left[\because \frac{\partial V}{\partial q_i} = 0 \right]$$

$$\Rightarrow \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 \quad (2)$$

Applicable to conservative system if derivative of Lagrangian function is conserved, i.e., $\dot{q}_i = \dot{q}_i(q_1, q_2, t)$

In case of "conservative" system, $L = L(q_1, \dot{q}_1)$

Cyclic coordinates: due to same reason when some of

the generalized coordinates (say q_k) do not occur explicitly in the expression of Lagrangian, then these coordinates are called ignorable or cyclic coordinates.

* Lagrangian g^0 of motion has a cyclic coordinate q_k if

$$\int \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_k} \right) dt = 0 \quad (\therefore \frac{\partial L}{\partial q_k} = 0)$$

On integration,

$$\left[\frac{\partial L}{\partial \dot{q}_k} = P_k = \text{constant} \right]$$

thus, because a coordinate q_k does not appear explicitly in L , the corresponding conjugate momentum is constant of motion.

Hence, the generalized momentum conjugate to a cyclic coordinate is conserved. The pair (P_k, p_k) is known as canonical or conjugate variables.

L does not depend on q_k , P_k , i.e., $\frac{\partial L}{\partial q_k} = 0$

→ $\dot{q}_k = \frac{\partial L}{\partial P_k}$

L does not depend on q_k , P_k , i.e., $\frac{\partial L}{\partial P_k} = 0$

→ In case of motion of a free particle, all 3 coordinates, x, y, z and g are cyclic coordinates.

APPLICATIONS:

① MOTION OF FREE PARTICLE:

Let force = 0
i.e., potential, $V = 0$

$$L = \frac{1}{2} m(x^2 + y^2 + z^2)$$

→ Here, all the coordinates are cyclic as L is not explicitly depending on them though they are present in corresponding velocities.

→ So, q_j 's of motion are,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = \frac{\partial L}{\partial x} \quad \text{or, } m\ddot{x} = 0$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = \frac{\partial L}{\partial y} \quad \text{or, } m\ddot{y} = 0$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = \frac{\partial L}{\partial z} \quad \text{or, } m\ddot{z} = 0$$

② SIMPLE HARMONIC OSCILLATION:

→ Let x be considered a vibrating body which is acted upon by a force directed towards or away from a fixed point 0 (equilibrium position).

→ Let x be the displacement of the body at any instant. So, $F \propto -x$

So, $[F = -Kx]$, K is the spring or force constant

For a simple harmonic oscillator of mass m ,

$$P_E = \frac{1}{2} m \dot{x}^2 \quad \& \quad V = -\int F.dx = -\int Kx dx = \frac{1}{2} Kx^2$$

$$\frac{\partial L}{\partial x} = m\ddot{x} \quad \& \quad \frac{\partial L}{\partial \dot{x}} = -Kx$$

∴ Lagrange's eqn. of motion,

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{x}_i} \right) - \frac{\partial L}{\partial x_i} = 0$$

$$\Rightarrow \frac{\partial}{\partial t} (m\ddot{x}_i) + Kx_i = 0 \Rightarrow m\ddot{x}_i + Kx_i = 0$$

$$\Rightarrow \ddot{x}_i + \frac{K}{m} x_i = 0$$

$$\Rightarrow \boxed{\ddot{x}_i + \omega^2 x_i = 0}$$

$$\text{Time period, } T = \frac{2\pi}{\omega} = 2\pi \sqrt{\frac{m}{K}}$$

⑨ SIMPLE PENDULUM

KE of simple pendulum,

$$T = \frac{1}{2} m v_{\theta}^2$$

$$P.E., V = mg (r(1 - \cos\theta))$$

$$= mg(r(1 - \cos\theta))$$

Lagrangian,

$$L = T - V \quad \text{--- (1)}$$

$$\frac{\partial L}{\partial t} = m\dot{v}_{\theta}^2 \quad \frac{\partial}{\partial t} = -mg\dot{\theta}$$

so, Lagrangian eqn. of motion:

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{v}_{\theta}} \right) - \frac{\partial L}{\partial \theta} = 0$$

$$\Rightarrow \frac{\partial}{\partial t} (m\dot{v}_{\theta}^2) + mg\dot{\theta} = 0$$

$$m\ddot{v}_{\theta}^2 + mg\dot{\theta} = 0$$

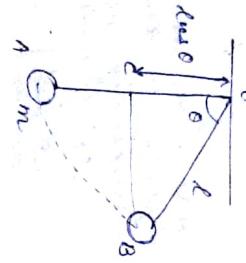
$$\Rightarrow \ddot{v}_{\theta} + g\sin\theta = 0$$

If amplitude of oscillation is small, $\sin\theta \approx \theta$.

$$\theta \approx \theta_0$$

$$\boxed{\ddot{v}_{\theta} + \omega^2 \theta = 0}$$

$$\text{Time period of oscillation, } T = \frac{2\pi}{\omega} = 2\pi \sqrt{\frac{1}{g}}$$



$$\omega = \sqrt{\frac{g}{L}}$$

HAMILTONIAN FORMULATION:

In general, $L = L(q_i, \dot{q}_i, t)$

If L is not an explicit function of time, then $L = L(q_i, \dot{q}_i)$

$$dL = \sum_j \frac{\partial L}{\partial \dot{q}_j} d\dot{q}_j + \sum_j \frac{\partial L}{\partial q_j} dq_j$$

$$ds, \frac{\partial L}{\partial t} = \sum_j \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right) \dot{q}_j + \sum_j \frac{\partial L}{\partial q_j} \cdot \frac{d}{dt} q_j$$

$$ds, \frac{\partial L}{\partial t} = \sum_j \frac{\partial}{\partial t} (p_j \dot{q}_j) + \sum_j p_j \frac{d}{dt} (q_j) \quad [p_j = \frac{\partial L}{\partial \dot{q}_j}]$$

$$ds, \frac{\partial}{\partial t} \left(\sum_j p_j \dot{q}_j - L \right) = 0$$

$$ds, \left(\sum_j p_j \dot{q}_j - L \right) = \text{constant}$$

This is known as Hamiltonian, H of the system.

if L is a conserved quantity

$$\boxed{H = \sum_j p_j \dot{q}_j - L}$$

However, when L is not a explicit func. of time, H is a constant of motion.

FORMULATION OF HAMILTON'S CANONICAL EQUATIONS OF MOTION

We can say, $H = H(p_j, q_j, t)$

$$\text{Now, } H = \sum_j p_j \dot{q}_j - L$$

$$dH = \sum_j p_j \frac{\partial L}{\partial \dot{q}_j} d\dot{q}_j + \sum_j p_j dq_j - dL \quad \text{--- (1)}$$

$$\text{and, } L = L(q_i, \dot{q}_i, t)$$

$$dL = \sum_j \frac{\partial L}{\partial \dot{q}_j} d\dot{q}_j + \sum_j \frac{\partial L}{\partial q_j} dq_j + \frac{\partial L}{\partial t} dt \quad \text{--- (2)}$$

Putting value of dL in (1),

$$dH = \sum_i \dot{q}_i dq_i + \frac{1}{2} \sum_{ij} q_i dq_j - \sum_{ij} \frac{\partial L}{\partial q_i} dq_j - \frac{\partial L}{\partial t} \frac{\partial q_i}{\partial t} - \frac{\partial L}{\partial t} dt \quad (3)$$

$$\text{Now, } \dot{p}_i = \frac{\partial L}{\partial \dot{q}_i} \quad \text{from Legendre's eqn}$$

$$\therefore$$

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = \frac{\partial L}{\partial q_i}$$

$$\therefore \dot{p}_i = \frac{\partial L}{\partial \dot{q}_i}$$

Substituting value of \dot{p}_i & \dot{p}_j in (3),

$$dH = \sum_i \dot{q}_i dq_i + \sum_{ij} \dot{q}_i dq_j - \sum_{ij} \dot{p}_i dq_j - \frac{\partial L}{\partial t} dt$$

$$\left[dH = \sum_i \dot{q}_i dq_i - \frac{1}{2} \sum_{ij} \dot{q}_i dq_j - \frac{\partial L}{\partial t} dt \right] \quad (4)$$

Again, $H = H(\dot{q}_i, \dot{p}_j, x)$

$$dH = \sum_i \frac{\partial H}{\partial \dot{q}_i} \cdot d\dot{q}_i + \sum_j \frac{\partial H}{\partial \dot{p}_j} \cdot dp_j + \frac{\partial H}{\partial t} \cdot dt \quad (5)$$

Comparing (4) & (5),

$$-\dot{p}_i = \frac{\partial H}{\partial \dot{q}_i} \quad \text{or, } \dot{p}_i = -\frac{\partial H}{\partial \dot{q}_i} \quad (6)$$

$$\text{and, } \dot{q}_i = \frac{\partial H}{\partial \dot{p}_i} \quad (7)$$

Eq 2 \dot{q}_i, \dot{p}_i & x are known as KAMILLIEN'S eq'n of motion

HAMILTONIAN Eqn. A. CONSERVATIVE SYSTEM

$$H = H(\dot{q}_i, \dot{p}_j, t) = \sum_i \dot{q}_i \dot{p}_i - L$$

For a conservative system, $V = V(\dot{q}_i)$

If generalized momentum, $p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial \dot{p}_i} \quad (\text{as } \frac{\partial V}{\partial \dot{q}_i} = 0)$

$$\text{or, } p_i = \frac{\partial}{\partial \dot{q}_i} \left(\sum_i \dot{q}_i \dot{p}_i - L \right) \quad [p = \sum_i \dot{q}_i \dot{p}_i]$$

$$= \sum_i \dot{q}_i \dot{p}_i \quad \left[\dot{q}_i = \sum_i \frac{1}{2m_i} \frac{\partial^2 L}{\partial \dot{q}_i^2} \frac{\partial \dot{q}_i}{\partial t} \right]$$

$$\text{Now, } H = \sum_i p_i \dot{q}_i - L = \sum_i p_i \dot{q}_i - \frac{1}{2} \sum_{ij} p_i p_j \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \quad (8)$$

$$\therefore$$

$$H = p_x \frac{dx}{dt} - \frac{1}{2} \sum_{ij} p_i p_j \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \quad (2)$$

Since, for a conservative system only, Hamiltonian indicates the total energy of the system. In this case, constraint are independent of time.

\rightarrow If constraints are time dependent, $H \neq E$. But, still total energy is conserved.

APPLICATIONS OF HAMILTONIAN FORMULATION

① SIMPLE HARMONIC OSCILLATOR

For a simple harmonic oscillator of spring constant, K ,

$$T = \frac{1}{2} m \dot{x}^2, \quad V = \frac{1}{2} Kx^2$$

$$\text{So, } L = p_x v = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} Kx^2 = \frac{p_x^2}{2m} - \frac{1}{2} Kx^2 \quad [\text{as } p_x = m\dot{x}]$$

$$\text{Now, } p_x = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \quad \Rightarrow \quad \dot{x} = \frac{p_x}{m} \quad (3)$$

$$\text{and, } H = \sum_i p_i \dot{q}_i - L = p_x \dot{x} - L$$

$$\Rightarrow H = p_x \frac{dx}{dt} - \left(\frac{p_x^2}{2m} - \frac{1}{2} Kx^2 \right)$$

$$\text{Hamiltonian eq'n of motion are:} \quad \frac{\partial H}{\partial \dot{x}} = \dot{p}_x \Rightarrow \frac{\partial H}{\partial p_x} = \dot{x} = \frac{p_x}{m} \quad (2)$$

$$\frac{\partial H}{\partial p_x} = -\dot{p}_x \Rightarrow \frac{\partial H}{\partial x} = -\dot{p}_x \Rightarrow \dot{p}_x = -Kx$$

$$\text{And, } p_x = m\dot{x} \quad (\text{given 3})$$

$$\dot{p}_x = -Kx \quad \text{or } \frac{d(m\dot{x})}{dt} + Kx = 0$$

$$\Rightarrow m'' + Kx = 0 \quad \Rightarrow \quad \ddot{x} + \frac{K}{m} x = 0$$

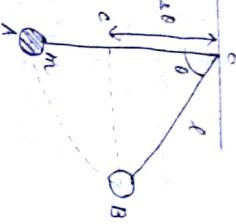
This is Hooke's law in Hookean eqⁿ of motion.

$$\text{Also, } \frac{d\theta}{dt} = \frac{d\theta}{dt} = \frac{2\pi}{\omega} \sqrt{\frac{m}{k}}.$$

(2) SIMPLE PENDULUM:

$$\begin{aligned} T &= \frac{1}{2} m L^2 \dot{\theta}^2, \quad V = mgL(1 - \cos\theta) \\ L &= \rho - v \\ &= \frac{1}{2} m L^2 \dot{\theta}^2 - mgL(1 - \cos\theta) \end{aligned}$$

$$\text{Now, } \ddot{\theta} = \frac{\partial L}{\partial \dot{\theta}} = mL^2 \ddot{\theta} \Rightarrow \ddot{\theta} = \frac{\ddot{\theta}_0}{mL^2}$$



$$\begin{aligned} H &= \sum T_i \dot{\theta}_i - L = \rho_0 \dot{\theta} - L \\ &= \frac{\rho_0^2}{2mL^2} - \left[\rho_0^2 L^2 - mgL(1 - \cos\theta) \right] \\ &= \frac{\rho_0^2}{2mL^2} + mgL(1 - \cos\theta) \end{aligned}$$

Now, Hamiltonian's eqⁿ of motion,

$$\ddot{\theta} = -\frac{\partial H}{\partial \dot{\theta}} = -mgL \sin\theta$$

$$\ddot{\theta} = \frac{\partial H}{\partial \theta} = \frac{\rho_0^2}{mL^2} \Rightarrow \rho_0 = mL^2 \cdot$$

$$\text{Now, } \rho_0 = -mgL \sin\theta$$

$$\frac{d}{dt} (\rho_0 L \dot{\theta}) + mgL \dot{\sin}\theta = 0$$

$$d\dot{\theta} \over dt$$

$$\Rightarrow mL^2 \dot{\theta} + mgL \sin\theta = 0$$

$$\Rightarrow \dot{\theta} + \frac{g}{L} \sin\theta = 0$$

$$\text{for small amplitude of oscillation, write } \approx 0 \\ \text{So, } \dot{\theta} + \frac{g}{L} \theta = 0 \Rightarrow \boxed{\ddot{\theta} + \omega^2 \theta = 0} \quad \omega = \sqrt{\frac{g}{L}}$$

This is Hookean eqⁿ of motion.

$$\text{And, } \rho = \frac{2\pi}{\omega} = 2\pi \sqrt{\frac{L}{g}}.$$

DIELECTRIC PROPERTIES

- NON POLAR MOLECULES:** material in which all the e are firmly bound to the atoms of the material.
- POLAR MOLECULES:** molecules under almost all conditions this atoms/pairs polarized under the influence of an external electric field \rightarrow can exert electrostatic field for a long time in it.
- e.g.: glass, mica, paper, air etc.

Dielectric constant: dielectric substance is characterized (or, relative permittivity) by a parameter known as dielectric constant.

ϵ_r is defined as the ratio of permittivity (ϵ) of the dielectric medium to that of free space:

$$\epsilon_{rf} = \frac{\epsilon_m}{\epsilon_0}$$

ϵ_0 for air (dry) and vacuum = 1

for water = 80 (now)

for paper & plastic = 2

\rightarrow depending on the separation betⁿ the centre of gravity of positive charges & the cosⁿ of -ve charges, the dielectrics are classified as

(a) POLAR MOLECULES MAKE POLAR DIELECTRIC

the cosⁿ of +ve charges is separated from that of -ve charges by a finite distance.

molecules of the dielectric have

intrinsic/ permanent dipole moment

Electric dipole

e.g.: N_2O , H_2O , $NaCl$, Na_3

In absence of electric field resultant dipole moment of the molecules dielectric is zero since the $-q$ -ve molecules are randomly oriented & they compensate each other.

(b) NON POLAR MOLECULES MAKE NON POLAR DIELECTRIC

cosⁿ of +ve charges coincide with cosⁿ of -ve charges.

has 0 electric dipole moment (no permanent

absence of electric field/no permanent electric dipole moment)

molecules have symmetrical structure

e.g.: Ne, Ar, Xe , H_2 , N_2 , O_2 , CO_2 (but CO_2 is linear sym. like $BeCl_2$)

POLARIZATION

Effect of electric field on polar & non-polar molecules:

(A) For non-polar molecules:

under no E , two θ -ne charges are very close to each other, so, there is no action between them.

under E , the charge is displaced a little from its equilibrium position in the dir's of E . And, -ve charge is displaced in the opp. dir's.

The displacement of these charges results in the creation of electric dipole.

thus the molecular phenomena due to which the molecules of a dielectric get aligned in the dir's of applied electric field & produce electric dipoles is called POLARIZATION.

(B) For polar molecules:

molecular permanent dipole present in the dielectric experience a torque which aligns them along the dir's of electric field.

The dielectric, thus, acquires a net dipole moment \vec{P} .

Note: Molecules with spherically symmetric charge are non-polar as the loc. of the θ -ne charge coincide.

ELECTRIC DIPOLE MOMENT?

* The dipole is an entity in which two equal θ -opp. charges are separated by a small distance.

* The atomic electric dipole moment $\vec{p} = q \vec{r}$

of the magnitude of charge of an atom of the separation (r) b/w the centres of the θ -ne charges. i.e.,

$$[\vec{p} = q \vec{r}]$$

p is a vector quantity directed from -ve to the +ve charge.

The unit is debye (D)

$$1 D = 3.3 \times 10^{-30} C \cdot m$$

POLARIZATION VECTOR (\vec{P})

The electric dipole moment per unit volume is called polarization (P). It is directed from -ve to +ve charge.

If n is the no. of molecules per unit volume & \vec{p} is the component of electric dipole moment of each molecule in the field dir's, the polarization vector is

$$[\vec{P} = n \vec{p}]$$

For a continuously polarized dielectric \vec{P} is defined with respect to the direction of electric field.

$$[\vec{P} = \lim_{\Delta r \rightarrow 0} \frac{\Delta \vec{p}}{\Delta V}]$$

Note: ① Polarization permittivity, $\epsilon_r = \frac{C}{C_0} = \frac{E_0}{E} = \frac{\nu_0}{V}$

$$\Rightarrow \vec{P} = \frac{\rho \vec{E}}{\epsilon_r} = \frac{\rho \vec{E}_0}{V}$$

② Displacement vector (\vec{D}) / Electric Flux Density per unit area ~~that substance~~ is called electric flux.

Flux density (per unit) = $\frac{F}{4\pi r^2}$
crossing normally

$$[\vec{D} = \frac{F}{4\pi r^2} \cdot \vec{n}]$$

\vec{D} is called electric displacement vector. Also, $\vec{D} = \epsilon_r \vec{E}$

ELECTRIC SUSCEPTIBILITY (χ_e)

When a dielectric material is placed in an electric field, the dielectric molecules become electrically polarized.

As a linearly homogeneous dielectric, the polarization vector (\vec{P}) is proportional to electric field (\vec{E}).

$$[\vec{P} = \chi_e \epsilon_0 \vec{E}]$$

χ_e is called the susceptibility of the dielectric.

$$[\chi_e = \frac{\vec{P}}{\vec{E} \epsilon_0}]$$

Thus, the electric susceptibility of a dielectric is defined as the ratio of the polarization per unit volume to the electric intensity in the dielectric.

It is a characteristic property of a dielectric.

POLARIZABILITY (α)

The net induced dipole moment of an atom of a dielectric substance, placed in an electric field is proportional to the applied electric field (E^{\rightarrow}). Also, it is proportional to the $\sin \theta$.

$$\vec{p} \propto \vec{E} \Rightarrow \vec{p} = \alpha \vec{E}$$

- * Thus, the atomic polarizability is the amount of induced electric dipole moment of an atom of a dielectric substance per unit electric field.

$$\alpha = \frac{p}{E}$$

$$\text{so unit of } \alpha = \frac{C \cdot m}{N \cdot m^{-1}} = F \cdot m^2$$

#

$$\text{value of } \vec{p} = n \alpha \vec{E}$$

$$\text{we know, } \kappa = \frac{p}{\epsilon_0 E} = \frac{n \alpha E}{\epsilon_0 E}$$

$$\Rightarrow \sqrt{\kappa} = \frac{n \alpha}{\epsilon_0}$$

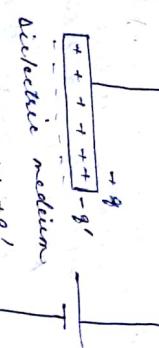
Dielectric Properties of Solids

* Gauss's law in free space

* Gauss's law in dielectric medium

* Gauss's law in dielectric places

$$\oint \vec{E} \cdot d\vec{s} = q/e_0$$



$$\text{Here, } \oint \vec{E} \cdot d\vec{s} = q - q'$$

$$\Rightarrow E \cdot A = \frac{q}{\epsilon_0} - \frac{q'}{\epsilon_0} \quad \text{--- (1)}$$

$$\left[\begin{array}{c} + + + + + \\ - - - - - \end{array} \right] - q'$$

$$+ + + + + - q'$$

dielectric medium

$$\Rightarrow \oint \vec{E} \cdot d\vec{s} = \frac{q}{\epsilon_0} + \frac{q'}{\epsilon_0}$$

$$\Rightarrow \frac{q}{\epsilon_0} = \frac{q}{\epsilon_0} + \frac{q'}{\epsilon_0} \quad (A \text{ is area of plate})$$

$$\Rightarrow \frac{q}{\epsilon_0} = \epsilon_0 \left(\frac{q}{\epsilon_0 \cdot \epsilon_0} \right) + \frac{q'}{\epsilon_0}$$

$$\Rightarrow q = \epsilon_0 E + p$$

On vector form, $\left[\vec{p} = \epsilon_0 \vec{E} + \vec{p} \right]$

* In free space (as vacuum), there is no polarization i.e. $\vec{p} = 0$, so,

$$\left[\vec{p} = \epsilon_0 \vec{E} \right]$$

Putting in (1),

$$\frac{E_0}{\epsilon_0} = \frac{q}{\epsilon_0} - \frac{q'}{\epsilon_0}$$

$$\text{Also, } E_1 = \frac{E_0}{4 \epsilon_0}$$

$$\text{Putting in (1), } \frac{q}{\epsilon_0} = \frac{q}{\epsilon_0} - \frac{q'}{\epsilon_0}$$

$$\Rightarrow \frac{q}{\epsilon_0} = q - q'$$

$\rightarrow q' < q$. So, induced charge within dielectric material is less than the excess charge within the capacitor plate.

$$\text{Now, } \oint \vec{E} \cdot d\vec{s} = \frac{q - q'}{\epsilon_0} = \frac{q}{\epsilon_0} - \frac{q}{\epsilon_0} \left(1 - \frac{1}{\epsilon_0} \right)$$

$$\Rightarrow \oint \vec{E} \cdot d\vec{s} = \frac{q}{\epsilon_0 \cdot \epsilon_0}$$

Relationship b/w electric field (E^{\rightarrow}), electric flux density (\vec{D}) and polarization (\vec{P}).

We know that induced charge in a dielectric,

$$q' = q \left(1 - \frac{1}{\epsilon_0} \right)$$

$$\Rightarrow \frac{q}{\epsilon_0} = q + q'$$

$$\Rightarrow q = \frac{q}{\epsilon_0} + q'$$

- Relationship betⁿ dielectric constant (ϵ_r) & electric susceptibility (χ)

We know that,

$$\vec{D} = \epsilon_0 \vec{E} = \epsilon_r \epsilon_0 \vec{E} \quad (1)$$

$$\text{and, } \vec{P} = \chi \epsilon_0 \vec{E} \quad (2)$$

Putting values of (1) and (2), in

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

$$\Rightarrow \epsilon_r \epsilon_0 \vec{E} = \epsilon_0 \vec{E} + \chi \epsilon_0 \vec{E}$$

$$\Rightarrow \epsilon_r = 1 + \chi$$

$$\Rightarrow \boxed{\chi = \epsilon_r - 1}.$$

- Relationship betⁿ electric polarization (\vec{P}) and dielectric constant (ϵ_r) in dielectric medium.

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

$$\Rightarrow \epsilon_0 \epsilon_r \vec{E} = \epsilon_0 \vec{E} + \vec{P}$$

$$\Rightarrow \boxed{\vec{P} = (\epsilon_r - 1) \epsilon_0 \vec{E}} \quad (3)$$

- Relationship betⁿ applied electric field (\vec{E}_0) & net electric field (\vec{E}) of the dielectric.

Net electric field within dielectric is given by,

(\vec{E}_p = electric field induced within dielectric)

$$\Rightarrow \vec{E} = \vec{E}_0 - \frac{\vec{P}}{\epsilon_r}$$

$$= \frac{\vec{P}}{\epsilon_r}$$

So, charge density, $\rho = \frac{-ze}{4\pi r^3}$

Charge inside the sphere of radius r ,

$$= \frac{4}{3}\pi r^3 n^3 = \frac{-ze}{R^3}$$

$$\Rightarrow \vec{E}_p (1+n) = \vec{E}_0$$

$$\Rightarrow \boxed{\vec{E}_p = \vec{E}_0}$$

$$\Rightarrow \boxed{\frac{\vec{E}_p}{\epsilon_r} = \frac{\vec{E}_0}{\epsilon_r}}$$

- Relationship betⁿ ϵ_r & α :

$$\text{We know that, } \chi = \frac{\vec{P}}{\epsilon_0 \vec{E}} = \frac{n \alpha \vec{E}}{\epsilon_0 \vec{P}} = \frac{n \alpha}{\epsilon_0}$$

$$\text{Also, } \epsilon_r - 1 = \chi$$

$$\Rightarrow \boxed{\epsilon_r = \frac{n \alpha}{\epsilon_0} + 1}$$

TYPES OF POLARIZATION:

The polarization that appears due to the displacement of electrons w.r.t atomic nucleus of a dielectric material under the action of external electric field, is called electronic polarization.



charge distribution
in absence of
electric field



in presence of electric
field

- Electric dipole moment is induced in the dirⁿ of applied electric field. Electric because it results from a shift of the cloud relative to the nucleus.

* Electronic polarization does not depend upon temp.

- Relationship betⁿ polarization (α) & atomic radius (a)

Consider an atom of atomic number Z

and radius r .

so, charge density, $\rho = \frac{-ze}{4\pi r^3}$

(1) atom in
absence of
electric field

$$\vec{E}$$



$$F_a = -zeE \quad (4)$$

→ total Coulomb force between the nucleus and the charge inside the sphere of radius r → $-ze^2/r^2$

and the charge inside the sphere of radius r → $-ze^2/r^3$

$$F_c = \frac{2e^2 z}{4\pi r^2 \epsilon_0} \frac{1}{r^2}$$

(2) polarization
equation

$$\rho_e = -2 \cdot e^2 n$$

At equilibrium, the Coulomb forces & valency forces are equal to each other as they acting in opp. dirn. so,

$$+2\mu E = \frac{4\pi R^3 n}{4\pi R^3} R^3$$

$$\Rightarrow \mu = \frac{4\pi n}{2e} R^3$$

Now, induced electric dipole moment.

$$\mu_i = 2eR$$

So, we may say, $\mu \propto e$

$$= 1/\mu_e = \alpha_e E \quad (1)$$

From (1) & (2), electric susceptibility

$$\mu_e = 4\pi e \cdot R^3$$

$$\text{So, } \overrightarrow{\rho_e} = m \alpha_e \overrightarrow{E}$$

$$\overrightarrow{\rho_e} = 2\pi n \alpha_e R^3 \overrightarrow{E}$$

relation betw. ϵ_r and radius of atom:

$$\text{We know, } \overrightarrow{\rho} = \chi \epsilon_0 \overrightarrow{E}$$

$$\text{or } \overrightarrow{\rho} = (\epsilon_r - 1) \epsilon_0 \overrightarrow{E}$$

$$\Rightarrow n \alpha \overrightarrow{E} = (\epsilon_r - 1) \epsilon_0 \overrightarrow{E}$$

$$\Rightarrow n \alpha \mu_e R^3 = (\epsilon_r - 1) \mu_0$$

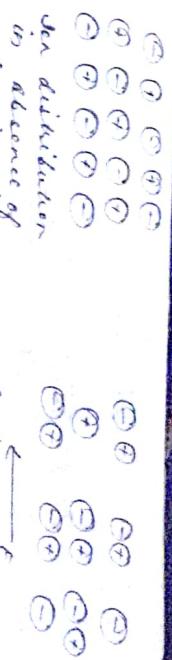
$$\Rightarrow \overrightarrow{\rho_e} = L + n \alpha R^3$$

Ionic / Atomic Polarization

In dielectric materials which possess ionic bond, e.g. NaCl, KCl, etc., appear due to mutual

attraction between positive & negative ions of the lattice displacement of positive & negative ions of the lattice expected due to the application of electric field on it, it is called ionic polarization.

* Ionic polarization does not depend upon temp.



Here, induced dipole moment (μ_i),

$$\Rightarrow \overrightarrow{\mu_i} = \alpha_i \overrightarrow{E}$$

$$\overrightarrow{\mu_i} = m \overrightarrow{\mu_e}$$

$$\Rightarrow \overrightarrow{\rho} = \overrightarrow{\mu_e} + \overrightarrow{\mu_i}$$

$$\Rightarrow \overrightarrow{\rho} = m (\alpha_e + \alpha_i) \overrightarrow{E}$$

III. ORIENTATIONAL OR DIPOLAR POLARIZATION:

observed only for polar dielectrics (which have permanent dipoles).

→ the polarization that appears due to the alignment of permanent dipoles in a material in the direction of applied electric field on it; it is called orientational polarization.

* strongly depends upon temp & decreases with increase of temp (field \propto $1/n^{1/2}$ of temp. of dielectric material)

Langevin's theory of polarization in polar dielectrics:

We know that, $\rho = n \rho_m$

→ the thermal energy of the molecules produces random dipole orientations.

* The probability of finding a molecule with energy E at temp T is $e^{-E/kT}$.

Now, $\rho \rightarrow \rho_e$ here the system is subjected to a field applied along the x dirn.

See potential energy associated with each dipole may be obtained as:

$$qE A/2 - qB$$

dipole may be obtained as:

TOTAL POLARIZATION

$$P = P_e + P_i + P_o$$

$$P = \eta_0 A E + \eta_1 A_i E + \eta_2 A_o E$$

BEHAVIOR OF DIELECTRIC IN ALTERNATING FIELD:

→ In charge due to poles-like prop. of the applied voltage on the dielectrics, $\tan \delta$ - presence of.

→ When an alternating electric field is applied on a dielectric

the dipole of the dielectric material try to get aligned themselves in the dir. of the oscillating electric field.

→ This implies that the Polarizability (α) of a dielectric substance or the electric displacement in a dielectric, is a function of time period or the frequency of the oscillating field.

→ or α is known as dipole moment.

DIELECTRIC LOSS:

When a dielectric material is placed in an alternating field, a part of

electrical energy is absorbed by the dielectric medium & wasted in the form of heat energy. This loss of energy is known as dielectric loss.

→ The resisting nature of the electric field that causes the dipole of the dipole to reverse is responsible for this dielectric loss.

→ The amount of dielectric loss depends upon the freq. of the applied field & the mechanism of polarization of the dielectric materials.



(i) 1 leads V by 90° (ii) 2 leads V by 0 in a

in an ideal dielectric commercial (as seen) dielectric

* the angle, $\theta = 90^\circ - \phi$, in real dielectric, is known as dielectric loss angle.

when a dielectric undergoes, during experiments, is subjected to an alternating voltage V having angular freq. ω , dielectric power loss is

$$P = V I \cos \delta$$

$$\text{Max. current, } I = \frac{V}{X_C} = \frac{V}{\omega C}$$

X_C = capacitive reactance

$$P = V^2 \cdot \frac{I}{2} \cos(90^\circ - \delta) = V^2 \cdot \frac{I}{2} \cos \delta$$

$$\Rightarrow P = V^2 \cdot \frac{I}{2} \cos \delta$$

where, $\cos \delta = \tan \delta$ for a small value of δ . δ is known as power factor (or, dissipation factor).

• Tan δ is known as power factor (or, dissipation factor). It indicates the amount of energy that is dissipated within the dielectric when an alternating electric field is applied across it.

DIELECTRIC STRENGTH:

If the E applied on a dielectric material is sufficiently large, it begins to pull electrons completely out of the molecules & then becomes conducting. When the dielectric becomes conducting, a dielectric breakdown is said to have occurred.

• The max. intensity that a dielectric can tolerate without breakdown is called dielectric strength of a material. Eg. Air 3, Rubber 2, Glass 30

MAGNETIC PROPERTIES

- the uniform magnetic field in which magnetic material is placed to magnetise is called magnetising field.

* MAGNETIC MOMENT (μ_m): Moment of the couple acting upon a magnet when it is placed with its axis at right angle to a uniform magnetic field of unit strength.

$$[\mu_m = m \times 2\pi]$$

$$\text{or } \mu_m = 1 \text{ m}^2$$

$$2\ell = \text{distance b/w the two poles}$$

$$\text{or unit of } \mu_m = 1 \text{ m}^2$$

→ here, the magnetic susceptibility of a magnetic material is defined as the ratio of intensity of magnetisation induced in it to the magnetising field.

→ for χ' , material can be magnetised more easily.

→ No wait.

$$\rightarrow \chi(\text{vacuum}) = 0 \text{ as } \frac{\mu_0}{\mu} = 0.$$

RELATION AMONG B , H AND χ

When a magnetic material is placed in a uniform magnetic field of intensity H , number of lines of force are passing through it. One is due to the magnetising field (H) and the other is due to the magnetisation $\chi(\mu)$.

∴ the magnetic induction (B) outside the material,

$$B = \mu_0 H + \mu_0 \chi H \quad \text{[to magnetic induction produced due to magnetisation of the material.]}$$

in free space

surrounding the source

$$\Rightarrow B = \mu_0 (H + \chi H)$$

RELATION BETWEEN PERMEABILITY (μ) AND MAGNETIC SUSCEPTIBILITY (χ)

We know,

$$\beta = \mu_0 (H + \chi H)$$

$$\Rightarrow \frac{B}{H} = \mu_0 (1 + \chi)$$

$$\therefore \mu = \mu_0 (1 + \chi).$$

thus, $\mu = \frac{\mu_0}{\chi} = 1 + \chi$.

$$\Rightarrow \chi = \frac{\mu_0}{\mu} - 1$$

ORIGIN OF MAGNETIC MOMENT OR AN APOM:

- When an e^- moves around a fixed point in a circular orbit, it produces magnetic field \perp to the plane of the orbit.

If the particle has an angular momentum,

→ so, if a charged particle has an angular momentum, it behaves as an elementary magnet.

→ thus, an atom possesses magnetic dipole moment μ due to the following three angular momenta-

- ① orbital angular momentum of the electrons in atom
- ② spin angular momentum of the nucleus
- ③ total angular momentum of the atom as the sum of these three moments.

I. OPERATIONAL MAGNETIC MOMENT OF THE ELECTRONS:

$$\mu_L = mev$$

L = radius of circular orbit
 v = velocity of revolution
 m = mass of e^-

→ dist' of L is along normal to the plane of e^- orbit (given by angular momentum rule.)

→ As the time period T of orbiting e^- is very small, ω is not treated as a single particle.

∴ the orbital motion of each e^- is around the nucleus is treated as a current loop. (This loop is equivalent to a current i due to a magnetic field B .)

∴ the electric current due to a moving e^- is,

$$I = -ev$$

$$\text{Now, } \frac{P}{A} = \frac{2\pi r}{T}$$

$$\text{So, } I = \frac{cv}{2\pi r}$$

∴ Area of current loop = πr^2

→ We know that current flowing through a circular coil produces a magnetic field in the dir' \perp to the plane of the coil. ∴ the magnitude of magnetic dipole moment is

$$\mu_m = IA = \frac{-ev \times r}{2m} \quad (I = \text{curr})$$

$$\Rightarrow \mu_m = -\frac{evL}{2m}$$

∴ we can observe that μ_m & μ_L are antiparallel

→ Thus, the magnetic susceptibility of a magnetic material is defined as the ratio of intensity of magnetisation induced in it to the magnetising field.

→ for χ , nature can be magnetised more easily.

→ χ (vacuum) = 0 as $\frac{\mu_r}{\mu_0} = 1$.

RELATION AMONG B , H AND χ

When a magnetic material is placed in a uniform magnetic field of intensity H , the flux of force ϕ passing through it, ϕ is due to the magnetising field (H) and the other is due to the magnetisation (χH) of the magnetic substance.

∴ magnetic induction (B) inside the material,

$$B = \mu_0 H + \mu_0 \chi H \quad \rightarrow \text{magnetic induction produced due to magnetisation of the material.}$$

in free space surrounding the source.

$$\Rightarrow B = \mu_0 (H + \chi H)$$

RELATION BETWEEN PERMEABILITY (μ) AND MAGNETIC SUSCEPTIBILITY (χ)

$$\text{No. Name, } \quad B = \mu_0 (1 + \chi H)$$

$$\Rightarrow \frac{B}{H} = \mu_0 (1 + \chi)$$

$$\Rightarrow \frac{B}{H} = \mu_0 (1 + \chi)$$

$$\text{Thus, } \chi = \frac{B}{\mu_0} - 1 = L + \chi.$$

$$\Rightarrow \boxed{\chi = \frac{B}{\mu_0} - L}$$

ORIGIN OF MAGNETIC MOMENT OF AN ATOM:

When an atom rotates around a fixed point in a circular orbit, it produces magnetic field L perpendicular to the orbit.

So, if a charged particle has an angular momentum, it behaves as an elementary magnet.

→ Thus, an atom possesses magnetic dipole moment by virtue of a magnetic dipole.

→ In an atom, the permanent magnetic moment arises due to the following three angular momenta-

(i) spin angular momentum of the electrons in atom
(ii) spin angular momentum of the nucleus.
The total angular momentum of the atom is the sum of these three momenta.

I. OPERATIONAL MAGNETIC MOMENT OF THE ELECTRONS:

$$\text{Orbital angular momentum of an e}^-$$

$$l = mev \quad m = \text{mass of e}^- \quad v = \text{velocity of revolution}$$

$$r = \text{radius of circular orbit}$$

→ Size of l is very small to see plane of e^- orbit (seen by right hand thumb rule).

→ As the time period T of orbital motion is very small, an e^- is not treated as a single particle.

The orbital motion of each e^- is around the nucleus is treated as a current loop.

∴ This sets up a magnetic field B the orbital motion of e^- is equivalent to a current.

→ The electric current due to a moving e^- is,

$$I = -ev$$

$$\text{Now, } I = \frac{2\pi}{\omega} = \frac{2\pi eL}{v}$$

$$\text{So, } \boxed{L = \frac{-ev}{2\pi}}$$

→ Area of current loop = πr^2

→ We know that current flowing through a circuit in the direction \rightarrow coil produces a magnetic field in the direction \rightarrow the plane of the coil. If the coil is identical to the plane of the dipole. Then, the magnitude of magnetic moment m' is,

$$m' = IA = \frac{-ev \times L}{2\pi r} = \frac{-evL}{2\pi r} \quad (\text{Ames})$$

$$\Rightarrow \boxed{\mu_m = -\frac{ev}{2\pi r}} \quad (\text{we sign indicate that } \mu_m \text{ and } L \text{ are antiparallel})$$

→ $1/e$ is a multiple of $h/2\pi$, i.e. L is an integral multiple of $h/2\pi$.

$$\text{So, } \mu_{\text{m}} = -\frac{1}{2} \frac{eL}{m} = -\frac{1}{2} \frac{e}{m} \left(\frac{mL}{2\pi} \right) = -\frac{e}{2m} \left(\frac{eL}{2\pi} \right) = -\frac{e^2 L}{4\pi m}$$

$$\text{or, } \mu_{\text{m}} = -n \left(\frac{e \hbar}{2m} \right) \quad \rightarrow \text{this indicates that } \mu_{\text{m}} \text{ due to orbital motion of an } e^- \text{ must be an integral multiple of } e\hbar/2m.$$

Least value of μ_{m} is $-\frac{e\hbar}{2m}$,

$$\mu_{\text{m}} = \frac{e\hbar}{2m} = \frac{e\hbar}{2m} \quad \text{A.U. is called Bohr magneton}$$

* $\mu_{\text{m}} = 9.27 \times 10^{-28} \text{ A.m}^2$ is unit of measurement of atomic magnetic moment of least value of sum of orbital

$$\mu_{\text{m}} = \frac{\mu_{\text{B}} e L}{2m} = \frac{1}{2} \frac{e\hbar L}{m} = \frac{\mu_{\text{B}} L}{2m}$$

$$e) \quad \mu_{\text{m}} = \frac{\mu_{\text{B}} L}{2m}$$

Note: ① If an atom be placed in a magnetic field B :

→ the total angular momentum L is in the direction of ext. magnetic field B , possible orientation of angular momentum vector is

$$L_{\text{ext}} = \frac{me}{2} \vec{t} \quad \text{m = number of subatomic particles}$$

$$\mu_{\text{m}} = \frac{-e}{2m} L_{\text{ext}} = -\frac{e\hbar}{2m} me = -\mu_{\text{B}} me$$

$$\Rightarrow \mu_{\text{m}} = -\mu_{\text{B}} me$$

② Corresponding energy of \vec{e} is $meB^2/2$.

ORBITAL HYDROMAGNETIC RATIO:

Ratio of magnetic moment of the atomic dipole to its angular momentum,

$$k_L = \frac{\mu_{\text{m}}}{L} = \frac{e}{2m}$$

II. SPIN ANGULAR MOMENTUM OR THE ELECTRON

gives spin magnetic moment (μ_s) since the e^- also has spinning motion other than orbital motion, it possesses spin magnetic moments.

$$\text{Here, } \mu_s = \frac{e \vec{s}}{2m}$$

where \vec{s} = spin angular momentum

$$= \frac{e \vec{t}_s}{2m}$$

$$\text{or, } \mu_s = \frac{1}{2} \left(\frac{e \vec{t}_s}{2m} \right) \quad \rightarrow \mu_s \text{ is half of } \mu_{\text{B}}$$

* Spin gyromagnetic ratio

$$Y_s = \omega \times \vec{n} = \vec{s} \times \vec{e} = \frac{e}{m} \Rightarrow Y_s = \frac{e}{m}$$

$$\mu_{\text{B}}, \mu_s = \frac{e}{2m} \times \vec{s} = \frac{1}{2} \frac{e \vec{t}_s}{2m} = \frac{\mu_{\text{B}} e}{2m}$$

* L-S coupling: If an atom contains more than one electron, then each electron may have different values of spin magnetic moment.

→ orbital angular momentum of an atom, $L = \vec{t}_1 + \vec{t}_2 + \dots + \vec{t}_N = \sum \vec{t}_i$

spin angular momentum of an atom, $\vec{s} = \sum \vec{s}_i$

total angular momentum, $\vec{J} = \vec{L} + \vec{s}$

Note: When we consider the e^- spin along the direction of external field, the magnetic moment component due to it spin along the field direction is, $\mu_{\text{ex}} = \theta \frac{e \vec{t}_s}{2m}$

here, θ is called spectroscopic splitting factor or factor of precession.

$$\theta = L + \frac{1}{2}(S+1) + \frac{1}{2}(S+1) - L(S+1)$$

NUCLEAR MAGNETIC MOMENT

→ Since the nucleus of an atom has an intrinsic spin, it has a nuclear magnetic moment. It passes in the nucleus, sum of the spin of all the protons in the nucleus of an atom gives rise to the nuclear spin.

$$\mu_h = \frac{e \vec{t}_n}{2m} = 8.65049 \times 10^{-28} \text{ J/T}$$

→ μ_n is 1296 times smaller than μ_B .

NOTE: The total magnetic moment of an atom will essentially be the vector sum of the orbital & spin magnetic moments.

CLASSIFICATION OR MAGNETIC MATERIALS:

Depending on the existence of permanent magnetic dipoles, magnetic materials can be classified:

A. DIAMAGNETIC MATERIALS:

- The substances which when placed in a magnetic field, become weakly magnetised in a direction opposite to that of the applied magnetising field are called diamagnetic substances. This magnetism is called diamagnetism.
- Such gases are diamagnetic as they have completely fixed electronic shells. They have no permanent magnetic moment.
- For a diamagnetic substance, susceptibility (χ) due to magnetisation is small & negative.

PROPERTIES:

- μ_r is less than unity
- χ is independent of temperature.
- Substance tends to magnetise stronger to weaker magnetised.
- Feeler repelled by a magnet.

UNPERTURBED FREQUENCY OR DIAMAGNETISM; LARMOR

ANGULAR FREQUENCY:

Karman explained diamagnetism from the electronic theory of matter.

Let the radius of the electronic orbit of an atom be r , & atomic number of the atom be Z . Also, let the velocity of e be v . So, in absence of an ext. magnetic field, centrifugal force of e equals coulomb force of nucleus

$$mv^2 = \frac{ZeV}{r}$$

[V = potential energy]

$$\omega_0 = \frac{eB}{2m}$$

$$\Rightarrow m\omega_0^2 = \frac{ze^2}{4\pi\epsilon_0 r^2} \quad (\text{as } V \rightarrow \text{constant})$$

$$\Rightarrow \omega_0^2 = \frac{ze^2}{4\pi\epsilon_0 m r^3}$$

→ When the atom is placed in a magnetic field (B), then the Larmor freq. experienced by the e ,

$$\Rightarrow \vec{F}_L = -e(\vec{v} \times \vec{B}) \quad \vec{T}_L = e(\vec{v} \times \vec{B})$$

$$\Rightarrow \omega_L = \frac{eB}{2m}$$

$$\Rightarrow m\omega_L^2 = m\omega_0^2 + e^2 B^2 \quad [\text{no longer antinodes, otherwise motion of } e \text{ will stop after } \omega_0]$$

$$\Rightarrow m(\omega_0 - \omega_L)(\omega_0 + \omega_L) = e^2 B^2$$

$$\Rightarrow \text{since } \omega \text{ differs slightly from } \omega_0 \text{ even in strongest magnetic field, we take } \omega_0 - \omega_L = \Delta\omega \Rightarrow \omega_0 + \omega_L = 2\omega_0$$

$$\Rightarrow \Delta\omega = \frac{e^2 B}{2m}$$

thus, the angular velocity (ω_L) of the e under the influence of applied magnetic field B ,

$$\omega = \omega_0 + \Delta\omega$$

$$\Rightarrow \omega = \omega_0 \pm \frac{eB}{2m} \quad (\omega_0 = eB/2m)$$

$$\Rightarrow \omega = \omega_0 \pm \omega_L \quad \omega_L \rightarrow \text{harmonic angular freq.}$$

and is equal to ω_0 .

LARMOR FREQUENCY: the change in angular freq. of a magnetic field is called Larmor freq.

INDUCED MAGNETIC MOMENT: the change in angular velocity of an orbit $\vec{\omega}$ due to application of an ext. \vec{B} , produces a change in μ_m . $\mu_{ind} = -2A = \frac{-e(r\omega)^2}{T} = \frac{-e^2 r^2 \omega^2}{2} = \frac{-e^2 r^2}{2\mu_0 \epsilon_0}$

$$\mu_{ind} = \frac{-e^2 r^2 \cdot B}{4\mu_0}$$

$$(\text{we note that result takes place in dir. opp. to } \vec{B})$$

SUSCEPTIBILITY OF MAGNETIC MATERIAL:

Considering that the orbit of e is normal to the applied magnetic field (\vec{B}).
 But the orbit can have any orientation with the app. mag. field.
 → The radius r of the orbit is replaced by projection (i.e.) of the radius of the orbit on a plane $\perp \vec{B}$ to the \vec{B} , i.e. in $x-y$ plane.

$$\text{Field} = -\frac{e^2 r^2}{4m} \cdot \vec{B}$$

If x, y, z are the components of radius along x, y, z axes respectively,
 $r^2 = x^2 + y^2 + z^2$

$$Now, any value of x, y, z are$$

$$\langle x^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle$$

$$\langle x^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle$$

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{3}{4} \langle r^2 \rangle$$

For spherically symmetric charge distribution,

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{3}{4} \left[\frac{-2e^2 B}{4m} \langle r^2 \rangle \right]$$

$$\therefore \langle x^2 \rangle = 2 \langle x^2 \rangle = \frac{2}{3} \langle r^2 \rangle$$

$$\therefore \text{So, } \langle x_1^2 \rangle = N \mu_0 \text{ and}$$

$$\frac{N}{V} = N \left(\frac{-2e^2 B}{4m} \right) \left(\frac{2}{3} \langle r^2 \rangle \right)$$

N = No. of atoms per unit volume.

$$\Rightarrow \frac{N}{V} = -N Z e^2 B \langle r^2 \rangle$$

$$\Rightarrow \frac{N}{V} = -N e^2 \mu_0 B \geq \langle r^2 \rangle$$

$$(B > \mu_0 H)$$

$$\text{Thus, } \chi = \frac{N}{V}$$

$$\checkmark \chi = -N Z e^2 \mu_0 \langle r^2 \rangle$$

This is known as TANGENT LAW.

→ Tangent law measures the susceptibility of a diamagnetic material & gives us the following info : (i) $\chi_{\text{air}} = -ve$
 (ii) does not depend on temp. of material
 (iii) " " " " " intensity of external magnetic field.

Note : (i) in $\chi = -\frac{e^2 \langle r^2 \rangle}{4m} B$

(ii) μ_0 (of exist e) = $\frac{e^2 \langle r^2 \rangle}{4m}$

PARAMAGNETIC MATERIALS:

→ The substance which when placed in a magnetic field are weakly magnetized in the direction of the applied field are called paramagnetic substances.

PROPERTIES : (i) Pt, Cu, O₂, Non-magnetic atom of this material has a permanent dipole.

- μ_0 is slightly more than 1.
- χ depends on temp. & it is zero at 0 K.
- χ is +ve.

• In a non uniform field, material is attracted towards stronger mag. field (i.e. tends to move from weaker to stronger mag. field)

O LANGEVIN'S THEORY OF MAGNETISM :

Assumptions : (i) Separation of dipoles in para. substances are such that their mutual magnetic interaction forces can be neglected (electrostatic).

(ii) These dipoles have all possible orientations.

→ $1/f_c$ to Maxwell Boltzmann statistics, the no. of atoms having PE E at temp. T is proportional to $e^{-E/k_B T}$.

$$K_B = \text{Boltzmann constant}$$

$$dN \propto e^{-E/k_B T} \sinh(\beta E)$$

• SUSCEPTIBILITY OF MAGNETIC MATERIAL:

Considering that the orbit of \vec{e} is normal to the applied magnetic field (\vec{B}).
 But the orbit can have any orientation with the app. mag. field.
 \rightarrow the radius r of the orbit is replaced by projection (i.e.) of the radius r of the orbit on a plane i.e. in $x-y$ plane.

$$\text{Mind} = -\frac{e^2 \vec{r}_x}{4m} \cdot \vec{B}$$

If x, y, z are the components of radius along x, y, z axes respectively

$$r_x^2 = x^2 + y^2 + z^2$$

Now, any values of r_x, θ, ϕ, ψ are

$$\langle r_x^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle$$

$$\langle r_y^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle$$

$$\langle r_z^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle$$

For spherically symmetric charge distribution,

$$\langle r_x^2 \rangle = \langle r_y^2 \rangle = \langle r_z^2 \rangle = \frac{3}{5} \langle r^2 \rangle$$

$$\text{So, } \langle r_x^2 \rangle = 2 \langle r^2 \rangle = \frac{2}{3} \langle r^2 \rangle$$

$$\text{of each atom has } 2 \vec{e}, \text{ total Mind} = -\frac{2e^2 B}{4m} \langle r^2 \rangle$$

$$\text{So, } \overline{M} = N \mu \text{ Mind}$$

$$\Rightarrow \overline{M} = N \left(\frac{-2e^2 B}{4m} \right) \left(\frac{2}{3} \langle r^2 \rangle \right)$$

volume.

$$\Rightarrow \overline{M} = -\frac{N e^2 B \langle r^2 \rangle}{6m}$$

$$(B = \mu_0 H)$$

$$\text{Thus, } \chi = \frac{M}{H}$$

$$\sqrt{\chi} = -\frac{Ne^2 \mu_0 \langle r^2 \rangle}{6m} \rightarrow \text{This is known as Langevin's formula.}$$

\rightarrow Langevin "g" measures the susceptibility of a diamagnetic material & gives us the following info:

- (i) χ is in $-ve$
- (ii) does not depend on temp. of material
- (iii) " " " " " intensity of external magnetic field.

$$\text{NOTE: (i) } g \text{ in gs, mean radius is given } \rightarrow \langle r^2 \rangle$$

$$(ii) \text{ Mind (of atom)} = \frac{e^2 \langle r^2 \rangle B}{4m}$$

B. PARAMAGNETIC MATERIAL:

\rightarrow the substance which when placed in a magnetic field are easily magnetized in "dipole" of the applied field are called paramagnetic substances.

e.g.: All Pt, Cu, O₂, Non

paramagnetic atom of this material has a permanent dipole.

- μ_n is slightly more than 1.
- χ depends on temp & β i.e. $\propto T$
- χ is $+ve$.

In a non uniform field, material is attracted towards stronger field (i.e. tends to move from weaker to stronger mag. field).

O LANGEVIN'S THEORY OF PARAMAGNETISM:

Assumptions: (1) Separation of dipoles in paramagnetic

are such that their mutual magnetic

interaction forces can be neglected.

(2) These dipoles have all possible orientations.

\rightarrow If χ to Maxwell Boltzmann statistics, the no. of atoms having PE E at temp T is proportional to $e^{-E/kT}$.

$K_B = \text{Boltzmann constant}$

\rightarrow the number of atoms per unit volume having an inclination between θ and $(\theta + d\theta)$ is proportional to

$$dN \propto e^{-E/kT} \sin \theta \cdot d\theta$$

$$dN = \frac{\mu_0}{4\pi} e^{-\epsilon/k_B T} \sin \theta \cdot d\theta$$

proportional constant

Therefore, the total no. of molecules along θ and π .

$$N = \int dN = \int e^{-\epsilon/k_B T} \sin \theta \cdot d\theta \quad (1)$$

θ

π

α

β

γ

δ

ϵ

ζ

η

κ

λ

μ

ν

ω

ρ

σ

τ

θ

ϕ

ψ

χ

$$\therefore M \propto N_A \left(\frac{1}{3} \right)$$

$$\text{Also, } M = N \mu_m \times \frac{\mu_0 H}{3 k_B T}$$

$$\therefore M = N \mu_m \frac{H}{3 k_B T}$$

$$\text{Also, } M = N \mu_m \left(\mu_0 \frac{H}{3 k_B T} \right)$$

$$\text{Similarly that } M \propto \mu_m \text{ is proportional to applied magnetic field}$$

$$\text{i.e. } \frac{M}{\mu_m} \propto \frac{H}{3 k_B T}$$

(2) Paramagnetic substance requires M in the dir'g of B .

Susceptibility: At high temp (at least $\overline{3k_B T}$)

$$\chi = \frac{N \mu_m^2}{3 k_B T} (\mu_0 \mu)$$

$$\Rightarrow \chi = \frac{N \mu_m^2}{3 k_B T} \quad \text{if it is always true.}$$

$$\chi = \frac{N \mu_m^2}{3 k_B T}$$

or, $\chi = \frac{C}{T}$ where $C = \frac{N \mu_m^2 \mu_0}{3 k_B}$ is known as Curie's constant.

$$\Rightarrow \chi \propto \frac{1}{T} \quad \text{Curie's law}$$

Curie's Law: There is also states that the susceptibility of a paramagnetic substance varies inversely with its absolute temperature.

→ Since paramagnetic susceptibilities of most temp., all paramagnetic materials become diamagnetic at high enough temp.

Molar Susceptibility: $\chi = \frac{N \mu_m^2 \mu_0}{3 k_B T} \quad N \mu_m^2 \text{ no. of dipole per mol}$

Molar susceptibility: $\chi = \frac{N \mu_m^2 \mu_0}{3 k_B T} \quad N = \text{no. of dipole per unit volume}$

(case a): when temp. is low & the field is strong.

for large value of μ_B , net $M_a \rightarrow L$
So, $L(a) \rightarrow (car Ra - \frac{1}{4} h) \rightarrow L$
and $[M = M_a]$ i.e. magnetization attains saturation state.

o Saturation state occurs due to the fact that at less temp all the magnetic dipoles are aligned in the direction of external strong magnetic field. Thus, at low temp.

Failure of Langevin's theory of paramagnetism: since it assumes that separation of magnetic dipoles are in large of their mutual interaction is little or zero, it is not applicable for substance that have large mutual interaction among their dipoles.

(iii) Also, failed to explain temp. dependency of χ .

o WEISS MOLECULAR FIELD THEORY

o Weiss theory accounted for intense magnetic moments due to mutual interaction among the atomic magnetic dipoles. These lead to an intense molecular magnetizing field (H_m).

$$\text{Now, } H_m \propto M \quad \Rightarrow \frac{1}{H_m} = \gamma M$$

So, net effective field,

$$H_{eff} = H + \gamma M$$

H = external/applied
magnetic field

$$\text{Now, } M = \frac{N \mu_m^2 \mu_0}{3 k_B T} H_{eff} = \frac{N \mu_m^2 \mu_0}{3 k_B T} (H + \gamma M)$$

$$\Rightarrow M = \frac{N \mu_m^2 \mu_0 H}{3 k_B T} \left[1 - \frac{N \mu_m^2 \mu_0 \gamma}{3 k_B T} \right] = \frac{N \mu_m^2 \mu_0 H}{3 k_B T} \left(1 - \frac{N \mu_m^2 \mu_0 \gamma}{3 k_B T} \right)$$

Magnetic Susceptibility

$$\chi = \frac{M}{H} = \frac{N\mu_0 I}{3kg - N\mu_0 H_0} = \frac{N\mu_0^2 I_0}{T - \left(\frac{N\mu_0^2 I_0}{3kg} \right)}$$

$$\Rightarrow \boxed{\chi = \frac{C}{T - \theta}}$$

(i) this is called Curie-Weiss Law

$$\begin{aligned} C &= \text{Curie temperature of para.} \\ \theta &= \text{Curie temperature of para.} \\ &= \frac{N\mu_0^2 I_0}{3kg} \end{aligned}$$

O PHYSICAL INTERPRETATION OF CURIE-WEISS LAW:

If temp (T) of paramagnetic substance

- ① $\theta < 0$, $\chi \rightarrow -\infty$ of para. substance becomes like diamagnetic

- ii) curie weiss law for para substance valid when $\theta > 0$.

→ Temperature below which paramagnetic substance mainly behave like a diamagnetic substance is called paramagnetic Curie Temperature.

C. FERROMAGNETIC MATERIALS:

→ the substances which when placed in a magnetic field are strongly magnetized in the dir. of applied magnetic field are said ferromagnetic materials.

Eg: Fe, Co, Ni & their alloys

→ of χ of ferro. substances:

↑ not a constant but varies w/ H if H is

↑ the H very large

↑ & with H above a certain temp. para. balance as para.

This temp is called paramagnetic Curie temp. (C_p).

O DOMAIN THEORY

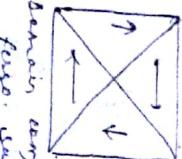
• stem of ferromagnetic materials possess nonzero magnetic moment due to spin motion of unpaired e. The ferromagnetic materials exhibit spontaneous magnetization, even in the absence of an external field.

→ the small volumes of ferro. material may consist of large no. of atomic dipole field response by force of exchange are called domains. Every domain is magnetically saturated due to the alignment of all the magnetic poles in the same direction.

→ the dir. of magnetization in diff. domains is diff. dom.

→ the boundary region betw. two domains is called a domain mag.

→ the magnetic domains within the material are so arranged that the dir. of magnetization varies from domain to domain. Form closed chains such that the magnetic effect of one another is nullified. The sample is said to be in a demagnetized state.



Magnetization: When ext. magnetic field is applied to ferro. materials, the substance becomes magnetized.

Reason ① If applied field is weak, domain boundaries get displaced.

② If field is strong, domains rotate in the dir. of magnetizing field.

→ transition metals like Fe, Co, Ni exhibit magnetization even when magnetizing field is removed.

O WEISS THEORY / MOLECULAR FIELD THEORY:

To explain spontaneous magnetization of ferro. materials, internal molecular field (H_i) taken into account.

$$\text{Now, } H_i \propto M$$

$$H_i = \gamma M$$

γ = molecular field constant

So, net magnetic field,

$$H_{eff} = H + \Delta H$$

Aren't Langevin's theory of paramagnetism,

$$M = Nm \angle(\alpha)$$

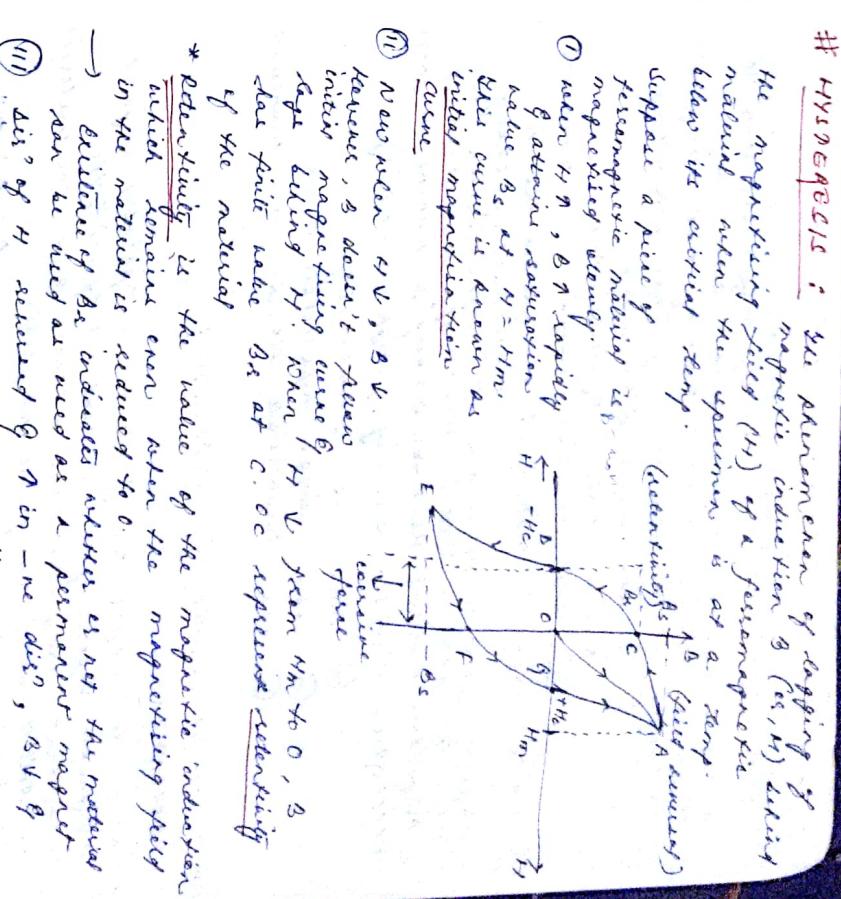
For very high temp., $\angle(\alpha) \approx \pi/2$ & $B = \mu_0 H_{eff}$

$$\text{so, } M = Nm \frac{\pi}{2} = \frac{Nm^2}{3} \frac{\mu_0 B}{K_B T}$$

$$= \frac{Nm^2 \mu_0 H_{eff}}{3 K_B T}$$

$$= \frac{Nm^2 \mu_0 (H + \Delta H)}{3 K_B T}$$

$$= \frac{Nm^2 \mu_0 H}{3 K_B T}$$



SOFT & HARD MAGNETIC MATERIALS:

- (A) soft magnetic materials: the material that can be placed in a weak magnetic field is called soft magnetic material, used for making electromagnets.

PROPERTIES:

- (1) has low coercivity & low retentivity
- (2) has larger permeability
- (3) has smaller hysteresis curve
- (4) has reversible domain wall movement

magnetized by strong field & can retain its magnetization even when the applied field is turned off is called hard magnetic material; used for making permanent magnets.

PROPERTIES:

- (1) high coercivity & high retentivity
- (2) has low permeability
- (3) has large hysteresis curve
- (4) has irreversible domain wall movement

ANTI-PERMAGNETIC MATERIALS:

PROPERTIES:

→ when the magnitudes of all the antiparallel aligned magnetic dipoles of a material are equal & the resultant magnetization becomes zero, the material is called antiperemagnetic material.
e.g.: NiO, Ba₂, PbO etc.

PROPERTIES:

- (1) the exchange forces b/w adjacent dipoles produces a tendency for antiparallel alignment of dipoles.
- (2) Net magnetization is 0.
- (3) $\chi \propto \text{N} \propto \frac{1}{T}$ i.e. $\chi = \chi_{\text{max}}$ at New temp.
- (4) $\chi \propto \text{New temp.}^2 \propto T^{-2}$ with temp. following "y"

$$\chi = \frac{C}{T+\theta} \quad (\theta \rightarrow \text{curie temp.})$$

FERRITE OR PERMI-MAGNETIC MATERIALS:

→ ferrites are special types of antiparallel magnetic materials in which anti-parallel aligned dipoles with different magnitudes produce a

large net magnetization produced a large magnetization even for small ext. field.



* PROPERTIES

- (1) have large magnetization even for small ext. field
- (2) possess a net magnetic moment
- (3) stable as para. above curie temp.
- (4) have negligible coercive force
- (5) low hysteresis loss
- (6) high magnetic permeability

* DIFF B/W FERRITES & FERROMAGNETIC:

- (1) ferrites have low electrical conductivity than iron
- (2) ferrites have higher permeability & lower hysteresis loss than ferro.

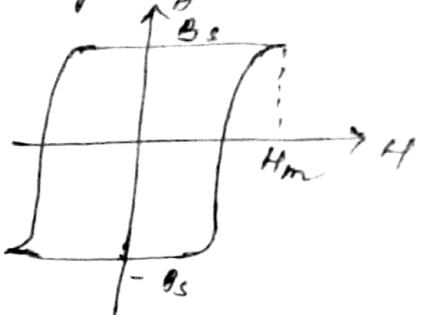
* APPLICATIONS OF FERRITE

- (1) Soft ferrites are used in transformers cores & in ac induction cores. also, in radio & communication devices.
- (2) Reason: Here, the material goes through complete cycle of magnetization continuously so, it ensures free dissipation of energy & ensures less heating of material.
- (3) → ensures small hysteresis loss.
- (4) ensures low eddy current loss.
- (5) manganese zinc ferrite Nickel zinc ferrite

(a) Hard ferrites (e.g. Ba ferrite & Sr ferrite) are more suitable to make permanent magnets that are used in loudspeakers & wiper motors.

(b) Ferrites are used in digital memory devices in computers.

Reason: Hysteresis curve of ferrites is almost a rectangle.



→ So, ferrite exhibits any of the saturated states of magnetic induction i.e either $+B_s$ or $-B_s$. These two states are analogous to binary states 0 & 1.

→ Reversal of ext. magnetic field can magnetize the material instantaneously to the same strength as before in the "reverse dir".