

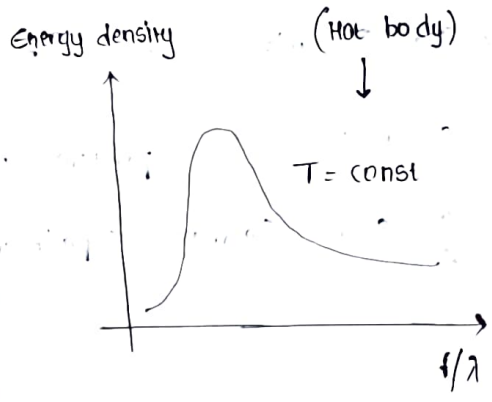
QUANTUM MECHANICS :

Planck's distribution :

(1900)

Planck $\rightarrow E_n = n(h\nu)$

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



* Energy density of obj b/w ν to $\nu + d\nu$

$\lambda \rightarrow$ freq (ω) wavelength

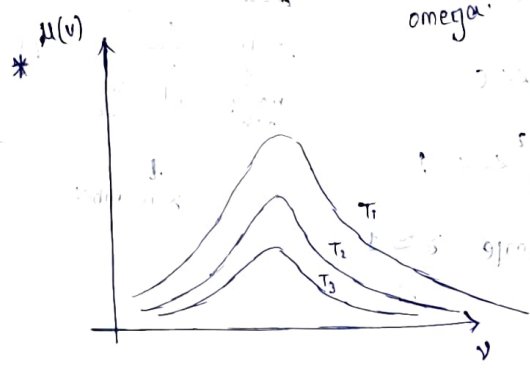
* $k_B \rightarrow$ Boltzman const.

$y \rightarrow$ Energy density.

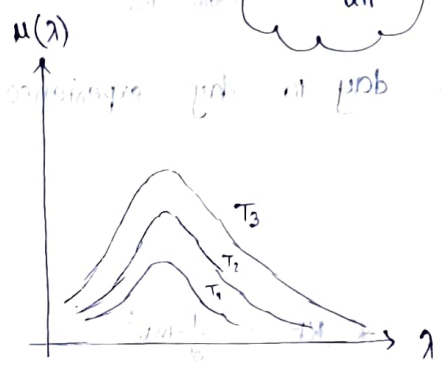
* $\mu(\nu)$ (ω) $\mu(\lambda)$ (ω) $\mu(\omega)$ (ω) $\mu(E)$

\downarrow
omega

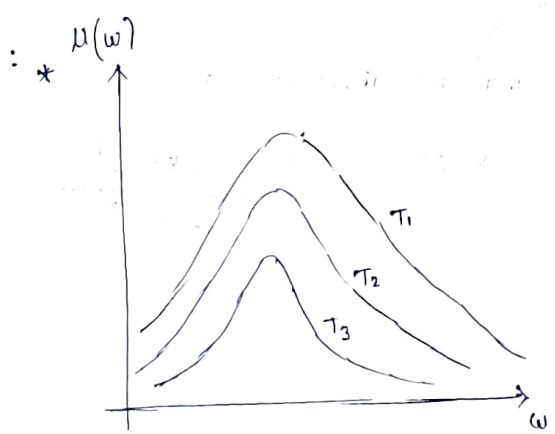
* $\hbar = \frac{h}{2\pi}$



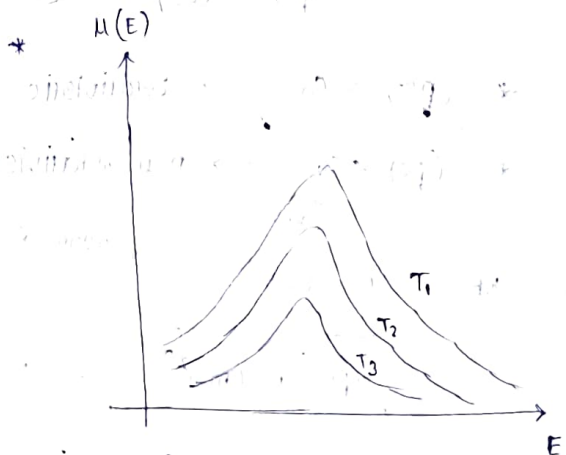
$T_1 \rightarrow 8000 \text{ K}$
 $T_2 \rightarrow 5000 \text{ K}$
 $T_3 \rightarrow 2000 \text{ K}$



① $\nu \propto T$
② $\lambda \propto \frac{1}{T}$



$\omega = 2\pi f$
 $\therefore \nu \propto T$
 $\omega \propto T$



$E = h\nu$
 $\nu \propto T$
 $E \propto T$

TOPICS :

- * De Broglie's relation ($\lambda = \frac{h}{p}$), $p \rightarrow mv$
- * Compton's effect (particle nature of wave)
- * Davisson Germer experiment (wave nature of ~~particle~~ ~~particle~~)

De BROGLIE'S

RELATION :

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2m KE}}$$

if eV is given, $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$

$$\lambda = \frac{h}{\gamma m_0 u} = \frac{h}{\gamma m}$$

γ moving mass

$$\gamma = \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$E = mc^2$$

$$E_0 = m_0 c^2$$

m_0 rest mass

$$\therefore m = \frac{m_0}{\sqrt{1 - \frac{u^2}{c^2}}} = \gamma m_0$$

\uparrow moving mass

remember

in day to day experience : $u \ll c$

$$\left(\frac{u}{c}\right)^2 \ll 1$$

$$\text{hence } \gamma \approx 1$$

$$* KE = \frac{1}{2} mv^2 \quad \text{E when there is velocity}$$

$$* KE = E - E_0 \rightarrow \textcircled{1}$$

$$* E^2 = p^2 c^2 + m_0^2 c^4$$

where there is no velocity (i.e. rest mass)

$$\text{Total energy} \Rightarrow E^2 = (pc)^2 + (E_0)^2 \rightarrow \textcircled{2}$$

E for wave = $\frac{hc}{\lambda} = pc$

$$E \text{ for particle} = \frac{mv^2}{2} = m_0 c^2$$

* $(pc) > E_0 \rightarrow$ relativistic \rightarrow then use above formula

* $(pc) < E_0 \rightarrow$ non-relativistic \rightarrow then use formula : $\lambda = \frac{h}{\sqrt{2m KE}}$

511 keV

$$* KE = E - E_0 \quad \leftarrow \text{Derivation of KE.}$$

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

$$= \sqrt{(m_0^2 c^4) \left(1 + \frac{p^2}{m_0^2 c^2}\right)} - m_0 c^2$$

$$= m_0 c^2 \left[1 + \frac{p^2}{m_0^2 c^2}\right]^{1/2} - m_0 c^2$$

$$= m_0 c^2 \left[1 + \frac{1}{2} \frac{p^2}{m_0^2 c^2} \right] - m_0 c^2 \quad [\text{Binomial}]$$

$$= \frac{1}{2} \frac{m_0^2 u^2 m_0 c^2}{m_0^2 c^2} = \frac{1}{2} m_0 u^2$$

⇒ Find de-Broglie λ of :

a) ball with velocity 30 m/s.

b) an e^- with velocity 10^7 m/s.

Soln a) $\frac{u}{c} = \frac{3 \times 10^1}{3 \times 10^8} = 10^{-7} \ll 1$

$$\gamma \approx 1 \Rightarrow \lambda = \frac{h}{m_0 u}$$

b) $\frac{u}{c} = \frac{10 \times 10^6}{3 \times 10^8} = 3.3 \times 10^{-2}$

$$\gamma \approx 1, \lambda = \frac{h}{m_0 u}$$

⇒ Find the KE of the proton where de-Broglie λ is 1 fm.

Soln find $pc, E_0 \rightarrow m_0 c^2$

$$p = \frac{h}{\lambda}, pc = \frac{hc}{\lambda}$$

Here we don't apply

$\lambda = \frac{h}{\sqrt{2mKE}}$ because proton has both wave (λ) & particle (mv^2).

~~$\lambda = \frac{h}{mv}$ but here~~

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mKE}} \Rightarrow KE = \frac{h^2}{2m\lambda^2} = \frac{(6.6 \times 10^{-34})^2}{2(1.6 \times 10^{-27})(10^{-15})^2}$$

$$KE = \dots$$

$$pc = \frac{hc}{\lambda} \Rightarrow pc = \frac{(6.6 \times 10^{-34})(3 \times 10^8)}{(10^{-15})}$$

~~$p = \frac{h}{\lambda} \Rightarrow m_0 u = \dots$~~

Soln) ~~$KE = \sqrt{(pc)^2 + (E_0)^2}$~~

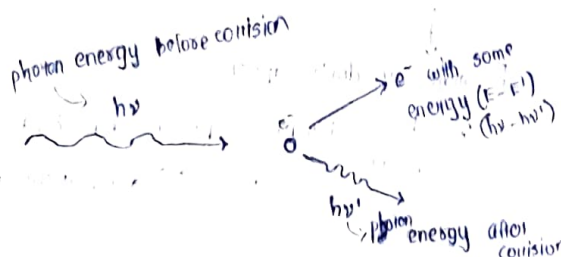
$$pc = \frac{hc}{\lambda} = \frac{6.6 \times 10^{-34} \text{ Js} \times 3 \times 10^8 \text{ m/s}}{10^{-15} \text{ m}} = 1.98 \times 10^{-11} \text{ J} = 1.2410 \text{ GeV}$$

$$E_0 = m_0 c^2 = 1.67 \times 10^{-27} \times (3 \times 10^8)^2 = 0.938 \text{ GeV}$$

$$E = \sqrt{(pc)^2 + (m_0 c^2)^2} = \sqrt{\quad} = 1.515$$

$$\therefore KE = E - E_0 = 1.515 - 0.938 = 637 \text{ MeV}$$

COMPTON EFFECT : (Particle wave nature of wave)



Treat this process as collision and derive the correlation b/w λ & λ' .

$$\Delta\lambda \doteq (\lambda' - \lambda)$$

after collision
before collision

$$\Delta\lambda = \lambda_c (1 - \cos \phi)$$

where

$$\lambda_c = \frac{h}{m_0 c} \quad (\text{Compton wavelength})$$

$$\lambda_c = \frac{h}{(m_0)_e c} = 2.426 \text{ pm} \quad \rightarrow \text{imp}$$

(photon energy (λ) & e^- energy (λ'))
so, photon λ & e^- (λ')

DAIRSSON GERMER : (WAVE NATURE OF PARTICLE)

Wave Nature	Particle Nature
Bragg's Theory	de-Broglie
λ_{Bragg}	$\lambda_{\text{de-brog}}$



$$\lambda_{\text{Bragg}} = \lambda_{\text{de-brog}}$$

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

HEISENBERG UNCERTAINTY THEORY :

$$* \Delta p_x \cdot \Delta x \geq \frac{\hbar}{2} = \frac{h}{4\pi}$$

$$\Delta p_y \cdot \Delta y \geq \frac{\hbar}{2}$$

$$\Delta p_z \cdot \Delta z \geq \frac{\hbar}{2}$$

$$* \Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

$$* \Delta J \cdot \Delta \phi \geq \frac{\hbar}{2}$$

$J \rightarrow$ angular momentum

$\phi \rightarrow$ angle

WAVE FUNCTION :

$$* \text{Notation} \rightarrow \Psi = \Psi(\vec{r}, t) \quad \text{Psi}$$

$$\psi = \psi(\vec{r}) \quad \text{psi}$$

* Ψ is in general complex.

* $|\Psi|^2$ has meaning, it represents the probability density of

$|\Psi|^2 \cdot dx$ is the probability of finding the object (e^- , proton, etc)

b/w x & $x+dx$.

$$P(x) = \int |\Psi|^2 dx$$

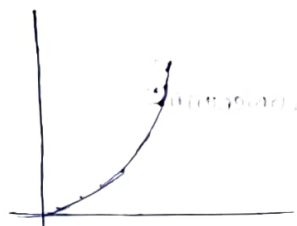
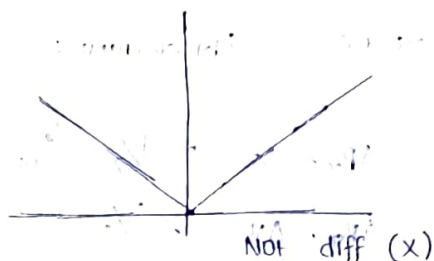
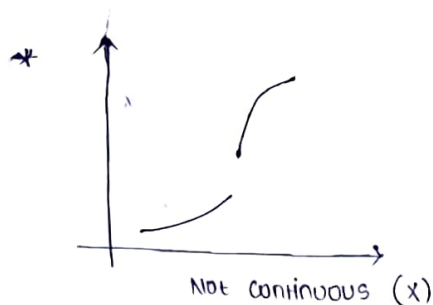
* Properties of Ψ :

i) Ψ is continuous, single values

ii) The derivative $\frac{\partial \Psi}{\partial x}$, $\frac{\partial \Psi}{\partial y}$, $\frac{\partial \Psi}{\partial z}$ are also continuous

iii) Ψ must be normalisable.

iv) Ψ goes to zero at $x \rightarrow \pm\infty$



$$m_p = 1.67 \times 10^{-27} \text{ kg} = m_H$$

$$m_e = 9.1 \times 10^{-31} \text{ kg}$$

* Zero point energy of e^- means $n=1$, principal quantum number

(1s, 2s, 2p, 3s, 3p, 3d) orbitals are possible for principal quantum number $n=3$.

orbitals are possible for principal quantum number $n=3$.

SCHRÖDINGER'S TIME DEPENDENT EGN : (SDE)

* we know :

$$\frac{1}{u^2} \frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2} \quad \text{where } f = f(x, t)$$

ODE : ordinary diff. eqn

PDE : partial DE

* Goal : We have to find differential eqn (ODE/PDE), which will describe the micro level or quantum level description of the particle.

* Wave eqn : $f(x, t) = Ae^{i(\omega t - Kx)}$

$$\frac{\partial f}{\partial t} = i\omega f$$

$$\frac{\partial f}{\partial x} = -iKf$$

$$\frac{\partial^2 f}{\partial t^2} = (i\omega)^2 f$$

$$\frac{\partial^2 f}{\partial x^2} = (-iK)^2 f$$

put in above eqn

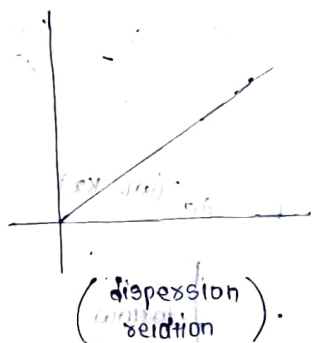
$$\frac{\omega^2}{u^2} = K^2$$

(or)

$$\omega = Ku$$

$$K = \frac{\omega}{c}$$

module-1



* For Quantum level :

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

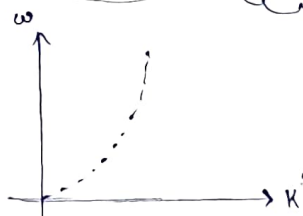
$$V(x) = 0$$

$$p = \hbar K$$

$$\hbar = \frac{h}{2\pi}$$

$$\Rightarrow \hbar \omega = \frac{\hbar^2 K^2}{2m}$$

$$\Rightarrow \omega \propto K^2$$



* If we have to satisfy this dispersion relation, what is the governing ODE/PDE ?

$$E = \frac{hc}{\lambda} = h\nu = 2\pi\hbar \left(\frac{\omega}{2\pi} \right) = \hbar\omega$$

~~p = mv~~
de-Broglie

$$\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda} \Rightarrow p = \frac{h\nu}{c} \Rightarrow p = \frac{h}{2\pi} \left(\frac{\omega}{c} \right) = \frac{\hbar K}{1} = \hbar K$$

* Assume the governing ODE/PDE solⁿ of the following.
 formal $f(x,t) = Ae^{i(\omega t - kx)}$

ω & k^2

$\omega \rightarrow$ relation to time derivatⁿ
 $k \rightarrow$ relation to space derivatⁿ

$\Rightarrow \omega = \delta k^2$ where $\delta = \text{const.}$

LHS \rightarrow one time derivatⁿ

RHS \rightarrow two space derivatⁿ

* $\frac{\partial f}{\partial t}$ & $\frac{\partial^2 f}{\partial x^2}$

* ω & k^2

$\Rightarrow i\omega f = \delta(-ik)^2 f$

$\Rightarrow \delta = \frac{i\omega}{k^2}$

$\frac{\partial f}{\partial t} = \delta \left(\frac{\partial^2 f}{\partial x^2} \right)$

$(-i\omega)f = \delta(ik)^2 f \rightarrow \textcircled{1}$

* $f = Ae^{i(\omega t - kx)}$

* $f = Ae^{i(kx - \omega t)}$

follow

follow

$\frac{\partial f}{\partial t} = i\omega f$

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

$\frac{\partial^2 f}{\partial x^2} = (-ik)^2 f$

$\frac{\partial^2 f}{\partial x^2} = (ik)^2 f$

* from eq $\textcircled{1}$:

$\delta = \left(\frac{i\omega}{k^2} \right) = \frac{i \left(\frac{E}{h} \right)}{\left(\frac{p}{h} \right)^2}$

$\frac{iE}{h} \cdot \frac{h^2}{p^2} = \frac{ihE}{p^2}$

$\Rightarrow \delta = \frac{ih}{2m}$

$\omega = 2\pi\nu = \frac{2\pi\nu}{\lambda} = \frac{2\pi\nu p}{h} = \frac{pv}{h} = \frac{hc/\lambda}{h} = \frac{E}{h}$

$\lambda\nu = \lambda f$

$k^2 = \frac{\omega^2}{c^2} = \left(\frac{\omega}{c} \right)^2 = \left(\frac{2\pi f}{c} \right)^2 = \left(\frac{h f}{h \lambda} \right)^2 = \left(\frac{p}{h} \right)^2$

$$\star \quad \frac{\partial f}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 f}{\partial x^2}$$

$$f \equiv \Psi(x,t) \quad \rightarrow \quad \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}, \text{ if } V(x) = 0$$

* In the presence of the potential $V(x)$, the薛定谔方程 (SDE) is:

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

→ This is not a derivation of SDE:

* ⇒ What would be the SDE in presence or absence of $V(x)$?

~~Solve~~ → may come in: FAT

Ans → above the pg.

$$\Psi(x,t) = \Psi(x) e^{-iEt/\hbar}$$

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \Psi$$

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~~# SCHRÖDINGER TIME INDEPENDENT EQ^N : (STIE)~~

* 1D (space) : $i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x) \Psi(x,t)$
 Cartesian

* 2D (space) : $i\hbar \frac{\partial \Psi(x,y,t)}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi(x,y,t)}{\partial x^2} + \frac{\partial^2 \Psi(x,y,t)}{\partial y^2} \right] + V(x,y) \Psi(x,y,t)$

* 3D (space) : $i\hbar \frac{\partial \Psi(x,y,z,t)}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi(x,y,z,t)}{\partial x^2} + \frac{\partial^2 \Psi(x,y,z,t)}{\partial y^2} + \frac{\partial^2 \Psi(x,y,z,t)}{\partial z^2} \right] + V(x,y,z) \Psi(x,y,z,t)$

SCHRÖDINGER TIME INDEPENDENT EQ^N : (STIE)

* STIE : $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x) \Psi$

$\therefore \Psi = \Psi(x,t)$

Assume : $\Psi(x,t) = f(x) g(t)$

$\frac{\partial \Psi}{\partial t} = f(x) \frac{dg}{dt}$

$\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 f}{dx^2} \cdot g$

$i\hbar f(x) \frac{dg(t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 f(x)}{dx^2} g(t) + V(x) f(x) g(t)$

* Divide LHS & RHS by $f(x) g(t)$

$i\hbar \frac{1}{g(t)} \cdot \frac{d(g(t))}{dt} = -\frac{\hbar^2}{2m} \frac{1}{f(x)} \frac{d^2 f(x)}{dx^2} + V(x) = E \text{ (const)}$

if $i\hbar \left(\frac{d(g(t))}{dt} \cdot \frac{1}{g(t)} \right) = \int E dt \Rightarrow g(t) = e^{-\frac{iEt}{\hbar}}$

$$\text{ii)} \quad -\frac{\hbar^2}{2m} \frac{1}{f(x)} \frac{d^2 f(x)}{dx^2} + V(x) = E$$

\therefore eqⁿ (ii) can be written as :

$$-\frac{\hbar^2}{2m} \frac{1}{f(x)} \frac{d^2 f}{dx^2} + V(x) = E$$

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

$$\psi = \psi(x) \rightarrow \frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi = 0 \} \rightarrow \text{S.T.E}$$

$$\Psi(x,t) = f(x) g(t)$$

is called separation
of variables.