12/03/18

- **Hamilton's eqns of motion** $\longrightarrow$

$$L = T - V = L(q_j, \dot{q}_j, t)$$

$$\downarrow \text{transform}$$

$$H = H(q_j, p_j, t) \Longrightarrow \text{Hamiltonian of the system}$$

where, p_j = generalised momentum

$$\boxed{p_j = \frac{\partial L}{\partial \dot{q}_j}}$$

» **Hessian matrix** :- (for transforming $\dot{q}_j \longrightarrow p_j$).

$$\left| \frac{\partial^2 L}{\partial \dot{q}_j \cdot \partial q_k} \right| \neq 0$$

» **Defn of Hamiltonian funcn** :-

$$\boxed{H(q_j, p_j, t) = \sum_{j=1}^{f} p_j \dot{q}_j - L(q_j, \dot{q}_j, t)} \quad \text{(1)}$$

$\Rightarrow$ d(LHS) = d(RHS)

$$\Downarrow$$

$$\sum_j \frac{\partial H}{\partial q_j} \cdot dq_j + \sum_j \frac{\partial H}{\partial p_j} dp_j + \frac{\partial H}{\partial t} dt$$

$\Rightarrow$ d(RHS) $\Rightarrow$

$$\sum_j p_j \cancel{d\dot{q}_j} + \sum_j \dot{q}_j dp_j - \sum \underbrace{\left\{\frac{\partial L}{\partial q_j}\right\}}_{\dot{p}_j} dq_j - \cancel{\sum \underbrace{\left\{\frac{\partial L}{\partial \dot{q}_j}\right\}}_{p_j} d\dot{q}_j} - \frac{\partial L}{\partial t} \cdot dt$$

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from d(LHS) & d(RHS) $\longrightarrow$

$$\boxed{-\dot{p}_j = \frac{\partial H}{\partial q_j} \;,\; \dot{q}_j = \frac{\partial H}{\partial p_j} \;,\; \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}}$$

<u>Hamilton's eq^{n}s of motion</u>

q_1 & p_1 $\longrightarrow$ canonically conjugate components

>> <u>from (1)</u> $\longrightarrow$

$H \neq H(q_\alpha)$

$\frac{\partial H}{\partial q_\alpha} = 0$

$\Rightarrow \dot{p}_\alpha = 0$

$\Rightarrow p_\alpha = \text{const.}$

If a particular generalised co-ordinate is cyclic wrt Hamiltonian of the system, then the corresponding generalized momentum will be a conserved quantity for a particular system.

$L \neq L(q_\alpha)$

$\Rightarrow \frac{\partial L}{\partial q_\alpha} = 0$

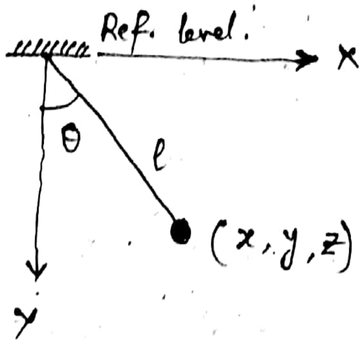
$\Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_\alpha}\right) = 0$

$\Rightarrow \dot{p}_\alpha = 0$

$\Rightarrow \frac{\partial H}{\partial q_\alpha} = 0 \Rightarrow \boxed{H \neq H(q_\alpha)}$

If a generalized co-ordinate is cyclic in Lagrangian, then that co-ordinate will be <u>cyclic</u> in Hamiltonian too.

⇒ Simple Pendulum :-



$x = l\sin\theta$

$y = l\cos\theta$

Generalised co-ordinate,

$q_1 = \theta$.

$$L = \frac{1}{2} m l^2 \dot{\theta}^2 + mgl\cos\theta$$

$$H(\theta, p_\theta, t) = p_\theta \cdot \dot{\theta} - L \qquad \text{--- } (1)$$

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} \qquad\qquad \dot{\theta} = \frac{p_\theta}{ml^2}$$

$$= ml^2 \dot{\theta}$$

∴ from (1) ⟶

$$H(\theta, p_\theta, t) = p_\theta \cdot \dot{\theta} - L$$

$$= ml^2\dot{\theta}^2 - \frac{1}{2} m l^2 \dot{\theta}^2 - mgl\cos\theta$$

$$= \frac{1}{2} m l^2 \dot{\theta}^2 - mgl\cos\theta$$

$$= \frac{1}{2} \cdot \frac{\cancel{(ml^2)}}{(ml^2)^{\cancel{2}}} \cdot p_\theta^2 - mgl\cos\theta$$

$$= \frac{p_\theta^2}{2ml^2} - mgl\cos\theta$$

$$\Rightarrow -\dot{p}_\theta = \frac{\partial H}{\partial \theta} \qquad \Rightarrow \boxed{\dot{p}_\theta = -mgl\sin\theta}$$

$$\Rightarrow \dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ml^2}$$

$$\Rightarrow \boxed{p_\theta = ml^2\dot{\theta}}$$

Replacing, we get ⟶

$$\cancel{m}l^{\cancel{2}}\ddot{\theta} = -\cancel{m}g\cancel{l}\sin\theta$$

$$\Rightarrow \boxed{\ddot{\theta} = -\frac{g}{l}\sin\theta}$$

$\boxed{\text{Phase Space}}$
↓
2f Dimension

» In case of Lagrangian eqⁿ of motion, there configuration of space = f. and generalised co-ordinate = q_j.

But in case of Hamiltonian eqⁿs of motion, generalised co-ordinate = $\dot{q}_j$ & p_j.
So, instead of config. of space, we write Phase space = 2f Dimension.

19/03/18

BAND THEORY OF SOLIDS

Solids ⟶ state of matter
↳ comprised of atoms
↳ nuclei of $e^{\ominus}$s
↓
follows the law of QM.

→ operator

$\hat{O} f(x) = \alpha f(x)$

↑ Eigen funcⁿ ↑ Eigen value

$\Rightarrow \frac{d}{dx} \cdot e^{\alpha x} = \alpha . e^{\alpha x}$.

Schrodinger Eqⁿ

$\hat{H}\Psi = E\Psi$

$\hat{H}$ → Total energy operator

$\hat{H} = KE + PE$

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

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

$$\left[\begin{array}{l} \hat{p} \longrightarrow -i\hbar\vec{\nabla} \\ \hat{V} \longrightarrow V \end{array}\right]$$

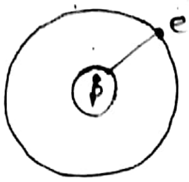
$\frac{d}{dx}$ for 1-D.

$\hat{H}\psi = E\psi$

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

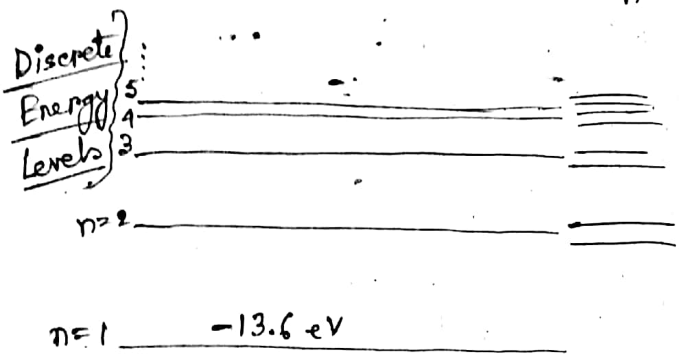
??

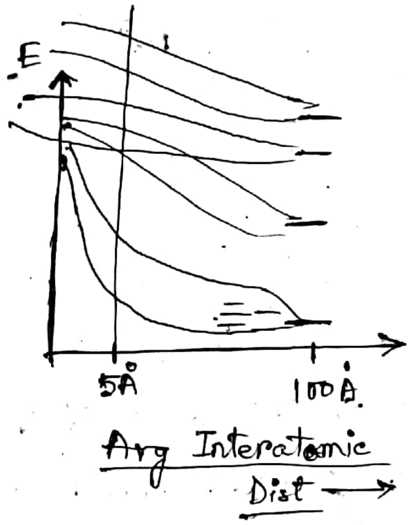
» <u>H - atom</u> :



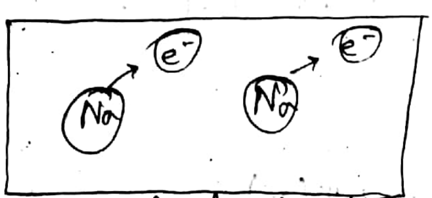
$$V(r) = \frac{(+e)(-e)}{r}$$

$$E_n = -\frac{13.6}{n^2}\ \text{eV}$$





» $_{11}$Na $\longrightarrow$ $\underbrace{1s^2\ 2s^2\ 2p^6}_{\text{core } e^- \text{'s}}$ $\underbrace{3s^1}_{\text{valence } e^- \text{'s}}$



→ Total no. of atoms in solid

[∵ $N \rightarrow 10^{22}$]

$N \longrightarrow Na^+$ atoms $(+Ne)$

$e^- \longrightarrow (N-1)$ no. of $e^\ominus \longrightarrow [-(N-1)e] \simeq (-Ne)$

∴ Total $\underline{V \approx 0}$ on e^-.

Hence valence $e^\ominus$s are <u>free electrons</u>.

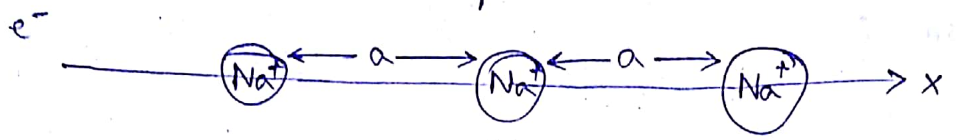
26/03/18

$\boxed{\text{Normal free } e^-}$ $\boxed{\text{free } e^- \text{ inside solid}}$

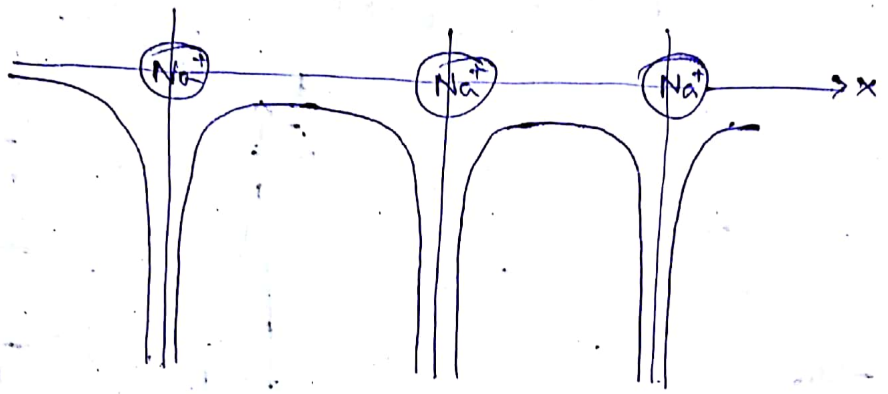
<u>1-D crystal lattice</u>

$a \rightarrow$ lattice const

Periodic potential



Potential funcⁿ, $V(x) = \frac{+ze.(-e)}{x} \propto -\frac{1}{x}$



» Inside a solid, a free $e^\ominus$ moves with periodic potential which a value equal to lattice const.

» For normal $e^\ominus$, $e^\ominus$ moves with ~~zero~~ periodic potential.

- <u>Quantum Mechanics in Periodic Potential</u> :-

» $V(x+a) = V(x)$

» $$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad \text{—— (1)}$$

<u>Th. (1)</u> :- If $V(x+a) = V(x)$, then $H(x+a) = H(x)$

$x + a = x'$

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

$$\frac{d}{dx'} \equiv \frac{d}{dx}$$

$$\Rightarrow H(x+a) = H(x')$$

$V(x+a) \rightarrow V(x)$

$$\Rightarrow \frac{d^2}{dx'^2} \equiv \frac{d^2}{dx^2}$$

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

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

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Th. (2) $H\psi = E\psi$

$\psi(x)$ is an Eigen func^n of $H(x)$ with Eigen value E. Lets define an operator $\hat{T}_a$ such that

$\hat{T}_a f(x) = f(x+a)$

↳ giving $f(x)$ a translational motion.

$\hat{T}_a \rightarrow$ lattice translational operator.

[$\{\hat{T}_a \psi(x)\}$ will be an eigen func^n of $H(x)$ with eigen value E.]

⇒ We know, $H(x)\,\psi(x) = E\psi(x)$

$\Rightarrow \hat{T}_a \{H(x)\,\psi(x)\} = \hat{T}_a \{E\psi(x)\}$

$\Rightarrow H(x+a)\,\psi(x+a) = E.\psi(x+a)$

$\Rightarrow \underbrace{H(x).\{\hat{T}_a\psi(x)\} = E\{\hat{T}_a\psi(x)\}}$ [applying, Th.(1)]

⇓

$\hat{T}_a \psi(x) = \psi(x+a) \quad \alpha\, \psi(x)$

$\Rightarrow \hat{T}_a \psi(x) = \psi(x+a) = \lambda\, \psi(x)$

$\lambda = ??$

» Floqvet's Th. :

If in a periodic lattice with $V(x) = V(x+a)$ and $\hat{T}_a\psi = \lambda\psi$ then, λ is a complex no. of unit modulus.

Let $u_1(x)$ & $u_2(x)$ are two independent sol^{n}s of Schrodinger Eq^n.

$u_1(x+a) = M_{11} u_1(x) + M_{12} u_2(x)$

$u_2(x+a) = M_{21} u_1(x) + M_{22} u_2(x)$

$\Downarrow$

$$\begin{pmatrix} u_1(x+a) \\ u_2(x+a) \end{pmatrix} = \underbrace{\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}}_{\text{Transfer matrix}} \begin{pmatrix} u_1(x) \\ u_2(x) \end{pmatrix}$$

$\psi(x) = A\, u_1(x) + B\, u_2(x)$ [Any func^n of $\psi(x)$ is a linear func^n of $u_1(x)$ & $u_2(x)$]

$\Rightarrow \psi(x+a) = A\, u_1(x+a) + B\, u_2(x+a)$

$\Rightarrow \lambda \psi(x) = A\left(M_{11} u_1(x) + M_{12} u_2(x)\right)$

$+ B\left(M_{21} u_1(x) + M_{22} u_2(x)\right)$ [$\because \psi(x+a) = \lambda \psi(x)$]

$\Rightarrow \lambda A\, u_1(x) + \lambda B\, u_2(x) = (AM_{11} + BM_{21})\, u_1(x)$

$+ (AM_{12} + BM_{22})\, u_2(x)$

$\Rightarrow AM_{11} + BM_{21} = \lambda A$

$AM_{12} + BM_{22} = \lambda B$

$(M_{11} - \lambda)A + M_{21} B = 0$

$M_{12} A + (M_{22} - \lambda) B = 0$

$$\begin{vmatrix} M_{11} - \lambda & M_{21} \\ M_{12} & M_{22} - \lambda \end{vmatrix} = 0 \begin{array}{l} \nearrow \lambda_1 \\ \searrow \lambda_2 \end{array}$$

[λ has 2 values so, 2 wave func^n can have]

$\psi_1(x+a) = \lambda_1 \psi_1(x)$

$\psi_2(x+a) = \lambda_2 \psi_2(x)$

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09/04/18

$$\lambda \begin{cases} \to \lambda_1 \Rightarrow \psi_1(x+a) = \lambda_1 \psi_1(x) \\ \to \lambda_2 \Rightarrow \psi_2(x+a) = \lambda_2 \psi_2(x) \end{cases}$$

<u>Define</u>, $\quad W(x) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

$$\Rightarrow W'(x) = \cancel{\psi_1'\psi_2'} + \psi_1\psi_2'' - \cancel{\psi_2'\psi_1'} - \psi_2\psi_1''$$

$$= \psi_1\psi_2'' - \psi_2\psi_1''$$

$$\psi_1'' + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi_1 = 0 \qquad \times \psi_2 \qquad \to \text{from } 1$$

$$\psi_2'' + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi_2 = 0 \qquad \times \psi_1$$

$$\psi_2\psi_1'' - \psi_1\psi_2'' = 0$$

$\therefore W'(x) = 0$

$\Rightarrow W(x) = \text{const wrt } x$

$\Rightarrow W(x+a) = W(x)$

$$\therefore W(x) = W(x+a) = \hat{T}_a W(x)$$

$$= \hat{T}_a\left[\psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)\right]$$

$$= \psi_1(x+a)\psi_2'(x+a) - \psi_2(x+a)\psi_1'(x+a)$$

$$= \lambda_1\psi_1(x)\lambda_2\psi_2'(x) - \lambda_2\psi(x)\lambda_1\psi_1'(x)$$

$$= \lambda_1\lambda_2\left[\psi_1\psi_2' - \psi_2\psi_1'\right]$$

$$= \lambda_1\lambda_2 W(x)$$

$$\Rightarrow \boxed{\lambda_1\lambda_2 = 1}$$

~~Now~~ $|\lambda| > 1 \qquad$ <u>say $\lambda = 5$</u>

$\Rightarrow \psi(x+a) = 5\psi(x)$

$\Rightarrow \psi(x+2a) = 5\psi(x+a) = 5^2\psi(x)$

$\Rightarrow \psi(x+na) = 5^n \psi(x)$

$\therefore$ Prob. of finding e^- at 1st lattice pt $= |\psi\psi^*|$.

" " " " " " nth " " $= 5^{2n}|\psi\psi^*|$

$\downarrow$

monotorically increasing.

Hence, $|\lambda| \not> 1$.

If $|\lambda| < 1$ say $\frac{1}{5}$

$\psi(x+na) = \frac{1}{5^n}\psi(x)$ ×

$\downarrow$

monotorically decreasing.

$\therefore \boxed{|\lambda| = 1}$

$\lambda = e^{\pm i\theta}$

$\hat{T}_a \psi_1(x) = \psi_1(x+a) = e^{i\theta}\psi_1(x)$

$\hat{T}_a \psi_2(x) = \psi_2(x+a) = e^{-i\theta}\psi_2(x)$.

$\theta \rightarrow$ angle , $\theta \propto a$

$\Rightarrow \theta = ka$

$[\theta] \longrightarrow$ dimensionless

$[a] \longrightarrow$ length, L

$\because K =$ Some kind of wave vector.

$\therefore [k] = \frac{1}{\text{length}}$

$\therefore \boxed{\psi(x+a) = e^{ika}\psi(x)}$

$\therefore \boxed{\psi(x+na) = e^{ikna}\psi(x)}$

BLOCH'S THEOREM.

are valid when $\psi(x) = e^{ikx}\cdot\phi(x)$

- Bloch Theorem : (in 1D)

If the potential $V(x)$ is periodic with periodicity of the lattice (a), then the solution $\psi(x)$ of the wave eqn, $H\psi = E\psi$ with $\rightarrow$

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

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at 1st lattice pt $= |\psi\psi^*|$

n nth " $n = 5^{2n}|\psi\psi^*|$

$\downarrow$

monotorically increasing

×

Hence, $|\lambda| \not> 1$

torically increasing

$,(x)$

$\psi_2(x)$.

a.

.a

is of the form, $\psi(x) = e^{ikx}\phi(x)$, for a given E where $\phi(x)$ is a periodic funcn,

$\phi(x+a) = \phi(x)$.

$\psi(x) = e^{ikx}\phi(x)$

$\Rightarrow \psi(x+a) = e^{ik(x+a)}\phi(x+a)$

$\Rightarrow \psi(x+a) = e^{ika}[e^{ikx}.\phi(x)]$

$= e^{ika}.\psi(x)$.

$\psi(x) \longrightarrow$ Bloch wave eqn.

20/03/18 PHYS (D.M.)

- **M-B Statistics :-**

$$N = \int_0^\infty N(E)\,dE \qquad \left[N = N_1 + N_2 + \cdots + N_i = \sum N_i \right]$$

$$= \int_0^\infty e^{-\alpha} \cdot e^{-\beta E} \cdot g(E)\,dE$$

$$= e^{\mu/KT} \cdot 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \int_0^\infty e^{-E/KT} \cdot E^{1/2}\,dE$$

Let, $\frac{E}{KT} = x$

$$\Rightarrow N = e^{\mu/KT} \cdot 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \cdot (KT)^{3/2} \underbrace{\int_0^\infty e^{-x} \cdot x^{1/2}\,dx}_{\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi}}$$

$$\Rightarrow N = e^{\mu/KT} \cdot V \left(\frac{2\pi m KT}{h^2}\right)^{3/2}$$

$$\Rightarrow \boxed{e^{\mu/KT} = \frac{N}{V\left(\frac{2\pi m KT}{h^2}\right)^{3/2}}}$$

- **M-B Energy Distribution Law :-**

$$N(E)\,dE = e^{-\alpha} \cdot e^{-\beta E} \cdot g(E)\,dE$$

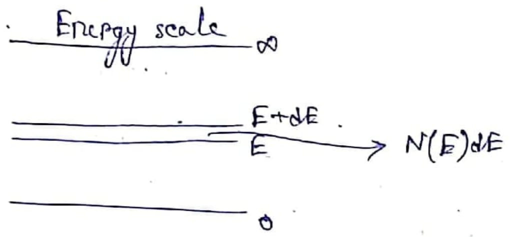
$$= \left[\frac{N}{\cancel{V}\left(\frac{2\pi \cancel{m} K T}{\cancel{h^2}}\right)^{3/2}} \times 2\pi \cancel{V} \left(\frac{\cancel{2m}}{\cancel{h^2}}\right)^{3/2}\right] \cdot e^{-E/KT} \cdot E^{1/2}\,dE$$

$$\boxed{N(E)\,dE = \left[\frac{2\pi N}{(\pi KT)^{3/2}}\right] \cdot e^{-E/KT} \cdot E^{1/2}\,dE}$$

(will be Given in paper)

- **Total Energy of gas molecules at T K :-**

$U = \sum E_i N_i$



$$U = \int_0^\infty E N(E) dE$$

$$= \frac{2\pi N}{(\pi KT)^{3/2}} \cdot \int_0^\infty e^{-E/KT} \cdot E^{3/2} dE$$

[Let, $x = \frac{E}{KT}$

$$= \frac{2\pi N}{(\pi KT)^{3/2}} \times (KT)^{5/2} \int_0^\infty e^{-x} \cdot x^{3/2} dx$$

$$= \frac{\cancel{2\pi} N}{(\cancel{\pi} \cancel{KT})^{3/2}} \times (KT)^{\cancel{5/2}} \times \frac{3}{2} \times \frac{1}{\cancel{2}} \times \cancel{\sqrt{\pi}}$$

$$\Rightarrow U = \frac{3}{2} NKT$$

$$\bar{U} = \frac{U}{N} = \frac{3}{2} KT$$

Avg Energy per degree of freedom $= \frac{1}{2} KT$

- **M-B Speed Distribution Law :-**

We know, $N(E) dE = \frac{2\pi N}{(\pi KT)^{3/2}} \cdot e^{-E/KT} \cdot E^{1/2} dE$

Here, total energy — (random particles)

$$E = \frac{1}{2} mv^2$$

$$\Rightarrow dE = mvdv$$

$$N(v)dv = \left[\frac{2\pi N}{(\pi KT)^{3/2}}\right] \cdot e^{-mv^2/2KT} \cdot \frac{1}{\sqrt{2}}\sqrt{m}.v.\ mv\,dv$$

$$\Rightarrow \boxed{N(v)dv = \left[\sqrt{2}\pi N \left(\frac{m}{\pi KT}\right)^{3/2}\right] . e^{-mv^2/2KT} . v^2\,dv}$$

Avg speed of gas molecules :-

H.W.

$$\bar{v} = \frac{\int_0^\infty v . N(v)\,dv}{N} = \sqrt{\frac{8KT}{\pi m}}$$

H.W.

$$v_{rms} = \sqrt{\frac{\int_0^\infty v^2 . N(v)\,dv}{N}} = \sqrt{\frac{3KT}{m}}$$

Most Probable Speed :-

We know, $N(v) = \left[\sqrt{2}\pi N\left(\frac{m}{\pi KT}\right)^{3/2}\right] . e^{-mv^2/2KT} . v^2$

$N(v) \longrightarrow$ No. of gas molecules per unit speed within the speed range v to $v+dv$.

$$\Rightarrow \ln[N(v)] = \ln A - \frac{mv^2}{2KT} + 2\ln v$$

$$\Rightarrow \frac{d\{\ln N(v)\}}{dv} = -\frac{mv}{KT} + \frac{2}{v}$$

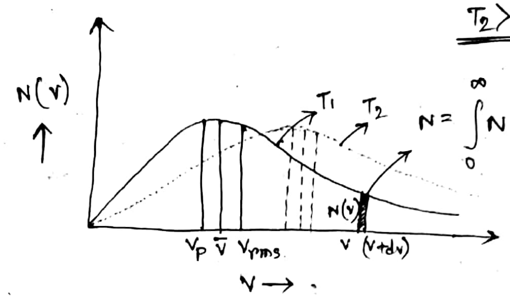
At, $v = v_p$ [for most probable speed]

$$\frac{d\{\ln N(v)\}}{dv} = 0 \qquad [\because N(v) \text{ is max}^m]$$

$$\Rightarrow -\frac{m v_p}{KT} + \frac{2}{v_p} = 0$$

$$\Rightarrow \boxed{v_p = \sqrt{\frac{2KT}{m}}}$$

$\underline{T_2 > T_1}$



$$N = \int_0^\infty N(v)\,dv$$

27/03/18

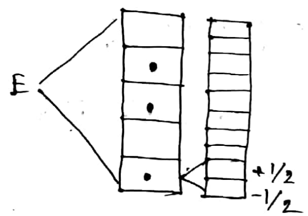
- **Fermi - Dirac Statistics :-** (conduction electrons)

F-D Energy Distribution law ⟶

$$N(E)dE = \frac{g(E)dE}{e^{\alpha+\beta E}+1}$$

$$g(E)dE = 2\pi V\left(\frac{2m}{h^2}\right)^{3/2} \cdot E^{1/2}\,dE$$ [have not consider spin of a particle

For particles, like e^-, we have two spin degeneracy, $S = \pm 1/2$



for each $e^{\ominus}$, there will be 2 allowed energy states corresponding to two possible spin orientation.

Taking spin into consideration —

$$\boxed{g(E)\,dE = 2 \times 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \times E^{1/2}\, dE}$$

» $\alpha = -\dfrac{\mu}{KT}$, $\mu(T = 0K) = \varepsilon_f$ [$\varepsilon_f \rightarrow$ Fermi Energy]

$\mu(300) = 0.998\, \varepsilon_f$

In general we can write →

$$\boxed{\alpha = -\frac{\varepsilon_f}{KT}}$$

» $\beta = \dfrac{1}{KT}$

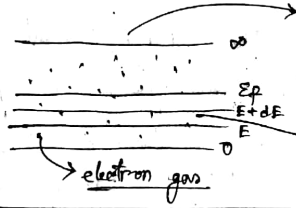
» $f(E) \longrightarrow$ Fermi distribution func^n

$f(E) = \dfrac{N(E)}{g(E)} = \dfrac{\text{The no. of particles per unit energy within the energy range E and E+dE}}{\text{" " " energy states per unit energy within the energy range E to E+dE.}}$

$$f(E) = \frac{1}{e^{\alpha + \beta E} + 1}$$

$$\Rightarrow f(E) = \frac{1}{e^{\frac{E - \varepsilon_f}{KT}} + 1}$$

»

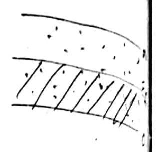


Energy scale for conduction $e^{\ominus}$ in metal

$\Rightarrow N = \int_0^{\infty} N(E)\, dE$ [N = total no. of conduction e^- in metal]

Fermi distribution func^n at T = 0 K and T > 0 K in metal :-

» **case - 1** : $E < \varepsilon_f$ and $T = 0\,K$



$$f(E) = \frac{1}{e^{\frac{E - \varepsilon_f}{KT}} + 1} = \frac{1}{e^{\frac{-(\varepsilon_f - E)}{KT}} + 1}$$

$$= \frac{1}{e^{-\infty} + 1} = \frac{1}{0 + 1} = 1$$

[$f(E) \to$ fraction of occupied state]

$\therefore N(E) = g(E)$

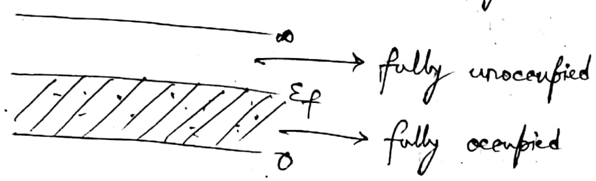
At T = 0 K, all the energy states in an energy level below fermi levels are fully occupied.

» **case - 2** : $E > \varepsilon_f$, at $T = 0\,K$.

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

$\therefore N(E) = 0$

At T = 0 K, all the energy states in an energy level above fermi level is fully unoccupied.



At T = 0 K, Fermi level is the energy level below which all the energy states are fully occupied. It is the highest occupied energy level at T = 0 K in metals.

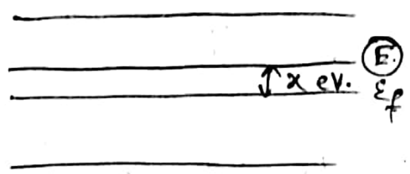
» case - 3 : $E = \varepsilon_f$ and $T > 0K$

$$f(E) = \frac{1}{e^{\frac{E-\varepsilon_f}{KT}}+1} = \frac{1}{e^0+1} = \frac{1}{2}$$

At $T > 0$ K, fermi level is the energy level at which the probability of finding the particle is $= \frac{1}{2}$.

(SEM) » Fraction of occupied states in the energy level above fermi level :-

$E = \varepsilon_f + x$



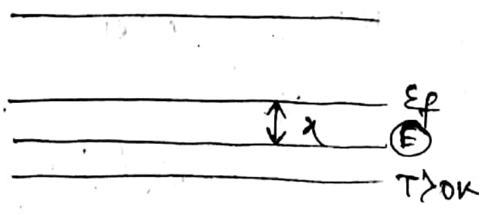
$$f(E) = \frac{1}{e^{\frac{E-\varepsilon_f}{KT}}+1}$$

[f(E) = fraction of occupied states]

$$\Rightarrow f(E_f + x) = \frac{1}{e^{x/KT}+1}$$

» Fraction of unoccupied states in the energy level below fermi level :-

$E = \varepsilon_f - x$



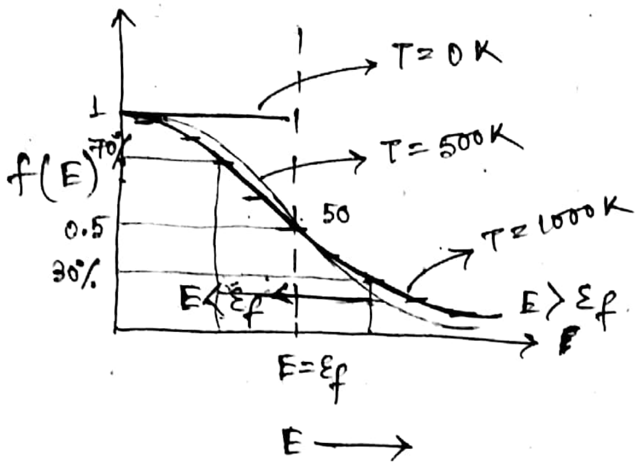
$$1 - f(E) = 1 - \frac{1}{e^{\frac{E-\varepsilon_f}{KT}}+1}$$

$$= \frac{1}{1 + e^{-\frac{(E-\varepsilon_f)}{KT}}}$$

[1 - f(E) = fraction of unoccupied states]

$$\Rightarrow 1 - f(E_f - x) = \frac{1}{1 + e^{x/KT}}$$

i) $f(E)$ vs. E at $T = 0K$, $T > 0K$:-



• Value of fermi energy at T = 0 K in metal :-

$$N = \int_0^\infty N(E)\,dE \qquad [N = \text{conduction } e^{\ominus}]$$

$$= \int_0^\infty f(E)\,g(E)\,dE$$

$$= \int_0^{\varepsilon_f} \underbrace{f(E)}_{1}\,g(E)\,dE + \int_{\varepsilon_f}^\infty \underbrace{f(E)}_{0}\,g(E)\,dE$$

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

$$N = \left[2 \times 2\pi V \left(\frac{2m}{h^2}\right)^{3/2}\right] \int_0^{\varepsilon_f} E^{1/2}\,dE$$

$$\Rightarrow N = 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} \times \frac{2}{3}\,\varepsilon_f^{3/2}$$

$$\Rightarrow \boxed{\varepsilon_f = \left(\frac{3N}{8\pi V}\right)^{2/3} \cdot \frac{h^2}{2m}}$$

$\left[\frac{N}{V} \longrightarrow \text{free } e^{\ominus} \text{ conc}^n\right]$ It varies from metal to metal

6 marks (problem will come)

⇒ At $T = 0K$, Na ⟶ atomic wt. = 23,

density of Na atom = 0.97×10^{3} kg/m^{3}

ε_f = ??

Soln :- $\left(\frac{N}{V}\right)_{Na-atom} = \dfrac{\text{density of Na}}{\left(\dfrac{\text{Atomic wt.}}{\text{Avogadro No.}}\right)}$

$$= \frac{0.97 \times 10^{3} \times 10^{3}}{\left(\dfrac{23}{6.023 \times 10^{23}}\right)}$$

Here, each Na atom ~~are free~~ contribute 1 free/conduction e^{-}.

$$\left(\frac{N}{V}\right)_{e^-} = \left(\frac{N}{V}\right)_{Na-atom}$$