

SAGAR DAM
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Problem 2: →

Given relation between χ & ν is:

$$\nu^2 = \frac{2\pi\tau}{P\chi^3} \Rightarrow \chi^3 = \frac{(P\nu^2)^{1/3}}{2\pi\tau},$$

$$\therefore K = \frac{2\pi}{\chi} = 2\pi \cdot \left(\frac{P\nu^2}{2\pi\tau} \right)^{1/3}.$$

$$\text{So: } \frac{dK}{d\nu} = 2\pi \cdot \left(\frac{P}{2\pi\tau} \right)^{1/3} \cdot \frac{2}{3} \nu^{-1/3} = \frac{4\pi}{3} \left(\frac{P}{2\pi\tau} \right)^{1/3} \nu^{-1/3}$$

So the density of states in the ν space
be given by,

$$J(\nu) d\nu = \frac{L_x}{2\pi} \times \frac{L_y}{2\pi} dK_x \times dK_y,$$

(\because This many full waves can fit in the
 $L_x \times L_y$ space in 2d region.)

$$= \frac{A}{4\pi^2} \times 2\pi K dK$$

$$= \frac{A}{2\pi} \cdot 2\pi \left(\frac{P\nu^2}{2\pi\tau} \right)^{1/3} \cdot \frac{4}{3}\pi \left(\frac{P}{2\pi\tau} \right)^{1/3} \nu^{-1/3} d\nu.$$

$$= \frac{4\pi A}{3} \left(\frac{P}{2\pi\tau} \right)^{2/3} \nu^{1/3} d\nu.$$

Now according to Debye model; (here the
name ~~is~~ should not be phonon as they are

Used in metals) the energy carriers are holes which follow B-E distn (with $g(E)$ derived as before)

The total surface energy will be given by:

$$E = \int_0^{v_D} h\nu f(v) g(v) dv.$$

$$\left(f(v) = \frac{1}{e^{\beta h v} - 1} \text{ for Bosons, with } E = h\nu. \right)$$

Here the Debye freq is given by:

$$\int_0^{v_D} g(v) dv = 2N_A \quad (2 \text{ as we are in 2 dimension})$$

However:

$$E_{\text{total}} = \int_0^{v_D} \underbrace{\frac{4}{3}\pi A \cdot \left(\frac{P}{2\pi\sigma}\right)^{1/3}}_C \cdot \frac{v^{1/3} \times h\nu}{e^{\beta h v} - 1} dv.$$

$$= \int_0^{v_D} C \times \frac{x^{1/3}}{(\beta h)^{1/3}} \cdot \frac{dx}{e^x - 1} \times \frac{m}{\beta}.$$

$$\left(\beta h v = x \Rightarrow v^{1/3} = \frac{x^{1/3}}{(\beta h)^{1/3}} ; dx = \frac{dx}{\beta h} \right)$$

$$= \frac{C}{(\beta h)^{1/3} \cdot \beta} \int_0^{\infty} \frac{x^{1/3} dx}{e^x - 1}$$

At low temperature $T \rightarrow 0$

$$\alpha_p = \frac{h\nu p}{kT} \rightarrow \infty$$

So changing the integral limit upto ∞ :

$$E_{\text{tot}} = \frac{c}{\beta (\beta h)^{4/3}} \int_0^\infty \frac{x^{4/3} dx}{e^x - 1}$$

Using mathematica the integral terms out to be:

$$\int_0^\infty \frac{x^{4/3} dx}{e^x - 1} = \Gamma\left(\frac{7}{3}\right) \cdot \Gamma\left(\frac{17}{3}\right) \simeq 1.685 \dots$$

Surface energy of the liquid at low temperature be given by:

$$E_{\text{tot}} = \frac{1.685}{\beta \cdot (\beta h)^{4/3}} \times \frac{4}{3} \pi A \left(\frac{P}{2\pi r} \right)^{2/3}$$
$$= \frac{2.073 A}{\beta \cdot (\beta h)^{4/3}} \cdot \left(\frac{P}{r} \right)^{2/3} \quad \left(\beta = \frac{1}{k_B T} \right)$$

(collecting all numerical constants)

Answer

Problem: 4

a. GaAs is a Semiconductor material. The concentration of e- & holes in the intrinsic semiconductor is given by:

$$n_i = p_i = 2 \cdot \left(\frac{KT}{2\pi h^2} \right)^{3/2} \cdot (m_e \cdot m_p)^{3/4} \cdot e^{-\frac{E_f}{2KT}}$$

(Using values [m_e, m_p] from given info])
 $= 1.73 \times 10^{12} \text{ m}^{-3}$.

So the intrinsic conductivity is given by:

$$\sigma_{int} = e n_i (m_e + m_h)$$

values of m_e & m_h are given.

$$\text{So; } \sigma_{int} = 5.55 \times 10^{-7} \text{ S/m}$$

This is very small as occurs in intrinsic semiconductor.

(The calculation has been done on desmos online calculator & the link has been sent.)

∴ The Chemical potential is:

$$\mu = \frac{1}{2} (E_{valence} + E_{conduction}) + \frac{3}{4} K_B T \ln \left(\frac{m_p}{m_e} \right)$$

$$= \frac{1}{2} (E_v + E_c) + 6.011 \times 10^{-21} \text{ J}$$

$$= \frac{1}{2} (E_v + E_c) + 0.0375 \text{ ev.}$$

So here the Fermi Level is shifted by +0.0375 ev from the middle of valence band & conduction band.

Ans

b. Here we use the formula:

$$\mu = E_{\text{comd}} - k_B T \ln \left(\frac{m_c}{m_d} \right) \quad \dots (1)$$

where $M_d = \text{total no of donors.} = 10^{22} \text{ m}^{-3}$ (given)

$m_c = \text{no of donors in conduction band}$

$$= 2 \left(\frac{m_e k T}{2\pi \hbar^2} \right)^{3/2} \rightarrow \begin{aligned} & \text{(from the normalization)} \\ & \text{at dist } \infty \text{ fm.} \\ M &= \frac{\sqrt{2}}{2\pi^2} \int_0^\infty e^{-\frac{Bk^2 \hbar^2}{2m_e}} k^2 dk \\ &= \sqrt{2} \left(\frac{m_e k T}{2\pi \hbar^2} \right)^{3/2} \end{aligned}$$

Ans 2 due to spin

so from (1) we get:

$$\mu = E_{\text{comd}} - k_B T \ln \left(\frac{m_c}{m_d} \right)$$

$$\therefore E_{\text{comd}} = 1.545 \times 10^{-20} \text{ J}$$

$$\therefore E_{\text{comd}} = 0.096 \text{ ev.}$$

Ans

$$\begin{array}{c} E_{\text{comd}} \\ \hline \mu \end{array} \} 0.096 \text{ ev.}$$

c. In part (a) it was evaluated that ~~the~~
 n_i (intrinsic) $\sim 10^{12} \text{ m}^{-3}$.

Here due to doping the concentration of
e-h holes has changed by a ~~very~~ huge amount.

As given $M_{\text{acc}} \sim 10^{21}$ & $M_{\text{donor}} \sim 10^{22} \text{ m}^{-3}$.

So the conductivity is given by:

$$\begin{aligned}\sigma &= \mu_m (\mathcal{N}_{\text{donor}} + \mathcal{N}_i) e \mu_e + (\mathcal{N}_{\text{acceptor}} + \mathcal{N}_i) \mu_n e \\ &= (10^{22} + 1.73 \times 10^{12}) e \mu_e + (2 \times 10^{21} + 1.73 \times 10^{12}) e \mu_n \\ &\approx 2.69 \times 10^3 \text{ S m}^{-1} \quad \underline{\text{Any}}$$

(This is much larger than $\sigma_{\text{intrinsic}}$ in part a. Which reveals the difference between doped & intrinsic semiconductor.)

So the no of valence band conductors be given by:

$$N_{\text{valence}} = 2 \times \left(\frac{m_e k_B T}{2\pi \hbar^2} \right)^{3/2}$$

(Same formula; only μ_e replaced by μ_n as we're dealing with valence band.)

$$\therefore N_{\text{valence}} = 7.59 \times 10^{24} \text{ m}^{-3}.$$

Now as we are in large energy (conduction bands) regime; we can approximate:

$$\frac{N_e}{N_{\text{tot}}} = \frac{1}{e^{\frac{(E-\mu)}{kT}} + 1} \approx e^{-\frac{(E-\mu)}{kT}}.$$

$$\begin{aligned} \text{So: } N_e &= N_{\text{cons.}} e^{(\mu - E) \beta} \\ N_p &= N_{\text{val.}} e^{(E_v - \mu) \beta} \end{aligned}$$

$$\therefore \frac{m_e}{m_p} \approx \frac{N_{coms}}{N_{val}} e^{\beta(2\mu - E_c - E_v)}$$

$$\Rightarrow e^{\beta(2\mu - E_c - E_v)} = \frac{m_e N_{val}}{m_p N_{coms}}$$

$$\Rightarrow 2\mu - E_c - E_v = \frac{1}{\beta} \ln \left(\frac{m_e N_{val}}{m_p N_{coms}} \right)$$

$$\Rightarrow \mu = \frac{1}{2} (E_c + E_v) + \frac{1}{2\beta} \ln \left(\frac{m_e N_{val}}{m_p N_{coms}} \right)$$

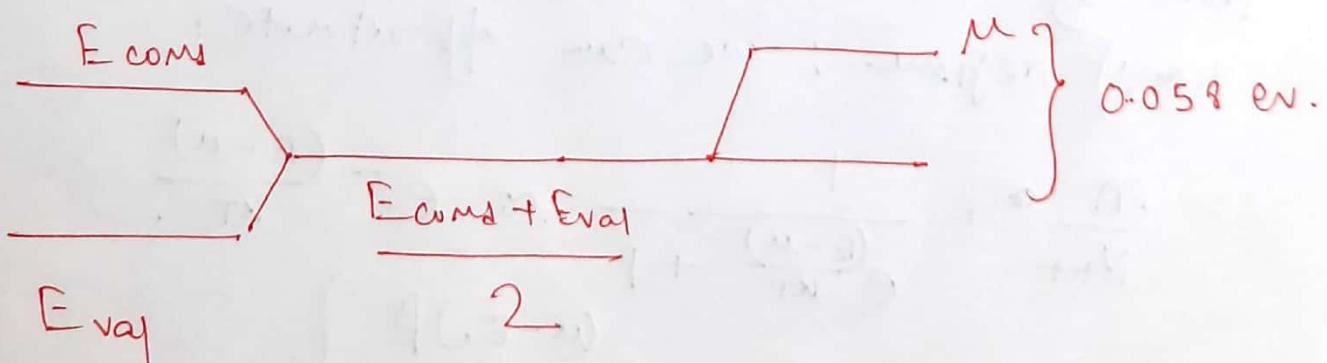
using $T = 300 \text{ K}$; $m_e = m_i + m_{deform}$

$$m_p = m_i + m_{acc}; N_{val} = 7.59 \times 10^{24} \text{ m}^{-3} \text{ (evaluated)}$$

$$N_{coms} = 4.166 \times 10^{23} \text{ m}^{-3}$$

$$\mu = \frac{E_{coms} + E_{val}}{2} + 9.344 \text{ J}$$

$$= \frac{E_{coms} + E_{val}}{2} + 0.058 \text{ ev.}$$



Problem: 3

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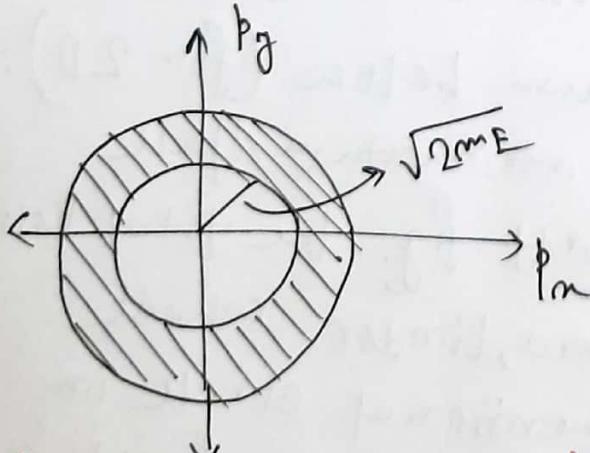
3.a Firstly ignoring spin; I'm going to derive the no of energy states  $n(E)$  in  $d$  dimension in the energy range between  $E$  &  $E+dE$ .

For non-relativistic free particle the  $E-p$  relation will be given by:

$$E = \sum_{i=1}^D \frac{p_i^2}{2m}$$

So for a  $D$ -dimensional case; total no of phase points between the ~~hyperSpheres~~ hyperSpheres satisfying conditions:

$$E + dE \geq \sum_{i=1}^D \frac{p_i^2}{2m} \geq E \quad \text{if the volume between the hyperSpheres divided by the volume of unit cell size.}$$



(fig representing the case of 2-d)

Now in  $d$ -dimension, the sphere of radius  $R$  has the volume:

$$V = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2} + 1)} \cdot R^d$$

Here  $R = \sqrt{2mE}$ ; So we get:

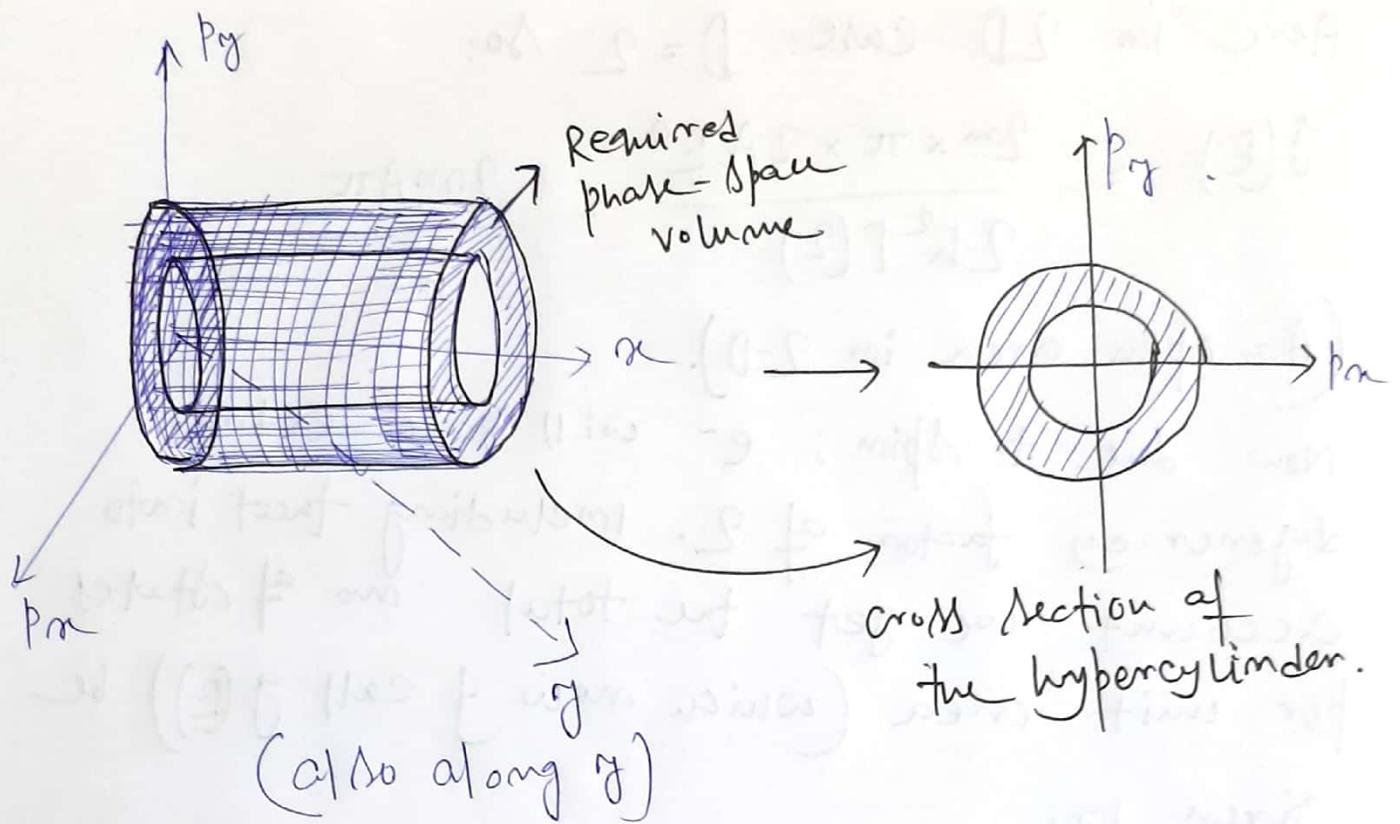
$$\tau = \frac{\pi^{D/2}}{\Gamma(D/2+1)} \cdot (2mE)^{D/2}.$$

$\therefore d\tau = \text{vol between spheres of radius } E \text{ & } E+dE$

$$= \frac{(2m)^{D/2} \pi^{D/2}}{\Gamma(\frac{D}{2}+1)} \cdot \frac{D}{2} E^{\frac{D}{2}-1}$$

As the particles are free we don't need to include the position ~~and~~ coordinates in the previous calculation. It will now be multiplied by a whole factor.

So in the phase space: the total volume (phase space vol) contained in that energy limit is although restricted by those values of momentum ( $p_i D$ ); the total volume is this volume multiplied by the physical volume accessible to the particles. Like I have drawn below (for 2D): the restricted region in momentum space is the shaded region in first fig; the total volume is the 4 dimensional hypercylinder whose cross section is the 2 dimensional circle in p space & other two extensions are freedom along  $x_j$  (position space).



So: total phase space volume  $d\Gamma = V \otimes dE$ .  
 (V is the D dimensional volume of open for the particle.)

$$\therefore d\Gamma = \frac{(2m)^{D/2} \cdot \pi^{D/2} D V E^{D/2}}{2 \Gamma(\frac{D}{2} + 1)} \cdot dE.$$

If the unit cell volume is  $h^D$  ( $h \sim n_i p_i$ )  
 then no of phase points in region  $d\Gamma$

$$= dN(E) = \frac{d\Gamma}{h^{D+1}} = \frac{(2m)^{D/2} \pi^{D/2} D V E^{D/2}}{2 \Gamma(\frac{D}{2} + 1) h^D} dE.$$

So density of states (without spin) in D-dimension

be given by:

$$g(E) = \frac{dN(E)}{dE} = \frac{(2m)^{D/2} \pi^{D/2} D V E^{D/2}}{2 \Gamma(\frac{D}{2} + 1) \cdot h^D}$$

Here in 2D case:  $D=2$  so:

$$g(E) = \frac{2m \times \pi \times 2A E^0}{2h^2 \Gamma(2)} = \frac{2mA\pi}{h^2}$$

( $A$  = open area in 2-D).

Now due to spin;  $e^-$  will have extra degeneracy factor of 2. Including that into account we get the total no of states per unit area (which now I call  $g(E)$ ) be given by:

$$g(E) = \frac{2}{A} \times \frac{2mA\pi}{h^2} = \frac{4mA\pi}{h^2}$$

Proved

3.b. Electron gas in metal follows F-D distribution given by:

$$f(E) = \frac{1}{e^{\frac{E-E_F}{kT}} + 1}$$

If total no of free  $e^-$  be  $N$  then we get:

$$\int_0^{E_F} f(E) \cdot g(E) dE = N.$$

In 3-d  $J(E)$  = density of state =  $\frac{4m\sqrt{m}\pi\sqrt{2}\sqrt{E}}{h^3} \times 2$   
(2 due to spin of  $e^-$ )

Now as  $T \rightarrow 0$  we get  $f(E)$  taking the form:

$$f(E) = 1 \quad E < E_F \\ = 0 \quad \text{otherwise}$$

$$\therefore N = \int_0^{E_F} f(E) g(E) dE = \frac{8m\sqrt{m}\pi v\sqrt{2}}{h^3} \int_0^{E_F} \sqrt{E} dE \\ = \frac{8m\sqrt{m}\pi v\sqrt{2}}{h^3} \cdot \left. \frac{E^{3/2}}{3/2} \right|_0^{E_F} \\ = \frac{2}{3} \times \frac{8m\sqrt{m}\pi v\sqrt{2}}{h^3} E_F^{3/2}.$$

$$\text{So; } E_F = \left( \frac{3h^3}{16m\sqrt{m}\pi v\sqrt{2}} \times \frac{N}{V} \right)^{2/3} \\ = \frac{\hbar^2}{2m} (3PV^2)^{2/3}. \quad \left( P = \frac{N}{V} \right)$$

Now for copper; free electron density (from online) is given by,

$$f = 8.5 \times 10^{28} \text{ m}^{-3}.$$

$$\text{So; } E_F \approx 1.128 \times 10^{-19} \text{ J} \\ = 7.05 \text{ eV.}$$

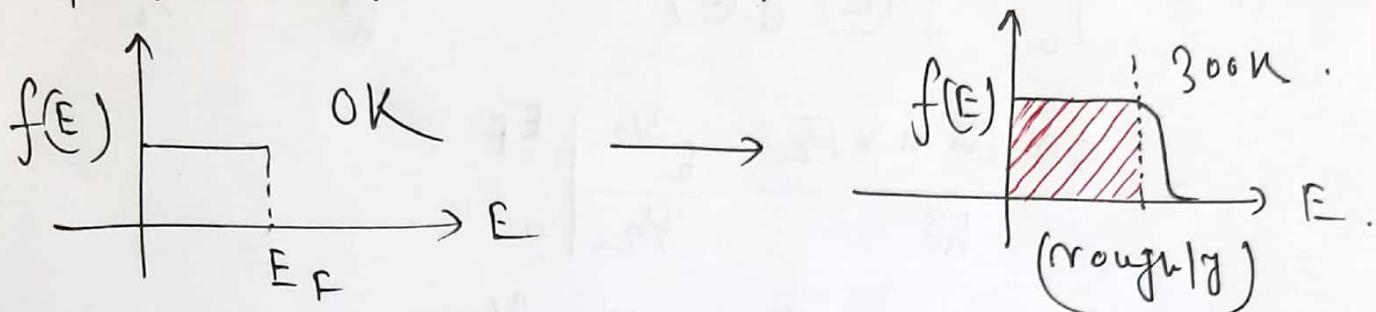
$$\therefore \text{Fermi temperature is given by } T_F = \frac{E_F}{k} \\ = 81748 \text{ K.}$$

which is very higher than room temp.

At room temp avg K.E of e- in copper be

$$\sim \frac{3}{2}kT \text{ i.e. } \sim 0.0308 \text{ ev.}$$

So at room temperature the function  $f(E)$  looks almost similar to the step form (i.e. at 0K)



So the part shaded by red is almost filled up. As  $g(E) \sim \sqrt{E}$ ; so upto a finite  $E$  ( $\sim E_F$ ) all degeneracies are filled by electrons.

$$(\text{i.e. } g(E)f(E) \cdot dE > f(E)dE)$$

So the electron gas in copper lies in degenerate states at room temp.

We can also show this by another way:

$$E_{\text{tot}} = \int_0^{\infty} Ef(E) g(E) dE = \int_0^{\infty} \frac{8\pi m \sqrt{m} \sqrt{2} \sqrt{E} \cdot E}{(e^{\frac{E-E_F}{kT}} + 1) h^3} dE$$

$$\text{Using expression of } E_F = \frac{\hbar^2}{2m} \left( \frac{3\pi^2 N}{V} \right)^{2/3}.$$

we get

$$E_{\text{tot}} = \int_0^{\infty} \frac{8\pi m \sqrt{m} E^{3/2}}{h^3} \times \frac{V}{\exp \left\{ \beta \left( E - \frac{\hbar^2}{2m} \left( \frac{3\pi^2 N}{V} \right)^{2/3} \right) \right\} + 1} dE.$$

Here as I've shown that  $f(E) \sim \text{const}$   $E < E_F$   
 $\sim 0$   $0/\infty$

$$\text{So } E_{\text{tot}} = \int_0^{k_F} \frac{\hbar^2 k^2}{2m} \times \frac{V k^2}{\pi^2} dk \quad \text{as } \infty \left( E = \frac{\hbar^2 k^2}{2m} \right)$$

$$= \frac{\hbar^2 k_F^5 V}{16 m \pi^2} = \frac{\hbar^2}{10 m \pi^2} \cdot \left( 3\pi^2 N_A \right)^{5/3} V^{-2/3}.$$

$$\therefore \frac{dE}{dV} = \frac{\hbar^2}{10 m \pi^2} \times \left( -\frac{2}{3} \right) \times 3\pi^2 \left( \frac{N_A}{V} \right)^{5/3}.$$

but this is the expression of degeneracy pressure  $P$ . ( $P = \frac{\partial E}{\partial V}$ )

$\therefore P$  ( $T = \text{room temp}$  / generally at sufficiently low temp  $T \ll T_F$ )

$$\therefore \sim \frac{\hbar^2}{m} \times P^{5/3}.$$

Using values:  $P \sim 2 \times 10^{10} \text{ N m}^{-2}$ .

which is quite much high.

So it means degeneracy is indeed present here at room temperature

Copper.

(I've not shown the full derivation of degeneracy pressure using complete form of  $f(E)$ .)  
 as it is lengthy and takes too much time  
 w.r.t exam time.

$$\text{So, } \frac{\partial E_{\text{tot}}}{\partial V} = \frac{8\pi m^{3/2}}{h^3} \int_0^\infty \frac{\partial}{\partial V} \frac{V E^{3/2} dE}{\exp\left(\beta\left(E - \frac{\hbar^2 k_F^2}{2m} \left(\frac{3\pi^2 N}{V}\right)^{2/3}\right)\right) + 1}$$

$$= \frac{8\pi m^{3/2}}{h^3} \times \int_0^\infty \frac{-E^{3/2} dE}{1 + \exp(\beta(E - E_F))}$$

$$= \frac{\sqrt{E}^{3/2}}{(1 + \exp(\beta(E - E_F)))^2} \times \beta(E - E_F)$$

$$= \frac{\sqrt{E}^{3/2}}{\beta \times \frac{\hbar^2}{2m} \times (3\pi^2 N)^{2/3} \cdot \left(-\frac{2}{3}\right)} \times (-1) \times V^{-5/3} dE.$$

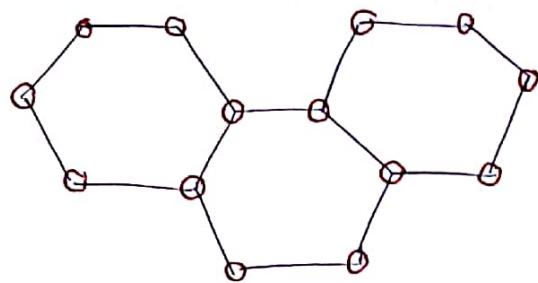
$$= \frac{8\pi m^{3/2}}{h^3} \left\{ \int_0^\infty \frac{E^{3/2} dE}{1 + e^{\beta(E - E_F)}} \right\}$$

$$= \frac{2}{3} \frac{\beta \hbar^2}{2m} \times (3\pi^2 N)^{2/3} \sqrt{-\frac{2}{3}} \int_0^\infty \frac{E^{3/2} e^{\beta(E - E_F)}}{(1 + e^{\beta(E - E_F)})^2} dE$$

Now,  $E = \frac{\hbar^2 k^2}{2m}$ ;  $\therefore k_F = \frac{\sqrt{E_F \times 2m}}{\hbar}$ .

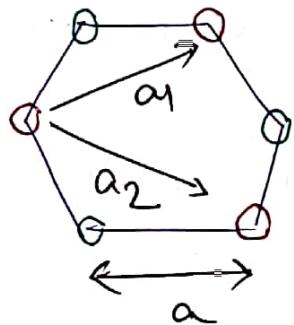
$$\therefore g(k) \Rightarrow f(E) \Rightarrow G(k) = \frac{V}{\pi^{1/2}} k^2 dk$$

### 3.c Energy band in Graphene with tight binding:-



Graphene is effectively a 2-dimensional honeycomb structure of Carbon atoms. From

fig we can see the lattice is not Bravais. The primitive lattice vectors are given by:

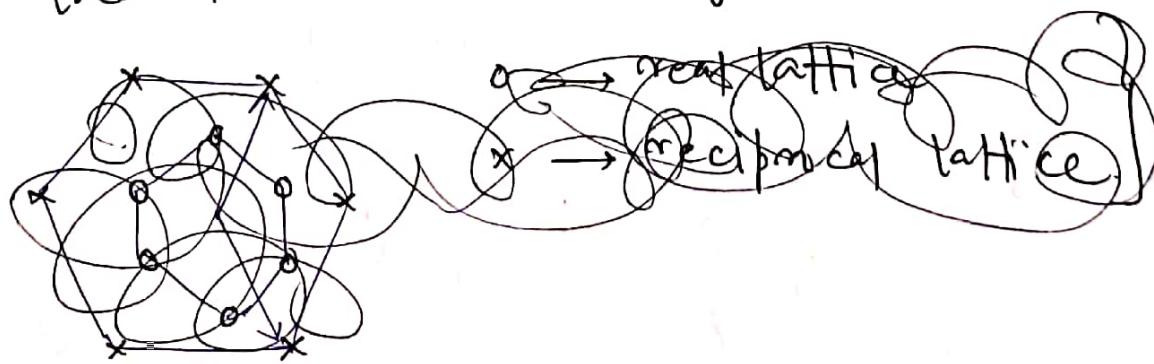


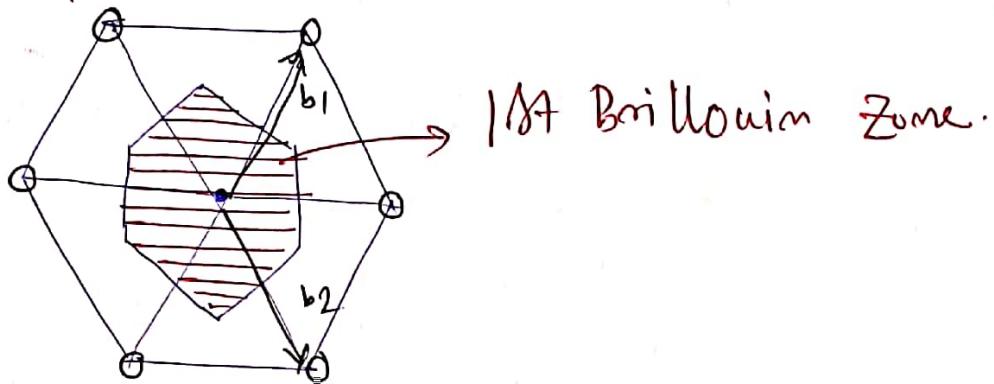
$$\left. \begin{aligned} \mathbf{a}_1 &= \frac{a\sqrt{3}}{2} (\sqrt{3}, 1) \\ \mathbf{a}_2 &= \frac{a\sqrt{3}}{2} (\sqrt{3}, -1) \end{aligned} \right\} \begin{array}{l} \text{using} \\ \text{law of} \\ \text{triangle.} \end{array}$$

Clearly the reciprocal vectors in 2-d be given by (using  $a_{ij} = 2\pi\delta_{ij}$ )

$$\mathbf{b}_1 = \frac{2\pi}{3a} (1, \sqrt{3}) ; \mathbf{b}_2 = \frac{2\pi}{3a} (1, -\sqrt{3})$$

So if we draw the reciprocal lattice then it will be given by:





1st Brillouin Zone.

If the hopping parameter is given by  $t$ ; then the tight binding Hamiltonian is given by, the interaction between nearest neighbours.

~~Bravais~~ However here as the lattice is not Bravais; there are two effective triangular lattice & hence the nearest neighbour of one A lattice point is another B lattice point.

So the Hamiltonian is given by,

$$H = -t \sum \left( |\vec{a}_A \times \vec{a}_B| + |\vec{a}_A \times \vec{a} + \vec{a}_1, B| + |\vec{a}_A \times \vec{a} + \vec{a}_2, B| + h.c \right) + E_0 |\vec{a} \times \vec{a}|$$

Now as the energy eigenstates are plain waves; but they are common to A & B so by intuition the state be given by:

The energy eigenstates are

$$|\Psi(\vec{k})\rangle = \frac{1}{\sqrt{A}} \sum_{\vec{a}} e^{i\vec{k} \cdot \vec{a}} (g_1 |\vec{a}, A\rangle + g_2 |\vec{a}, B\rangle)$$

Now over  $N$  cells there will be  $2N$  sites due to A & B type lattice.

Plugging  $|\psi(\mathbf{k})\rangle$  in Schrodinger eq we get:

$$H |\psi(\mathbf{k})\rangle = E(\mathbf{k}) |\psi(\mathbf{k})\rangle$$

On the left hand side

But using the expression of  $|\psi(\mathbf{k})\rangle$  we get the elements of  $\hat{H}$  be given by,

$$H_{11} = \langle \alpha_A | H | \alpha_A \rangle$$

In  $\hat{H}$  there is no term like  $|\alpha_A \times \alpha_A\rangle$

$$\text{So } H_{11} = 0.$$

$$\begin{aligned}
 H_{11,22} &= \sum_{\mathbf{m} \in \mathbb{Z}^2} \left( \langle \vec{\alpha}_A | \vec{\alpha}_A \times \vec{\alpha}_B | \vec{\alpha}_B \rangle + \right. \\
 &\quad \left. \langle \vec{\alpha}_A | \vec{\alpha}_A \times \vec{\alpha}_{A+\vec{a}_1, B} | \vec{\alpha}_B \rangle + \right. \\
 &\quad \left. \langle \vec{\alpha}_A | \vec{\alpha}_A \times \vec{\alpha}_{A+\vec{a}_2, B} | \vec{\alpha}_B \rangle + \right. \\
 &\quad \left. \langle \vec{\alpha}_A | \vec{\alpha}_B \times \underbrace{\vec{\alpha}_A}_{e^{i\vec{k} \cdot \vec{a}_1}} | \vec{\alpha}_B \rangle + \right. \\
 &\quad \left. \langle \vec{\alpha}_A | \vec{\alpha}_B \times \underbrace{\vec{\alpha}_A}_{e^{i\vec{k} \cdot \vec{a}_2}} | \vec{\alpha}_B \rangle + \right. \\
 &\quad \left. \langle \vec{\alpha}_A | \vec{\alpha}_B \times \underbrace{\vec{\alpha}_A}_{0} | \vec{\alpha}_B \rangle + \right. \\
 &\quad \left. \langle \vec{\alpha}_A | \vec{\alpha}_{A+\vec{a}_1, B} \times \underbrace{\vec{\alpha}_A}_{0} | \vec{\alpha}_B \rangle \right) \\
 &\quad + \langle \vec{\alpha}_A | \vec{\alpha}_{A+\vec{a}_2, B} \times \underbrace{\vec{\alpha}_A}_{0} | \vec{\alpha}_B \rangle
 \end{aligned}$$

$$\text{So } H_{12} = -t (1 + e^{i\vec{k}_0 \cdot \vec{\alpha}_1} + e^{i\vec{k}_0 \cdot \vec{\alpha}_2}) = \alpha \text{ (let)}$$

(I've used  $\langle \vec{r}_1, \alpha | \vec{r}_2, \beta \rangle = \delta_{\alpha\beta}$   
in this case  $\alpha, \beta = [A, B]$ )

by similar reason of (1):  $H_{22} = 0$

$$\therefore H_{21} = \alpha^*$$

$$\therefore \hat{H} = \begin{pmatrix} 0 & \alpha \\ \alpha^* & 0 \end{pmatrix} |\vec{\alpha} A\rangle \\ |\vec{\alpha} B\rangle \\ \langle \vec{\alpha} A| \langle \vec{\alpha} B|$$

Ans Schrodinger eq gives:

$$\begin{pmatrix} 0 & \alpha \\ \alpha^* & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \dots (2)$$

(clearly without hopping we would get)  
 $H = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

Solving for  $E$  we get:

$$\det \begin{vmatrix} -E & \alpha \\ \alpha^* & -E \end{vmatrix} = 0$$

$$\Rightarrow E = \alpha\alpha^* = |\alpha|^2 = t^2 \left(1 + e^{i\vec{k} \cdot \vec{\alpha}_1} + e^{i\vec{k} \cdot \vec{\alpha}_2}\right)^2$$

~~∴ E^2 = t^2 | 1 + e^{i \frac{3}{2} k\_m a} \cdot e^{i \frac{\sqrt{3}}{2} k\_g a} + e^{i \frac{3}{2} k\_m a} \cdot e^{-i \frac{\sqrt{3}}{2} k\_g a} |^2~~

$$\therefore E^2 = t^2 \left| 1 + e^{i \frac{3}{2} k_m a} \cdot e^{i \frac{\sqrt{3}}{2} k_g a} + e^{i \frac{3}{2} k_m a} \cdot e^{-i \frac{\sqrt{3}}{2} k_g a} \right|^2 \\ = t^2 \left| 1 + 2e^{\frac{3i k_m a}{2}} \left( \frac{e^{i \frac{\sqrt{3}}{2} k_g a} + e^{-i \frac{\sqrt{3}}{2} k_g a}}{2} \right) \right|^2.$$

$$= t^2 \left| 1 + 2e^{\frac{3i k_m a}{2}} \cos \left( \frac{k_g \sqrt{3} a}{2} \right) \right|^2.$$

$$= t^2 \left| 1 + 2 \cos \left( \frac{3k_m a}{2} \right) \cos \left( \frac{\sqrt{3} a k_g}{2} \right) + 2i \sin \left( \frac{3k_m a}{2} \right) \cos \left( \frac{\sqrt{3} a k_g}{2} \right) \right|^2.$$

$$= t^2 \left| \left( 1 + 2 \cos \left( \frac{3k_m a}{2} \right) \cos \left( \frac{\sqrt{3} a k_g}{2} \right) \right)^2 + 4 \sin^2 \left( \frac{3k_m a}{2} \right) \cos^2 \left( \frac{a \sqrt{3} k_g}{2} \right) \right|$$

$$= t^2 \left( 1 + 4 \cos^2 \left( \frac{\sqrt{3} a k_g}{2} \right) + 4 \cos \left( \frac{3k_m a}{2} \right) \cos \left( \frac{\sqrt{3} k_g a}{2} \right) \right)$$

i.e.  $E = \pm \sqrt{t \left( 1 + 4 \cos^2 \left( \frac{\sqrt{3} a k_g}{2} \right) + 4 \cos \left( \frac{3k_m a}{2} \right) \cos \left( \frac{\sqrt{3} k_g a}{2} \right) \right)}$

Ans

Problem :- I

a. Given that the system only has two energy states with energy values  $\Delta \neq 0$ .

The partition function is given by:  $Z = \sum_E e^{-\beta E}$

$$\text{So Here, } Z = e^{-\beta \Delta} + e^{\beta \Delta} = 2 \cosh(\beta \Delta)$$

So the internal energy of the system is given

$$\text{by: } U = -\frac{\partial}{\partial \beta} (\ln Z) = -\frac{\partial}{\partial \beta} (\ln 2 + \ln(\cosh(\beta \Delta)))$$

$$= -\Delta \frac{\sinh(\beta \Delta)}{\cosh(\beta \Delta)} = -\Delta \tanh(\beta \Delta).$$

$$\therefore U = -\Delta \tanh\left(\frac{\Delta}{kT}\right) \quad \underline{\text{proved}}$$

$$\text{The specific heat is } C = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \left( -\Delta \tanh\left(\frac{\Delta}{kT}\right) \right)$$

$$= -\Delta \cdot \operatorname{Sech}^2\left(\frac{\Delta}{kT}\right) \cdot \left(-\frac{\Delta}{kT^2}\right)$$

$$\Rightarrow C = \left(\frac{\Delta}{kT}\right)^2 \times k \operatorname{Sech}^2\left(\frac{\Delta}{kT}\right) \quad \underline{\text{proved}}$$

b. This can be done by 2 methods:

i) for the given system,

$\Delta$  values are equally likely up to some upper bound  $\Delta_0$ .

So the density of state is given by,

$$g(\epsilon) = \begin{cases} \text{constant} & \epsilon < \epsilon_0 \\ 0 & \text{o.w.} \end{cases}$$

Assuming the system to be classical we get  
take  $f(E) \sim e^{-\beta E}$ .

$$\begin{aligned} \therefore E_{\text{total}} &= \int_0^{\infty} E f(E) g(E) dE \\ &= A \int_0^{\epsilon_0} \epsilon e^{-\beta \epsilon} d\epsilon \quad \left( \begin{array}{l} A \text{ is some} \\ \text{normalization} \\ \text{const} \end{array} \right) \\ &= A \cdot \left[ -\frac{e^{-\beta \epsilon} (1 + \beta \epsilon)}{\beta^2} \right]_0^{\epsilon_0} \\ &= \frac{A}{\beta^2} [1 - e^{-\beta \epsilon_0} (1 + \beta \epsilon_0)] \end{aligned}$$

As given:  $\beta \epsilon_0 \gg kT$  i.e.  $\frac{\epsilon_0}{kT} = \beta \epsilon_0 \gg 1$

So we assume  $e^{-\beta \epsilon_0} \approx 0$ .

$$\therefore E_{\text{total}} = \frac{A}{\beta^2} (1 - 0) = \frac{A \beta}{\beta^2} = A' T^2.$$

$$\therefore C = \frac{\partial E_{\text{total}}}{\partial T} = 2A' T. \quad (\text{for some const } A')$$

$$\boxed{C \propto T}$$

Proved

Method: 2

From the result of part 2(a) if we integrate from the result of part 2(a) if we integrate over  $\Delta$  from 0 to  $\Delta_0$  for the whole sample with weight factor A (= const as given) then the specific heat becomes:

$$C = \int_0^{\Delta_0} A \frac{\Delta^2}{kT^2} \operatorname{sech}^2\left(\frac{\Delta}{kT}\right) d\Delta.$$

$$= \frac{A}{kT^2} \int_0^{\Delta_0} \Delta^2 \operatorname{sech}^2\left(\frac{\Delta}{kT}\right) d\Delta.$$

but substituting  $\frac{\Delta}{kT} = x$  i.e  $d\Delta = dx \cdot kT$

$$C = \frac{A}{kT^2} \cdot \int_0^{\Delta_0/kT} x^2 \operatorname{sech}^2(x) \cdot kT \cdot dx$$

$$= Ak^2 T \int_0^{\Delta_0/kT} x^2 \operatorname{sech}^2(x) dx$$

but  $kT \ll \Delta_0 \Rightarrow \frac{\Delta_0}{kT} \rightarrow \infty$ . So we get:

$$C = Ak^2 T \int_0^{\infty} x^2 \operatorname{sech}^2(x) dx$$

using mathematica-

$$= Ak^2 T \times \frac{\pi^2}{12}$$

So  $C \propto T$

Ans

L.C for A cold Solid; the Specific ~~heat~~ heat is calculated in two ways.

# 1) Sommerfeld model:-

According to Sommerfeld; the e- are free in metal & they follow F-D distn.

In that context the total energy & No of e- in the metal be given by:

$$E_{\text{tot}} = \int_0^{\infty} E g(E) f(E) dE \quad \left. \begin{array}{l} g(E) = \frac{4m\sqrt{m}\pi\sqrt{2}}{h^3} \times 2\sqrt{E} \\ f(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \end{array} \right\}$$

$$N_{\text{tot}} = \int_0^{\infty} g(E) f(E) dE \quad \left. \begin{array}{l} g(E) = \frac{4m\sqrt{m}\pi\sqrt{2}}{h^3} \times 2\sqrt{E} \\ f(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \end{array} \right\}$$

$$E_{\text{tot}} = 2 \int_0^{\infty} \frac{4m\sqrt{m}\pi\sqrt{2} E^{3/2}}{e^{\beta(E-\mu)} - 1} dE \quad \left. \begin{array}{l} g(E) = \frac{4m\sqrt{m}\pi\sqrt{2}}{h^3} \times 2\sqrt{E} \\ f(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \end{array} \right\}$$

$$N_{\text{tot}} = 2 \int_0^{\infty} \frac{4m\sqrt{m}\pi\sqrt{2} E^{1/2}}{e^{\beta(E-\mu)} - 1} dE \quad \left. \begin{array}{l} g(E) = \frac{4m\sqrt{m}\pi\sqrt{2}}{h^3} \times 2\sqrt{E} \\ f(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \end{array} \right\}$$

After some algebra the two expression reduces to:

$$\left. \begin{array}{l} E_{\text{tot}} = \frac{3KT\pi}{\lambda^3 \beta} f_{5/2}(z) \\ N_{\text{tot}} = \frac{2\pi}{\lambda^3} f_{3/2}(z) \end{array} \right\} \quad \left. \begin{array}{l} \lambda = \frac{h}{\sqrt{2\pi m k T}} \\ f_n(z) = \frac{1}{\Gamma(n)} \int_0^{\infty} x^{n-1} e^{-x} dx \\ z = e^{\beta(E-\mu)} \end{array} \right\}$$

$$\text{Now, } f_m(z) = \frac{1}{\Gamma(m)} \int_0^{\infty} \frac{x^{m-1} dx}{z^m e^x + 1}$$

$$\Rightarrow \Gamma(m) f_m(z) = \int_0^{\infty} \frac{x^{m-1} dx}{z^m e^x + 1} = \int_0^{\infty} + \int_{\infty}^{\infty} \frac{x^{m-1} dx}{z^m e^x + 1}$$

$$\begin{aligned}
 f_m(z) \Gamma(m) &= \int_0^{\beta m} x^{m-1} \left(1 - \frac{1}{1+ze^{-x}}\right) dx \\
 &\quad + \int_{\beta m}^{\infty} \frac{x^{m-1}}{z^m e^{m+x}} dx \\
 &= \frac{(\log z)^m}{m} - \int_0^{\beta m} \frac{x^{m-1}}{1+ze^{-x}} dx + \int_{\beta m}^{\infty} \frac{x^{m-1} dx}{z^m e^{m+x}}
 \end{aligned}$$

Substituting  $\eta_1 = \beta m - x$  in 1st integral }  
 $\eta_2 = x - \beta m$  in 2nd }

$$\begin{aligned}
 f_m(z) \Gamma(m) &= \frac{(\ln z)^m}{m} - \int_0^{\beta m} \frac{(\beta m - \eta_1)^{m-1}}{1+e^{\eta_1}} d\eta_1 \\
 &\quad + \int_0^{\infty} \frac{(\beta m + \eta_2)^{m-1}}{1+e^{\eta_2}} d\eta_2
 \end{aligned}$$

(using approximation  $\beta m \gg 1$ )

$$\begin{aligned}
 &= \frac{(\ln z)^m}{m} + \int_0^{\infty} \frac{(\beta m + \eta)^{m-1} - (\beta m - \eta)^{m-1}}{1+e^{\eta}} d\eta
 \end{aligned}$$

Using Taylor expansion:

$$\begin{aligned}
 (\beta m + \eta)^{m-1} - (\beta m - \eta)^{m-1} &\approx (\beta m)^{m-1} \left[ \left(1 + \frac{\eta}{\beta m}\right)^{m-1} - \left(1 - \frac{\eta}{\beta m}\right)^{m-1} \right] \\
 &\approx (\beta m)^{m-1} \left\{ 1 + (m-1) \frac{\eta}{\beta m} - 1 + (m-1) \frac{\eta}{\beta m} \right\} \\
 &\approx 2(m-1)\eta (\beta m)^{m-2}.
 \end{aligned}$$

$$\text{So, } f_m(z) \Gamma(m) = \frac{(\ln z)^m}{m} + 2(m-1)(\ln z)^{m-2} \int_0^\infty \frac{\eta}{e^{\eta} + 1} d\eta$$

$$\begin{aligned} \text{But } \int_0^\infty \frac{\eta}{1+e^\eta} d\eta &= \int_0^\infty \frac{d\eta e^{-\eta}}{1+e^{-\eta}} \\ &= \int_0^\infty \eta \sum_{m=1}^\infty e^{-\eta m} \cdot (\Gamma)^{m+1} d\eta \\ &= \sum_{m=1}^\infty (\Gamma)^{m+1} \int_0^\infty \eta e^{-\eta m} d\eta \\ &= \sum_{m=1}^\infty \frac{(\Gamma)^{m+1}}{m^2} \int_0^\infty u e^{-u} du \\ &\quad \downarrow = 1. \end{aligned}$$

$$2 \sum_{m=1}^\infty \frac{(\Gamma)^{m+1}}{m^2} = 1 - \frac{1}{2^2} + \frac{1}{3^2} - \dots$$

$$= \left( 1 + \frac{1}{2^2} + \dots \right) - 2 \left( \frac{1}{2^2} + \frac{1}{4^2} + \dots \right)$$

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

$$= \left( 1 - \frac{1}{2} \right) \cdot \Gamma(2) = \frac{1}{2} \cdot \frac{\pi^2}{6} = \frac{\pi^2}{12}.$$

$$\text{So: } f_m(z) \approx \frac{(\ln z)^m}{\Gamma(m+1)} \left\{ 1 + \frac{\pi^2 m(m-1)}{c (\ln z)^2} + \dots \right\}$$

Using the expression:

$$E \approx \frac{V}{5\pi^2 h^3} (2m)^{3/2} \mu^{5/2} \left( 1 + \frac{5\pi^2}{8} \cdot \left( \frac{K_B T}{\mu} \right)^2 + \dots \right)$$

$$f N \approx \frac{V}{3\pi^2 h^3} (2m\mu)^{3/2} \left( 1 + \frac{\pi^2}{8} \left( \frac{K_B T}{\mu} \right)^2 + \dots \right)$$

~~Now I compute  $E$  by inverting denominator  
series expansion by using mathematica. That gives:~~

$$E = \frac{1}{5\pi^2 h^3} (2m)^{3/2} \mu^{5/2} \left( 1 + \frac{5\pi^2}{81} \left( \frac{k_B T}{\mu} \right)^2 \right)$$

$$\text{Now } N = \int_0^\infty f(E) g(E) dE \quad | \text{ at } T = 0$$

$$= \frac{8\pi m \sqrt{m} \sqrt{\pi} \sqrt{2}}{h^3} \int_0^{E_F} \sqrt{E} dE$$

$$= \frac{8\pi m \sqrt{m} \sqrt{\pi} \sqrt{2}}{h^3} \cdot E_F^{3/2} \cdot \frac{2}{3}$$

$$\text{So; } E_F = \frac{h^2}{2m} \left( \frac{3N\pi^2}{V} \right)^{2/3}$$

Using this we get:

(Using mathematica for long algebra)  
(taken series expansion upto 2nd order)

$$\mu = E_F \left( 1 - \frac{\pi^2}{12} \left( \frac{k_B T}{E_F} \right)^2 + \dots \right)$$

Now I have calculated  $\frac{E}{N}$

from the above expression & replaced  $\mu$  by the expansion term in  $E_F$ .

All calculation has been done in  
mathematica & upto 2nd order correction.

$$\frac{E}{N} \approx \frac{3E_F}{5} \left( 1 + \frac{5\pi^2}{12} \left( \frac{K_B T}{E_F} \right)^2 + \dots \right)$$

As  $E_F = \text{const of temp}$ .

So,

$$C_v^e = \left( \frac{\partial E}{\partial T} \right)_{N,V} = \frac{3E_F N}{5} \cdot \frac{5\pi^2}{12} \cdot \frac{2K_B^2 T}{E_F^2}$$

$$= \frac{\pi^2}{2} \cdot N K_B^2 \cdot \frac{T}{E_F}$$

ii) Debye model of phonons:-  
 According to Debye model; the phonons are like bottom & they carry energy according to the formula  $E = \text{thv}$ :  
 Now there are three modes of vibration (one longitudinal; two transverse) so the density fm of phonon be:

$$g(\omega) = 4\pi N \left( \frac{1}{c_L^3} + \frac{2}{c_T^3} \right) \frac{\omega^2 dw}{4\pi^2 \times 2\pi} \quad x$$

$$(x = \frac{N}{2\pi^2} \frac{\omega^2 dw}{\cancel{\omega^2}})$$

$\therefore$  Total energy of the phonon mode be given by:

$$E = \int_0^{\omega_p} f(\omega) \cdot g(\omega) \cdot \text{thv} dw$$

$$f(\omega) = \frac{1}{e^{\beta \text{thv}}} \quad \text{for phonon of } \cancel{\text{bottom}} \text{ they are bottom.}$$

$$\therefore E = \frac{N \times x}{2\pi^2} \int_0^{\omega_p} \frac{\omega^2 \text{thv}^3 dw}{e^{\beta \text{thv}} - 1}$$

here  $\omega_p$  is the limit given by debye

$$\text{as: } \int_0^{\omega_p} g(\omega) dw = 3N_A \quad (\text{for 1 mole})$$

which gives

$$\omega_D = 2\pi \cdot \left\{ \frac{9N_A}{4\pi v \left( \frac{1}{C_l^3} + \frac{2}{C_h^3} \right)} \right\}^{1/3} \sim \frac{N_A^{1/3} C_{\text{solid}}}{v^{1/3}}$$

however;  $E = \frac{V \times X}{2\pi^2} \int_0^{T_D/T} \frac{\alpha^3 K^3 T^3}{h^3} \cdot \frac{KT}{h} \frac{d\alpha}{e^\alpha - 1}$

$\Rightarrow \left( \frac{\hbar\omega}{KT} = \alpha; \quad T_D = \frac{\hbar\omega_D}{K} \right)$

$$\Rightarrow E = \frac{V \times (KT)^4}{2\pi^2 h^3} \int_0^{T_D/T} \frac{\alpha^3 d\alpha}{e^\alpha - 1}$$

Now the  $T^3$  law which comes from Debye  
law is ~~not~~ valid for low temp. Here.

$$\omega_D \sim \frac{N_A^{1/3} C_{\text{solid}}}{v^{1/3}} \text{ which is pretty big.}$$

but the exponential makes the integrand very  
small at large enough  $\omega$ .

$\therefore$  we can take (for cold solid)  $T_D/T \gg 1$   
i.e.  $T \ll T_D$  and the limit to be infinite.

$$\therefore E = \frac{V \times (KT)^4}{2\pi^2 h^3} \int_0^\infty \frac{\alpha^3 d\alpha}{e^\alpha - 1}$$

$$= \frac{V \times (KT)^4}{2\pi^2 h^3} \cdot \frac{\pi^4}{15}$$

So the Specific heat will be given by:

$$C_V = \frac{\partial E}{\partial T} = \frac{4V\pi^2 \times K_B T^3}{30 h^3}$$

So in general; we conclude that specific heat  $C$  can depend on ~~the~~ temperature by:

$$C = \alpha T + \beta T^3$$

↓

from Sommerfeld theory of free  $e^-$       → from Debye's theory of phonon.

For  $e^-$ ; no of free  $e^-$  is higher & hence  $\alpha$  is sufficiently large. (In insulator) On the other hand  $\beta$  is larger & phonon are predominant.

(As  $e^-$  are not free so their vibration mode or phonon mode is the only energy contributor in that case.)

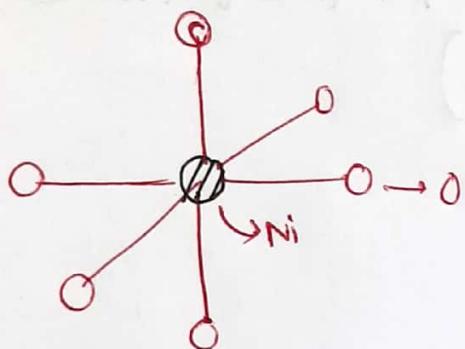
Here the material shows linear behaviour but still it is insulator.

At low temp insulating phase exhibits a finite energy gap  $E_F$ . The electron ~~corr~~ correlation of transition metal oxide (here  $Mn$  is transition metal) in different dimension is strong. So electron correlation plays a significant role in determining the thermal properties (or other) of such materials in lower ~~excited~~ excited state.

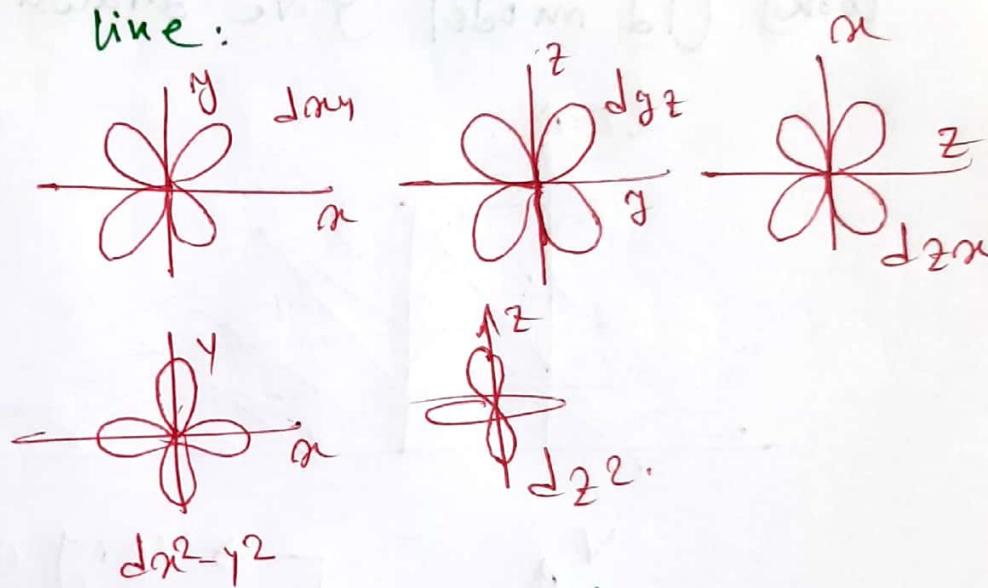
Answer

5.a. Ni is a d-element with e<sup>-</sup> configuration  
 $\rightarrow 4d^2 3d^8$ .

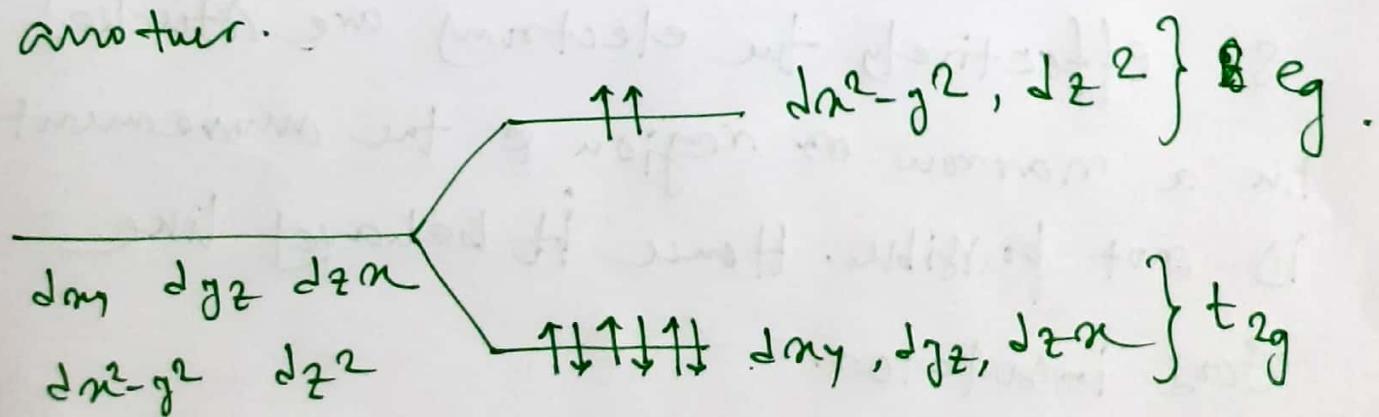
Now  $\text{NiO}$  has the same structure like  
 Nacl. 1 Ni atom is surrounded by 6 O atoms  
 from 6 faces of cube.



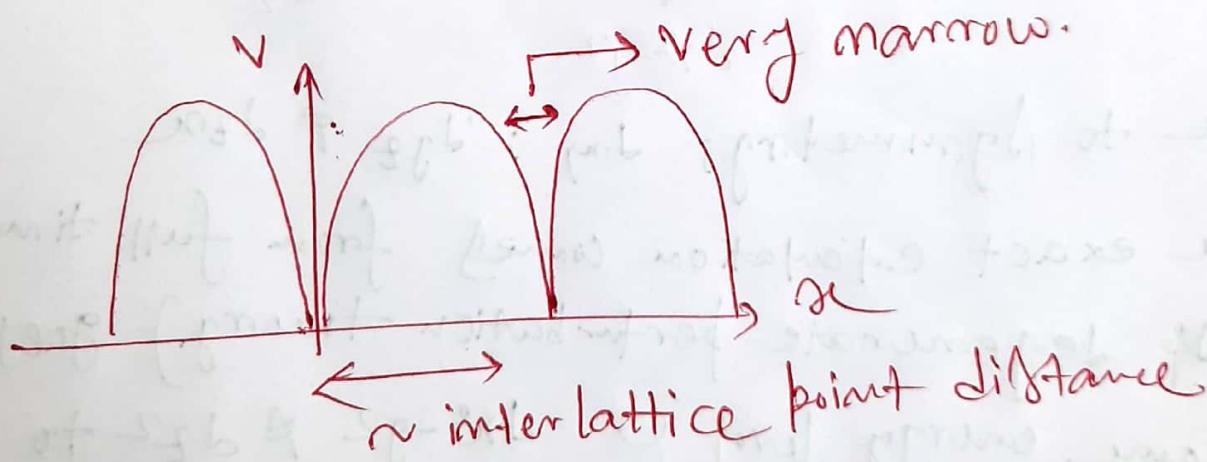
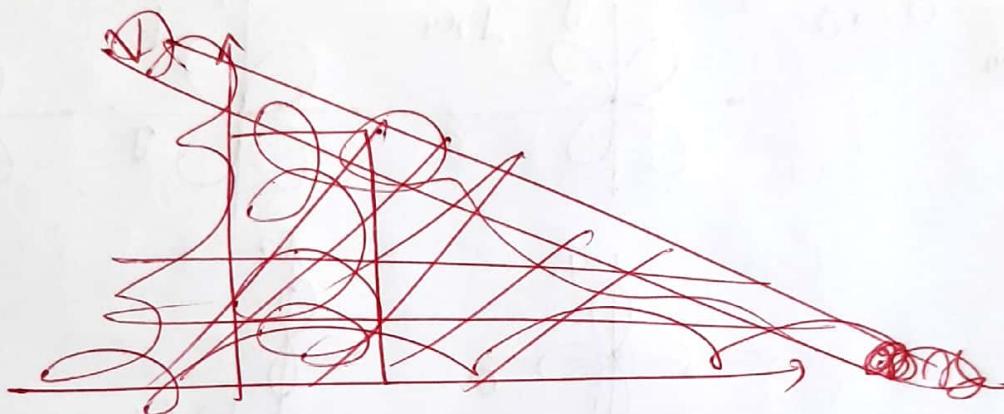
Now the d orbital looks like:



due to  $\Delta$  symmetry;  $d_{xy}$ ;  $d_{yz} \neq d_{zx}$   
 (The exact calculation comes from full time  
 inst degenerate perturbation theory.) goes  
 to some energy level  $\otimes$   $d_{x^2-y^2} \neq d_{z^2}$  to  
 another.



5.b NiO is a MOTT insulator. In NiO (for other MOTT) the electron repulsion is quite high (~~electrostatic~~  $V_{\text{Coulomb}}$  interaction  $\sim 10 \text{ eV}$ ) which stops the movement of electrons. i.e. the effective potential in the lattice looks (1d model I've drawn;)



So effectively the electrons are stucked in a narrow ~~as~~ region & the movement is not possible. Hence it behaves like good insulator.