Solid State Assignment - 2

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1. Kohn Anomaly:—

The dispersion relation is given by:

$$w^2 = \frac{2}{M} \sum_{p>0}' C_p \left(1 - \cos pka\right)$$

but $C_p = A \dfrac{\sin pk_0 a}{pa}$

$$\therefore w^2 = \frac{2A}{Ma} \sum_{p>0}' \frac{\sin pk_0 a}{p} \left(1 - \cos pka\right) \quad \cdots (1)$$

Now we get

$$\sum_{m>0} \frac{\sin ma}{m} = \sum_{m>0} \frac{e^{ima} - e^{-ima}}{2im}$$

$$= \frac{1}{2i} \left\{ \sum_{m>0} \frac{e^{ima}}{m} - \sum_{m>0} \frac{e^{-ima}}{m} \right\}$$

$$= \frac{1}{2i} \left[\left\{ e^{ia} + \frac{(e^{ia})^2}{2} + \frac{(e^{ia})^3}{3} + \cdots \right\} - \left\{ e^{-ia} + \frac{(e^{-ia})^2}{2} + \frac{(e^{-ia})^3}{3} + \cdots \right\} \right]$$

$$= \frac{1}{2i} \left[\ln\left(1 - e^{ia}\right) - \ln\left(1 - e^{-ia}\right) \right]$$

[using $\ln(1+z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots$
for $|z| \leqslant 1$ & here $z = e^{ia}$ & $|e^{ia}| = 1$]

$$= \frac{1}{2i} \ln\left(\frac{1-e^{ia}}{1-e^{-ia}}\right)$$

$$= \frac{1}{2i} \ln\left\{\frac{e^{ia}(e^{-ia}-1)}{(1-e^{-ia})}\right\} = \frac{1}{2i} \ln\left(-e^{ia}\right)$$

$$= \frac{1}{2i} \left\{ \ln(e^{ia}) + \ln(-1) \right\}$$

Using the principle value of $\ln(-1) = e^{i\pi}$:

$$w^2 = \frac{1}{2i} \left\{ ia + i\pi \right\} = \frac{a+\pi}{2}.$$

So from (1):

$$w^2 = \cancel{} \frac{2A}{Ma}\left[\frac{k_0 a + \pi}{2} + \sum_{p>0} \frac{\sin pk_0 a \cos pka}{p}\right] \quad \cdots (2)$$

The second sum be given by:

$$\sum_{p>0} \frac{\sin(pk_0 a)\cos(pka)}{p} = S \text{ (let)}$$

$$= \sum_{p>0} \left(\frac{e^{ipk_0 a} - e^{-ipk_0 a}}{2ip}\right)\left(\frac{e^{ipk_0 a} + e^{-ipka}}{2}\right)$$

$$= \frac{1}{4i}\left\{ \sum_{p>0} \frac{e^{ip(k+k_0)a}}{p} + \sum_{p>0} \frac{e^{ip(k_0-k)a}}{p} + \sum_{p>0} \frac{e^{ip(k-k_0)a}}{p} + \sum_{p>0} \frac{e^{-ip(k+k_0)a}}{p} \right\}$$

Using the previous calculation we get:

$$S = \frac{1}{4i}\Big[\ln\left(1-e^{i(k+k_0)a}\right) + \ln\left(1-e^{i(k_0-k)a}\right)$$
$$- \ln\left(1-e^{i(k-k_0)a}\right) - \ln\left(1-e^{-i(k+k_0)a}\right)\Big].$$

$$= \frac{1}{4i}\ln\left\{\frac{\left(1-e^{i(k+k_0)a}\right)\cdot\left(1-e^{i(k_0-k)a}\right)}{\left(1-e^{i(k-k_0)a}\right)\cdot\left(1-e^{-i(k+k_0)a}\right)}\right\}.$$

$$= \frac{1}{4i}\ln\left\{\frac{e^{i(k+k_0)a}\cdot e^{i(k_0-k)a}\left(e^{-i(k+k_0)a}-1\right)\left(e^{i(k-k_0)a}-1\right)}{\left(1-e^{-i(k+k_0)a}\right)\left(1-e^{i(k-k_0)a}\right)}\right\}$$

clearly at $k \neq k_0$ the value of S is given by:

$$S\Big|_{k\neq k_0} = \frac{1}{4i}\ln\left\{e^{ia(k+k_0+k_0-k)} \times (-1)\times(-1)\right\}.$$

$$= \frac{1}{4i}\ln\left(e^{2iak_0}\right) = \frac{2iak_0}{4i} = \frac{ak_0}{2}.$$

So at $k \neq k_0$ the term

$$S = \frac{a+k_0}{2}.$$

at $k = k_0$: $S = \sum \frac{\sin(pk_0a)\cos(pk_0a)}{p}.$

$$= \frac{1}{2}\sum \frac{\sin(2pk_0a)}{p}.$$

Using previous result:

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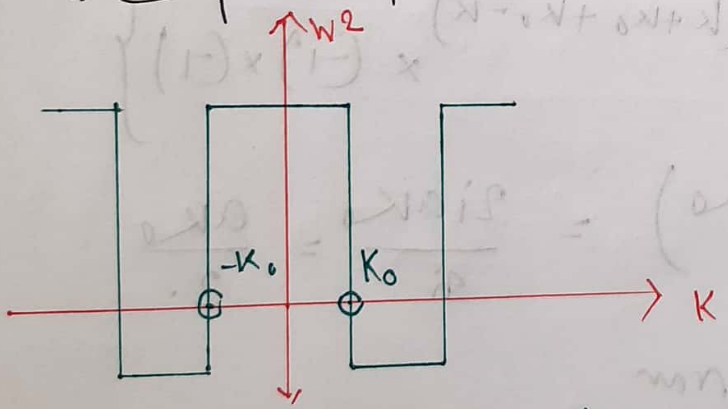
$$S\big|_{k=k_0} = \frac{1}{2}\left(\frac{\pi + 2k_0 a}{2}\right)$$

$$\therefore\ W^2 = \frac{2A}{Ma}\left[\frac{\pi + k_0 a}{2} + \frac{k_0 a}{2}\right] \quad k \neq k_0$$

$$= \frac{2A}{Ma}\left[\frac{\pi + k_0 a}{2} + \frac{k_0 a}{2} + \frac{\pi}{2}\right] \quad k = k_0.$$

So there is a vertical tangent at $k = k_0$ in the plot of W^2 vs k. i.e at $k = k_0$; the graph is not smooth. (that is also true for $k = \frac{3k_0}{2}, 4k_0, \ldots$ etc)

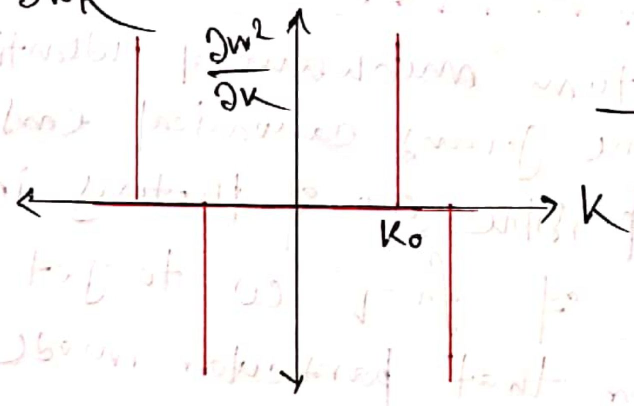
The plot of W^2 with k is given by:



I have shown the actual plot (for $k_0 a = 2.5$) in the mathematical file. For more and more terms in the summation; the result tends to this periodic ~~...~~ box function.

Clearly $\frac{\partial W^2}{\partial K} = 0$ for $K \neq K_0$
$= \infty$ for $K = K_0$ } i.e $\sim \delta(K - K_0)$

the $\frac{\partial W^2}{\partial K}$ is of the form:



→ periodic delta spikes.

This has also been shown in the mathematica file.

$$\therefore \quad W^2 = \frac{2A}{Ma}\left[\frac{\pi}{2} + K_0 a\right] \quad K \neq K_0$$
$$= \frac{2A}{Ma}\left[\pi + K_0 a\right] \quad K = K_0$$

& $\frac{\partial W^2}{\partial K} = 0 \quad K \neq \tilde{K}_0$ } $\tilde{K}_0 = K_0, \frac{3K_0}{2}, \ldots$

$= \frac{2A}{Ma} \times \frac{\pi}{2} \; \delta(K - \tilde{K}_0)$ } → $K = \tilde{K}_0$

Proved

(In question it was told to show that $\frac{\partial W^2}{\partial K}$ = finite for $K = K_0$; however that was not true and was corrected by prof Kaloborar's student, when I asked.)

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2.a Gruneisen Constant:-

Photon is a quantum mechanical identical particle. So we deal with the grand canonical ensemble by populating all possible no of photons in a particular mode of freq ω to get the partition fn for that particular mode of frequency.

Now at mode of freq ω; the energy of population of n no of photons be given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega.$$

($\because$ photon is a boson; n runs from 0 to ∞)

$$\therefore \quad Z_\omega = \sum_{n=0}^{\infty} \exp(-\beta E_n)$$

$$= \sum_{n=0}^{\infty} e^{-\frac{\beta\hbar\omega}{2}} \cdot e^{-n\beta\hbar\omega}.$$

$$= e^{-\frac{\beta\hbar\omega}{2}} \left(1 + e^{-\beta\hbar\omega} + e^{-2\beta\hbar\omega} + \cdots\right)$$

$$= \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\frac{\beta\hbar\omega}{2}}} = \frac{1}{e^{a} - e^{-a}} \qquad \left(a = \frac{\beta\hbar\omega}{2}\right)$$

So; the free energy is given by:

$$F_\omega = -K_BT \ln Z_\omega = K_BT \ln\left\{2\left(\frac{e^{a} - e^{-a}}{2}\right)\right\}$$

$$\Rightarrow F_\omega = k_BT \ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) = k_BT \ln\left(2\sinh\frac{\hbar\omega}{2k_BT}\right)$$

proved

2.b. Given: $F(\Delta,T) = \dfrac{B\Delta^2}{2} + k_BT\sum_k \ln\left(2\sinh\left(\dfrac{\beta\hbar\omega_k}{2}\right)\right)$

$\therefore$ For minimum value of F w.r.t Δ:

$$0 = \frac{\partial F}{\partial \Delta} = B\Delta + k_BT\sum_k \frac{\beta\hbar}{2}\coth\left(\frac{\beta\hbar\omega_k}{2}\right)\cdot\left(\frac{\partial\omega_k}{\partial\Delta}\right)$$

$$= B\Delta + \sum \frac{\hbar}{2}\coth\left(\frac{\beta\hbar\omega_k}{2}\right)\cdot\frac{\partial\omega_k}{\partial\Delta}$$

$\left(\because \beta = \dfrac{1}{k_BT}\right)$

Now comes one rough assumption.

given: $\dfrac{\partial\omega}{\omega} = -\gamma\,\partial\Delta$ when $\Delta = \dfrac{\delta V}{V}$.

taking for constant V: $\delta V \sim V$ we get:

$$d\Delta = \frac{d(\delta V)}{V} \sim \frac{dV}{V} \sim \Delta.$$

$$\therefore \frac{\partial\omega}{\omega} \sim -\gamma\,\delta\Delta \quad \text{i.e.}\ \frac{\partial\omega}{\partial\Delta} \sim -\gamma\omega.$$

Substituting:

$$0 = B\Delta + \frac{\hbar}{2}\sum_k(-\gamma\omega_k)\cdot\coth\left(\frac{\beta\hbar\omega_k}{2}\right)$$

$$\Rightarrow B\Delta = \gamma\sum_k\frac{\hbar\omega_k}{2}\coth\left(\frac{\beta\hbar\omega_k}{2}\right)$$

proved

for free mode ω

The energy of the system be given by:

$$U_\omega = -\frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial \beta} \ln\left(2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)$$

$$= \frac{\hbar\omega}{2} \coth \frac{\beta\hbar\omega}{2} = U_\omega(T)$$

So from last result:

$$\beta\Delta = \gamma \sum_k U_{\omega_k} = \gamma\, U(T)$$

$$\Rightarrow \Delta = \frac{\gamma . U(T)}{\beta}$$ proved

2.c

$$\frac{\delta\omega}{\omega} = -\gamma\Delta = -\gamma \frac{\delta V}{V}.$$

but the Debye temperature θ is defined by: $K\theta = \hbar\omega \Rightarrow K\, d\theta = \hbar\, d\omega$

i.e $$\frac{d\omega}{\omega} = \frac{d\theta}{\theta}.$$

So; $$\frac{\delta\omega}{\omega} = -\gamma\frac{\delta V}{V} = \frac{\delta\theta}{\theta}$$

$$\Rightarrow \gamma = -\gamma \frac{V}{\theta}\frac{\delta\theta}{\delta V} = -\gamma \frac{V}{\theta}\frac{\partial\theta}{\partial V}$$

$$= -\gamma \frac{\partial(\ln\theta)}{\partial(\ln V)}$$ proved

4. Sommerfield vs Debye model:—

1) Sommerfield model:—

According to Sommerfield; the e^- are free in metal & they follows F-D distn. In that context the total energy & No of e^- in the metal be given by:

$$E_{tot} = \int_0^\infty E\, g(E)\, f(E)\, dE$$
$$N_{tot} = \int_0^\infty g(E)\, f(E)\, dE$$

$$g(E) = \frac{4m\sqrt{m}\,\pi V\sqrt{2}}{h^3} \times 2\sqrt{E}$$
$$f(E) = \frac{1}{e^{\beta(E-\mu)}-1}$$

$$\therefore E_{tot} = 2\int_0^\infty \frac{4m\sqrt{m}\,\pi V\sqrt{2}\,E^{3/2}}{e^{\beta(E-\mu)}-1}\, dE$$

$$N_{tot} = 2\int_0^\infty \frac{4m\sqrt{m}\,V\pi\sqrt{2}\,E^{1/2}}{e^{\beta(E-\mu)}-1}\, dE$$

After some algebra the two expression reduces to:

$$E_{tot} = \frac{3KTV}{\lambda^3\beta} f_{5/2}(z)$$
$$N_{tot} = \frac{2V}{\lambda^3} f_{3/2}(z).$$

$$\lambda = \frac{h}{\sqrt{2\pi m K T}}$$
$$f_\nu(z) = \frac{1}{\Gamma(\nu)}\int_0^\infty \frac{x^{\nu-1}\,dx}{z^{-1}e^x+1}$$
$$z = e^{\beta\mu}.$$

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

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

$$f_m(z)\,\Gamma(m) = \int_0^{\beta\mu} x^{m-1}\left(1 - \frac{1}{1+ze^{-x}}\right) dx$$

$$+ \int_{\beta\mu}^{\infty} \frac{x^{m-1}}{z^{-1}e^{x}+1}\, dx$$

$$= \frac{(\log z)^m}{m} - \int_0^{\beta\mu} \frac{x^{m-1}}{1+ze^{-x}}\, dx + \int_{\beta\mu}^{\infty} \frac{x^{m-1}\, dx}{z^{-1}e^{x}+1}.$$

Substituting $\left.\begin{array}{l}\eta_1 = \beta\mu - x \text{ in 1st integral} \\ \eta_2 = x - \beta\mu \quad " \quad 2nd \quad "\end{array}\right\}$

$$f_m(z)\,\Gamma(m) = \frac{(\ln z)^m}{m} - \int_0^{\beta\mu} \frac{(\beta\mu - \eta_1)^{m-1}}{1+e^{\eta_1}}\, d\eta_1$$

$$+ \int_0^{\infty} \frac{(\beta\mu + \eta_2)^{m-1}}{1+e^{\eta_2}}$$

(using approximation $\beta\mu >> 1$)

$$= \frac{(\ln z)^m}{m} + \int_0^{\infty} \frac{(\beta\mu+\eta)^{m-1} - (\beta\mu-\eta)^{m-1}}{1+e^{\eta}}\, d\eta.$$

Using Taylor expansion:

$$(\beta\mu+\eta)^{m-1} - (\beta\mu-\eta)^{m-1} \simeq (\beta\mu)^{m-1}\left\{\left(1+\frac{\eta}{\beta\mu}\right)^{m-1} - \left(1-\frac{\eta}{\beta\mu}\right)^{m-1}\right\}$$

$$\simeq (\beta\mu)^{m-1}\left\{1 + (m-1)\frac{\eta}{\beta\mu} - 1 + (m-1)\frac{\eta}{\beta\mu}\right\}$$

$$\simeq 2(m-1)\eta(\beta\mu)^{m-2}.$$

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

but $\int_0^\infty \frac{\eta}{1+e^\eta}\, d\eta = \int_0^\infty \frac{d\eta\, e^{-\eta}.\eta}{1+e^{-\eta}}$

$= \int_0^\infty \eta \sum_{m=1}^{\infty} e^{-m\eta}.(-1)^{m+1}\, d\eta$

$= \sum_{m=1}^{\infty} (-1)^{m+1} \int_0^\infty \eta e^{-m\eta}\, d\eta.$

$= \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m^2} \underbrace{\int_0^\infty u e^{-u}\, du}_{=1}$

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

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

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

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

So: $f_n(z) \simeq \frac{(\ln z)^n}{\Gamma(n+1)} \left\{ 1 + \frac{\pi^2 n(n-1)}{6(\ln z)^2} + \cdots \right\}$

Using the expression:

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

& $N \simeq \frac{V}{3\pi^2\hbar^3} (2m\mu)^{3/2} \left(1 + \frac{\pi^2}{8}\left(\frac{K_B T}{\mu}\right)^2 + \cdots\right)$

$$\cancel{\frac{E}{V} = \frac{1}{5\pi^2\hbar^3}(2m)^{3/2}\cdot\mu^{5/2}\left(1+ \quad (\mu)\right)}$$

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

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

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

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

Using this we get!
(Using mathematica for long algebra):
(taken series expansion upto 2nd order)

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

Now I have calculated $\frac{E}{N}$ from the above expression & replaced μ by the expansion term in E_F.

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

$$\frac{E}{N} \simeq \frac{3E_F}{5}\left(1 + \frac{5\pi^2}{12}\left(\frac{K_BT}{E_F}\right)^2 + \cdots\right)$$

As E_F = const of temp.

So,

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

$$= \frac{\pi^2}{2} \cdot NK_B^2 \cdot \frac{T}{E_F}.$$

Ans

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ii) Debye model of phonons:-

According to Debye model; the phonons are like bosons & they carry energy according to the formula $E = \hbar\omega$.

~~Also~~ Now as there are three modes of vibration (one ~~to~~ longitudinal; two transverse)

So the density fn of phonons be:

$$g(\omega) = 4\pi V \underbrace{\left(\frac{1}{C_L^3} + \frac{2}{C_t^3}\right)}_{X} \frac{\omega^2 \, d\omega}{4\pi^2 \times 2\pi}$$

$$= \frac{V X}{2\pi^2} \omega^2 \, d\omega$$

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

$$E = \int_0^{\omega_D} f(\omega) \cdot g(\omega) \cdot \hbar\omega \, d\omega$$

$$f(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}$$ for phonon as ~~bo~~ they are boson.

$$\therefore E = \frac{V\hbar X}{2\pi^2} \int_0^{\omega_D} \frac{\omega^3 \, d\omega}{e^{\beta\hbar\omega} - 1}.$$

here ω_D is the limit given by debye as:

$$\int_0^{\omega_D} g(\omega) \, d\omega = 3N_A. \quad (\text{for } 1 \text{ mole})$$

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which gives:

$$\omega_D = 2\pi \cdot \left\{ \frac{9N_A}{4\pi V\left(\frac{1}{c_l^3} + \frac{2}{c_t^3}\right)} \right\}^{1/3} \sim \frac{N_A^{1/3} C_{solid}}{V^{1/3}}.$$

however; $$E = \frac{V\hbar X}{2\pi^2} \int_0^{T_D/T} \frac{x^3 K^3 T^3}{\hbar^3} \cdot \frac{KT}{\hbar} \frac{dx}{e^x - 1}$$

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

$$\Rightarrow E = \frac{V X}{2\pi^2 \hbar^3} (KT)^4 \int_0^{T_D/T} \frac{x^3\, dx}{e^x - 1}$$

Now the T^3 law which comes from Debye law is ~~valid~~ valid for low temp. Here $\omega_D \sim \frac{N_A^{1/3} C_{solid}}{V^{1/3}}$ which is pretty big.

but the exponential makes the integrand very small at large enough ω.

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

$$\therefore E = \frac{V x (KT)^4}{2\pi^2 \hbar^3} \int_0^\infty \frac{x^3\, dx}{e^x - 1}$$

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

So the specific heat be given by:

$$C_V^l = \frac{\partial E}{\partial T} = \frac{4 V \pi^2 x K_B^4 T^3}{30 \hbar^3}$$

So; $\dfrac{C_V^e}{C_V^L} = \dfrac{\cancel{\pi^2}}{\cancel{2}} N\cancel{K_B}^{\cancel{2}} \dfrac{\cancel{T}}{E_F} \times \dfrac{\overset{15}{\cancel{30}}\, \hbar^3}{4 \cancel{\pi^2} X \underset{K_B^2 T^2}{\cancel{K_B^4}\cancel{T^3}} V}$

$$= \frac{15 N \hbar^3}{4 K_B^2 T^2 V E_F X}$$

$$X = \left(\frac{1}{C_l^3} + \frac{2}{C_t^3}\right)$$

b.) When; $\dfrac{C_V^e}{C_V^L} = 1$ i.e $C_V^e = C_V^L$

at $T = T^*$ then.

$$\frac{15 N \hbar^3}{4 K_B^2 T^2 V E_F X} = 1$$

$$\Rightarrow T^* = \sqrt{\left(\frac{4 K_B^2 E_F X}{15 \rho \hbar^3}\right)^{-1}} \qquad \rho = \frac{N}{V}.$$

$$= \left\{\frac{4 K_B^2 E_F \left(\frac{1}{C_l^3} + \frac{2}{C_t^3}\right)}{15 \rho \hbar^3}\right\}^{-1/2}.$$

$$= \sqrt{\frac{15 \rho \hbar^3}{4 K_B^2 E_F \left(\frac{1}{C_l^3} + \frac{2}{C_t^3}\right)}}$$

c: I've calculated value of T^* for Na

Now for Na (from Online):

$C_{Na} \simeq 3200$ m/s

$E_F = 3.24$ eV.

$\rho \simeq 2.225 \times 10^{29}$ m^{-3}.

And assuming $C_L \simeq C_t$ we get:

$$T^*_{Na} \simeq \sqrt{\frac{15 \times 2.225 \times 10^{29} \times (1.054 \times 10^{-34})^3 \times 3200^3}{3 \times 4 \times (1.039 \times 10^{-23})^2 \times 3.24 \times 1.6 \times 10^{-19}}} \ K$$

$\simeq 4.371$ K.

Similarly:

For Li: $C_{Li} \simeq 6000$ m/s

$\rho \simeq 4.90 \times 10^{28}$ m^{-3}

$E_F \simeq 4.74$ eV.

$\therefore T^*_{Li} \simeq 13.623$ K.

For K $\rho_K = 1.356 \times 10$ m^{-3}

$C_K = 2000$ m/s

$E_F = 2.12$ eV.

$\therefore T^*_K \simeq 2.084$ K.

5. Hall effect & Sterio magnetic conductivity:

Given: $\vec{j} = nq\vec{v} = \frac{ne^2\vec{E}\tau}{m}$.

Now in presence of electron collision; the equation gives,

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right)\vec{v} = -e\left(\vec{E} + \frac{1}{c}(\vec{v}\times\vec{B})\right).$$

Here $\vec{B} = B\hat{z}$.

$$\therefore \vec{v}\times\vec{B} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ v_x & v_y & v_z \\ 0 & 0 & B \end{vmatrix} = \hat{i}Bv_y - \hat{j}v_xB.$$

So the vector eqn for motion gives:

$$\left.\begin{aligned} m\frac{dv_x}{dt} + \frac{mv_x}{\tau} &= -eE_x - \frac{eBv_y}{c} \\ m\frac{dv_y}{dt} + \frac{mv_y}{\tau} &= -eE_y + \frac{eBv_x}{c} \\ m\frac{dv_z}{dt} + \frac{mv_z}{\tau} &= -eE_z. \end{aligned}\right\}$$

At static current condition; $\vec{j}$ = constant.

i.e $\frac{\partial\vec{j}}{\partial t} = 0$. But to satisfy that; we must have $\left.\frac{\partial\vec{v}}{\partial t}\right|_{static} = 0$. $(\because \vec{j} = nq\vec{v})$

$\therefore \frac{dv_x}{dt} = 0 = \frac{dv_y}{dt} = 0 = \frac{dv_z}{dt}$ gives,

$$\left.\begin{aligned} m\frac{v_x}{\tau} &= -eE_x - \frac{eBv_y}{c} \\ \frac{mv_y}{\tau} &= -eE_y + \frac{eBv_x}{c} \\ m\frac{v_z}{\tau} &= -eE_z \end{aligned}\right\}$$

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Now ; $v_i = \frac{j_i}{nq}$.

So in terms of j the eqns give :

$$\left.\begin{aligned} \frac{m\dot{j}_x}{nq\tau} &= -eE_x - \frac{eBj_y}{nqc} \\ \frac{m\dot{j}_y}{nq\tau} &= -eE_y + \frac{eBj_x}{nqc} \\ \frac{m\dot{j}_z}{nq\tau} &= -eE_z \end{aligned}\right\}$$

i.e

$$\left.\begin{aligned} \frac{j_x}{nq\tau} + \frac{\omega j_y}{nq} &= -\frac{eE_x}{m} \\ \frac{j_y}{nq\tau} - \frac{\omega j_x}{nq} &= -\frac{eE_y}{m} \\ \frac{j_z}{nq\tau} &= -\frac{eE_z}{m} \end{aligned}\right\} \quad \omega = \frac{eB}{mc}$$

in matrix form :

$$\frac{1}{nq\tau}\begin{pmatrix} 1 & +\omega\tau & 0 \\ -\omega\tau & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = -\frac{e}{m}\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = [j] = \left(-\frac{e\tau nq}{m}\right)\cdot\begin{pmatrix} 1 & \omega\tau & 0 \\ -\omega\tau & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}^{-1}\begin{pmatrix} E \end{pmatrix}$$

$$\Rightarrow [j] = \frac{ne^2\tau}{m(1+(\omega\tau)^2)}\begin{pmatrix} 1 & -\omega\tau & 0 \\ \omega\tau & 1 & 0 \\ 0 & 0 & 1+\omega^2\tau^2 \end{pmatrix}\begin{pmatrix} E \end{pmatrix}$$

(Evaluated the inverse in Mathematica) ($\because q = -e$ here) but $\frac{ne^2\tau}{m} = \sigma_0$ = conductivity in drude model.

$$\therefore \begin{pmatrix} j \end{pmatrix} = \frac{\sigma_0}{1+\omega^2\tau^2}\begin{pmatrix} 1 & -\omega\tau & 0 \\ \omega\tau & 1 & 0 \\ 0 & 0 & 1+(\omega\tau)^2 \end{pmatrix}\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

$$= \begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix}$$

Proved.

5.b. In high B limit i.e $\tau\omega = \frac{eB\tau}{mc} >> 1$

we get:

[comparing $[j] = [\sigma][E]$ when $[\sigma] = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$]

$$\sigma_{yx} = \frac{\sigma_0\omega\tau}{1+\omega^2\tau^2}$$

$$\therefore \lim_{\omega\tau\to\infty}\sigma_{yx} = \lim_{\omega\tau\to\infty}\frac{\sigma_0\omega\tau}{1+\omega^2\tau^2}$$

$$\approx \frac{\sigma_0\omega\tau}{\omega^2\tau^2} = \frac{\sigma_0}{\omega\tau}.$$

i.e $\lim_{\omega\tau\to\infty}\sigma_{yx} \simeq \frac{ne^2\tau}{m}\cdot\frac{mc}{eB\tau} = \frac{nec}{B}.$

And clearly we see $\sigma_{yx} = -\sigma_{xy}$.

$\therefore$ At $\omega\tau\to\infty$: $\sigma_{yx} = \frac{nec}{B} = -\sigma_{xy}$.

Proved

$$\lim_{\omega\tau\to\infty}\sigma_{xx} = \frac{\sigma_0}{1+\omega^2\tau^2}\Big|_{\omega\tau\to\infty}$$

$$= \frac{\sigma_0}{\omega^2\tau^2\left(1+\frac{1}{\omega^2\tau^2}\right)}$$

$$\approx \frac{\sigma_0}{\omega^2\tau^2}\cdot\left(1-\frac{1}{\omega^2\tau^2}+\cdots\right)$$

So $\lim_{\omega\tau \to \infty} \sigma_{xx} \simeq \dfrac{\sigma_0}{\omega^2\tau^2}$.

proved

5.c When both electrons & holes are present; the j is given by:

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \frac{\sigma_0^e}{1+\omega_e^2\tau^2} \begin{pmatrix} 1 & -\omega_e\tau & 0 \\ \omega_e\tau & 1 & 0 \\ 0 & 0 & 1+\omega_e^2\tau^2 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$$

$$\underbrace{+ \frac{\sigma_0^h}{1+\omega_h^2\tau^2} \begin{pmatrix} 1 & -\omega_h\tau & 0 \\ \omega_h\tau & 1 & 0 \\ 0 & 0 & 1+\omega_h^2\tau^2 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}}_{e^- + \text{ hole contribution}}$$

$$\omega_e = \frac{eB}{2m_e}; \quad \omega_h = \frac{-q_{hole}B}{2m_{hole}}.$$

$$\therefore \sigma_{yx} = \frac{\sigma_0^e \cdot \omega_e\tau}{1+\omega_e^2\tau^2} + \frac{\sigma_0^h \omega_h\tau}{1+\omega_h^2\tau^2}.$$

$$\therefore \lim_{\omega\tau \to \infty} \sigma_{yx} \simeq \frac{\sigma_0^e}{\omega_e\tau} + \frac{\sigma_0^h}{\omega_h\tau}.$$

taking $q_e = -q_h$

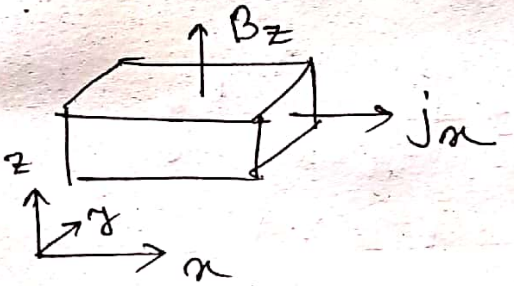
$$\sigma_{yx} \simeq \frac{n_e e^2\tau}{m_e} \cdot \frac{m_e c}{eB\tau} - \frac{n_h e^2\tau}{m_h} \cdot \frac{m_h c}{eB\tau}$$

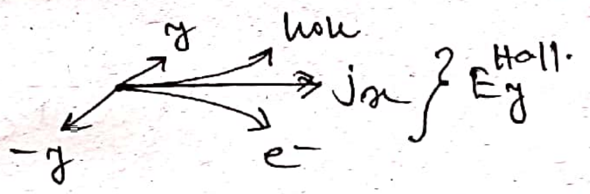
$$\Rightarrow \sigma_{yx} \simeq \frac{(n-p)ec}{B}$$ Proved

$(n_e = n;\ n_h = p)$.

5'd. The hall field is the amount of electric field developed across the direction of that is both perpendicular to $\vec{J}$ & $\vec{B}$ i.e due to the term $q(\vec{v}\times\vec{B}) \sim q(\vec{J}\times\vec{B})$ $(\because \vec{J}\propto\vec{v})$; the different accumulation of electrons & holes due to charge difference, makes this amount of field.

Here we have to calculate hall field along y direction. i.e that's caused by the current along x direction ($\because$ the $\vec{B}$ is along $\hat{z}$ only)





Taking $j_y = 0$ in $\vec{J} = \sigma\vec{E}$ eq:

$$\sigma_{yx}E_x + \sigma_{yy}E_y = 0 \quad (\because \sigma_{yz} = 0)$$

($\because$ Hall field just opposes the current at the maximum limiting amount)

$$\Rightarrow \left(\frac{\sigma_0^e \omega_e\tau}{1+\omega_e^2\tau_e^2} + \frac{\sigma_0^h\omega_h\tau}{1+\omega_h^2\tau_e^2}\right)E_x + \left(\frac{\sigma_0^e}{1+\omega_e^2\tau_e^2} + \frac{\sigma_0^h}{1+\omega_h^2\tau_h^2}\right)E_y = 0.$$

Now, $\dfrac{\sigma_0^e\omega_e\tau_e}{1+\omega_e^2\tau_e^2} \approx \dfrac{nec}{B}$.

$$\frac{\sigma_0^h\omega_h\tau_h}{1+\omega_h^2\tau_h^2} \approx -\frac{pec}{B}.$$

$$\frac{\sigma_0^e}{1+\omega_e^2\tau_e^2} \simeq \frac{\sigma_0^e}{\omega_e^2\tau_e^2} \simeq \frac{n\cancel{e^2}\cancel{\tau_e}}{\cancel{m_e}} \cdot \frac{m_e^{\cancel{2}}c^2}{\cancel{e^2}B^2} \cdot \frac{1}{\tau_e^{\cancel{2}}}$$

$$= \frac{n m_e c^2}{B^2\tau_e}$$

$$\& \quad \frac{\sigma_0^h}{1+\omega_h^2\tau_h^2} \simeq \frac{p m_h c^2}{B^2\tau_h}.$$

So; $$\frac{(n-p)ec}{B}E_x = -\left(\frac{n m_e c^2}{B^2\tau_e} + \frac{p m_h c^2}{B^2\tau_h}\right)E_y$$

$$\Rightarrow (n-p)E_x = -\left(\frac{n m_e c}{\tau_e\, eB} + \frac{p\, m_h c}{\tau_h\, eB}\right)E_y.$$

$$\Rightarrow (n-p)E_x = -\left(\frac{n}{\omega_e\tau_e} + \frac{p}{\omega_h\tau_h}\right)E_y$$

$$\Rightarrow E_y = -(n-p)\left(\frac{n}{\omega_e\tau_e} + \frac{p}{\omega_h\tau_h}\right)^{-1}E_x$$

proved

5.e. $$j_x = \sigma_{xx}E_x + \sigma_{xy}E_y$$

$$= \left(\frac{\sigma_0^e}{1+\omega_e^2\tau_e^2} + \frac{\sigma_0^h}{1+\omega_h^2\tau_h^2}\right)E_x - \left(\frac{\sigma_0^e\omega_e\tau_e}{1+\omega_e^2\tau_e^2} + \frac{\sigma_0^h\omega_h\tau_h}{1+\omega_h^2\tau_h^2}\right)E_y.$$

Using values:

~~j_x~~

$$j_x = \left(\frac{n m_e c^2}{B^2 \tau_e} + \frac{p m_h c^2}{B^2 \tau_h}\right) E_x$$

$$- \frac{(n-p)ec}{B} \underbrace{\left\{ -(n-p)\left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right)^{-1}\right\}}_{\text{from part d.}} E_x$$

$$\Rightarrow j_x = \frac{ec}{B}\left[\left(\frac{n\, m_e c}{\tau_e B e} + \frac{p\, m_h c}{\tau_h B e}\right) + (n-p)^2 \left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right)^{-1}\right] E_x$$

$$= \underbrace{\frac{ec}{B}\left[\left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right) + (n-p)\left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right)^{-1}\right]}_{\sigma_{eff}} E_x$$

So

$$\sigma_{eff} = \frac{ec}{B}\left[\left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right) + (n-p)\left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right)^{-1}\right]$$

proved

At $n=p$; the 2nd term goes to zero.

$$\therefore \sigma_{eff} = \frac{ec}{B}\left(\frac{n}{\omega_e \tau_e} + \frac{p}{\omega_h \tau_h}\right)$$

as $\omega \propto B$ so clearly in that situation,

$$\sigma_{eff} = \frac{(\cdots)}{B^2} \quad \text{i.e } \sigma_{eff} \propto B^{-2}$$

proves

If $m \neq p$:

$$\sigma_{eff} = \frac{Ec}{B}\left[\left(\frac{m m_e c}{\tau_e B e} + \frac{p m_h c}{\tau_h B e}\right) + (m-p)^2 \cdot \left(\frac{m m_e c}{\tau_e B e} + \frac{p m_h c}{\tau_h B e}\right)^{-1}\right]$$

$\therefore$ at $\underset{B \to \infty}{} \sigma_{eff}$ = (1st term goes zero)

$$+ Ec(m-p)^2 \left(\frac{m m_e c}{e \tau_e} + \frac{p m_h c}{e \tau_h}\right)^{-1}$$

= indp of B. proved

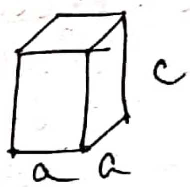
3. X-Ray diffraction of $La_{1.8}Ba_{0.2}Cu_{4-y}$.

a). In the S.C lattice; all lattice planes of the simple tetragonal Bravais lattice can refuct x-rays; since the geometric structure factor does not ~~play~~ affect when the basis is not taken into account.

For B.C tetragonal lattice; w.r.t the conventional cell; the basis has too points:

$d_1 = (0,0,0)$; $d_2 = \left(\frac{a}{2}, \frac{a}{2}, c\right)$

[$\because$ for b.c tetragonal $a = b \neq c$].



So; $\vec{K}$ = reciprocal vector

$$= 2\pi\left\{\frac{h\hat{e}_x}{a} + \frac{k e_y}{a} + \frac{l\hat{e}_z}{c}\right\}$$

And the structure const be given as:

$$S(K) = \sum_m e^{-i\vec{K}\cdot\vec{d}_m} = 1 + e^{-i\pi(h+k+l)}$$

clearly $S(K) = 2$ if $h+k+l$ = even
$= 0$ " " = odd

So the selection rule is; the lattice can reflect X-ray iff $h+k+l$ = even only; otherwise not.

b. From the given value of 2θ we compute $4\sin^2\theta$ & then use the eq:

$$4\sin^2\theta = m^2\lambda^2\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) \quad (\text{here } a = b)$$

then using trial and error method, for first few peaks of diffraction; we get the values of a, b, c.

Here the procedure gives:

2θ	$4\sin^2\theta$	$\bar{h}\ \bar{k}\ \bar{l}$	a (mm)	c (mm)
34.736	0.356483	1 0 3	0.37940	1.33152
37.442	0.41206	1 1 0	0.37806	1.33033
40.516	0.47955	1 1 2	0.37943	1.33162
45.576	0.60007	0 0 6	0.37939	1.33148
46.493	0.62311	1 0 5	0.37836	1.33149
48.690	0.67947	1 1 4	0.37839	1.33148
54.043	0.82564	2 0 0	0.37841	1.33156
56.0369	0.89232	2 0 2	0.37941	1.33155
60.421	1.012975	1 1 6	0.37838	1.33142
60.757	1.02297	1 0 7	0.37936	1.33136
61.598	1.04869	2 1 1	0.37841	1.33153
62.189	1.06689	0 0 8	0.37841	1.33154
63.007	1.09224	2 0 4	0.37939	1.33147
65.956	1.18194.	2 1 3	0.37939	1.33147

3-c. Here a & c have already been calculated in last part. However I have taken the mean & σ2 of a & c using python.

$a_{mean} = 0.37937$ mm ; $\sigma_a = 8.81933 \times 10^{-5}$ mm

$c_{mean} = 1.33142$ mm ; $\sigma_c = 0.0031$ mm

Ans