

QCMP-2014/15 — Quantum Condensed Matter Physics

Problem sheet 1: Lorentz dipole oscillator model, Drude model, Sommerfeld theory, lattices

1. Sapphire

A sapphire crystal doped with titanium absorbs strongly around 500 nm. Calculate the difference in the refractive index of the doped crystal above and below the 500 nm absorption band, if the density of absorbing atoms is $1 \cdot 10^{25} \text{ m}^{-3}$. The refractive index of undoped sapphire is 1.77.

Solution: We use

$$\epsilon(\omega) = \epsilon_{\infty} + \frac{\omega_p^2}{\omega_T^2 - \omega^2 - i\gamma\omega}$$

with $\omega_p^2 = \frac{(N/V)e^2}{\epsilon_0 m}$.

For $\omega \ll \omega_T$, this gives $\epsilon(\omega \ll \omega_T) = \epsilon_{st} = \epsilon_{\infty} + \omega_p^2/\omega_T^2$, and for $\omega \gg \omega_T$, we obtain $\epsilon(\omega \gg \omega_T) = \epsilon_{\infty}$.

The difference in permittivity above and below the resonance is $\Delta\epsilon = \omega_p^2/\omega_T^2$. For the quoted concentration and resonance wavelength, we obtain $\Delta\epsilon \simeq 2.3 \cdot 10^{-3}$.

The refractive index is $n(\omega) = \sqrt{\epsilon(\omega)}$, which gives $\Delta n = n(\omega \ll \omega_T) - n(\omega \gg \omega_T) = \sqrt{\epsilon_{\infty} + \Delta\epsilon} - \sqrt{\epsilon_{\infty}}$. Because $\Delta\epsilon \ll \epsilon_{\infty} = 1.77^2$, we can Taylor-expand this and obtain:

$$\Delta n = \frac{\Delta\epsilon}{2\sqrt{\epsilon_{\infty}}} \simeq 6.5 \cdot 10^{-4}$$

2. Reflectivity of metals

The phase velocity of light in a conducting medium is the speed of light divided by the refractive index $N(\omega) = \epsilon(\omega)^{1/2}$ where we may use for ϵ the Drude result

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} \quad . \quad (1)$$

In a “good” metal, we have $1/\tau \ll \omega_p$.

Show that

- (a) For $\omega \ll 1/\tau$, ϵ is large and imaginary, so that $|N| \gg 1$ and N has roughly equal real and imaginary parts,
- (b) For $1/\tau \ll \omega \ll \omega_p$, ϵ is real and negative, so that N is imaginary,
- (c) For $\omega > \omega_p$, ϵ is positive, and N is real.

Consider a light wave with the electric field polarised in the x -direction at normal incidence from the vacuum on a good Drude metal (with $1/\tau \ll \omega_p$) occupying the region $z > 0$. In the vacuum ($z < 0$), the incident E_1 and reflected E_2 waves give rise to a field

$$E_x = E_1 \exp(i\omega[z/c - t]) + E_2 \exp(-i\omega[z/c + t]) \quad , \quad (2)$$

whereas in the medium, the electric field is

$$E_x = E_0 \exp(i\omega[N(\omega)z/c - t]) \quad . \quad (3)$$

Matching the electric and magnetic fields on the boundary, show that

$$E_0 = E_1 + E_2 \quad , \quad (4)$$

$$NE_0 = E_1 - E_2 \quad , \quad (5)$$

and hence show that the reflection coefficient satisfies

$$R = \left| \frac{E_2}{E_1} \right|^2 = \left| \frac{1 - N}{1 + N} \right|^2 \quad . \quad (6)$$

Using the Drude formula above, show that

$$R \approx 1 - 2 \left(\frac{2\epsilon_0\omega}{\sigma(0)} \right)^{1/2} \quad \text{for } \omega \ll 1/\tau \quad (7)$$

$$\approx 1 - \frac{2}{\omega_p\tau} \quad \text{for } 1/\tau \ll \omega \ll \omega_p \quad (8)$$

$$\approx \frac{1}{16} \left(\frac{\omega_p}{\omega} \right)^4 \quad \text{for } \omega_p \ll \omega \quad (9)$$

and sketch the reflectivity $R(\omega)$.

To get the first two of these results with the minimum of fuss, you may find it helpful to expand in $1/N$, viz.

$$R = \frac{(1 - \frac{1}{N})(1 - \frac{1}{N^*})}{(1 + \frac{1}{N})(1 + \frac{1}{N^*})} \approx 1 - 4\Re(1/N) \quad (10)$$

Solution:

①

$$(-m\omega^2 - \frac{i}{\tau})x_\omega = q E_\omega$$

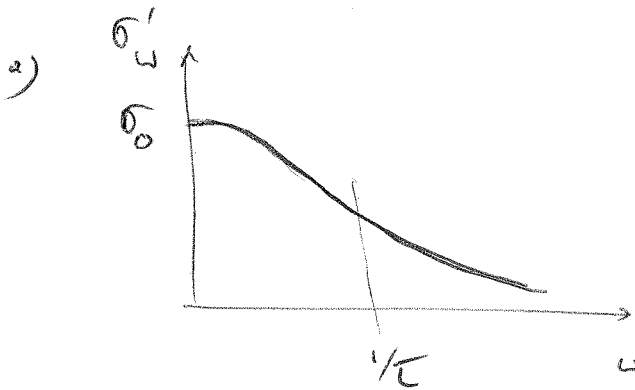
$$q n x_\omega = P_\omega = \frac{q^2 n}{-m} \frac{1}{\omega^2 + i\omega/\tau} E_\omega$$

$$\textcircled{*} \quad \epsilon E_\omega = D_\omega = \epsilon_0 E_\omega + P_\omega = \epsilon E_\omega \left(1 - \underbrace{\left(\frac{q^2 n}{\epsilon_0 m} \right)}_{\omega_p^2} \frac{1}{\omega^2 + i\omega/\tau} \right)$$

$$n q \dot{x} = j$$

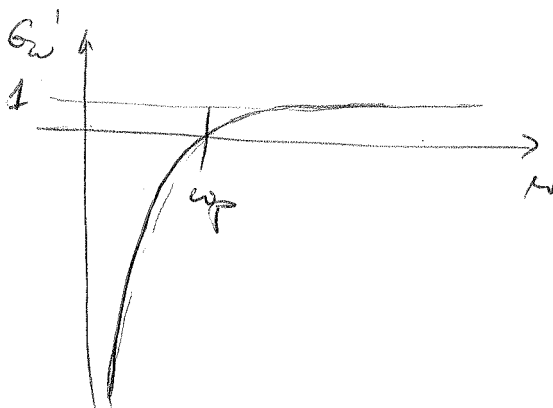
$$-n q i \omega x_\omega = j \omega = -i \omega P_\omega = \sigma_\omega E_\omega$$

$$\textcircled{*} \quad \sigma_\omega = -i \omega \epsilon_0 (\epsilon_\omega - 1) = \epsilon_0 \omega_p^2 \frac{\tau}{1 - i\omega\tau}$$

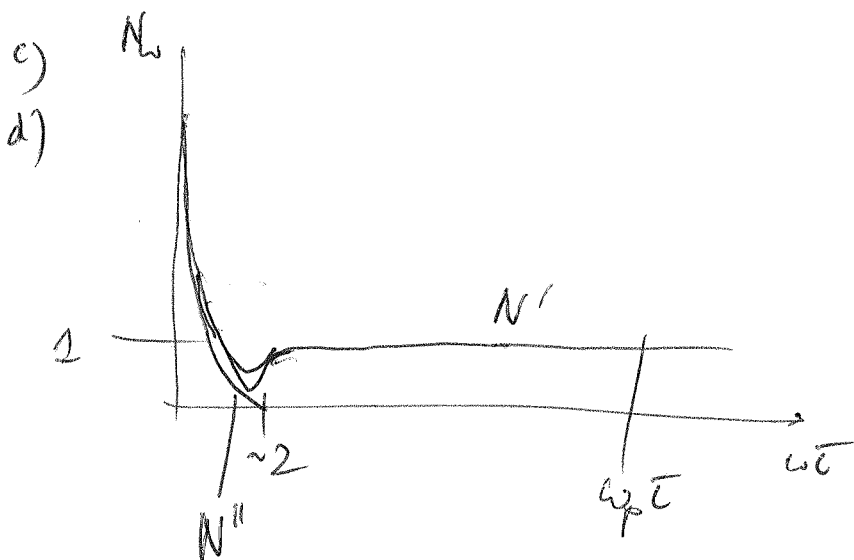


$$b) \quad \epsilon_\omega = 1 - \frac{\omega_p^2 \tau^2}{\omega^2 \tau^2 + i\omega\tau}$$

$$\omega_p \tau \approx 100$$



①



$$\begin{array}{c}
 E_1 e^{ikz} \uparrow \underline{E} \\
 \underline{k} \rightarrow \\
 E_2 e^{-ikz} \leftarrow
 \end{array}
 \quad \left| \quad \begin{array}{c} \uparrow x \\ \rightarrow z \end{array} \right.
 \quad \longrightarrow \quad E_0 e^{ik(\omega)z}$$

$$k(\omega) = \frac{\omega N(\omega)}{c}$$

at boundary:

$$\underline{E_1 + E_2 = E_0} \quad (1)$$

$$\nabla \times \underline{E} = - \dot{\underline{B}}$$

$$\left| \begin{array}{cc} 1 & E_x \\ k & \partial_z \end{array} \right| = \begin{pmatrix} 0 & \partial_z E_x \\ -\partial_z E_x & 0 \end{pmatrix} = - \begin{pmatrix} 0 & \dot{B}_y \\ \dot{B}_y & 0 \end{pmatrix}$$

$$\dot{B}_y = \partial_z E_x \Rightarrow (E_1 - E_2)k = E_0 k(\omega)$$

$$\underline{E_1 - E_2 = E_0 N(\omega)} \quad (2)$$

$$NE_1 + NE_2 = E_1 - E_2$$

$$E_1(N-1) = -E_2(N+1)$$

$$R = \left| \frac{E_2}{E_1} \right|^2 = \left| \frac{1-N}{1+N} \right|^2$$

① $R \approx 1 - 2 \left(\frac{2\epsilon_0 \omega}{\sigma_0} \right)^{1/2} \quad \text{for } \omega \ll 1/\tau$

$\frac{1}{N} = \frac{1}{\sqrt{\epsilon_\omega}}$. Denominator in $\epsilon_\omega = 1 - \frac{\omega_p^2 \tau^2}{\omega^2 \tau^2 + i\omega\tau}$

is dominated by term linear in $\omega\tau$

$\Rightarrow \epsilon_\omega \approx - \frac{\omega_p^2 \tau^2}{i\omega\tau}$

$\frac{1}{\sqrt{\epsilon_\omega}} = \frac{1-i}{\sqrt{2}} \frac{\sqrt{\omega\tau}}{\omega_p \tau}$

$\left| \frac{1 - 1/\sqrt{\epsilon}}{1 + 1/\sqrt{\epsilon}} \right|^2 \approx \left| 1 - 2/\sqrt{\epsilon} \right|^2 \approx 1 - 4 \operatorname{Re}(1/\sqrt{\epsilon}) =$

$= 1 - 2\sqrt{2} \frac{\sqrt{\omega\tau}}{\omega_p \tau} = 1 - 2 \left(\frac{2\omega\tau\epsilon_0}{\epsilon_0 \omega_p^2 \tau} \right)^{1/2} \quad \checkmark$

② $R \approx 1 - \frac{2}{\omega_p \tau} \quad 1 \ll \omega\tau \ll \omega_p \tau$

Denominator in ϵ_ω now dominated by $(\omega\tau)^2$

term. Taylor expand $\frac{1}{\sqrt{\epsilon}}$ (neglecting the leading 1)

$$\frac{1}{\sqrt{\epsilon_\omega}} = -i \left| \frac{(\omega\tau)^2 + i/\omega\tau}{(\omega_p\tau)^2} \right|^{1/2} = -i \frac{\omega\tau}{\omega_p\tau} \left(1 + \frac{i}{2\omega\tau} \right)$$

$$\operatorname{Re} \left(\frac{1}{\sqrt{\epsilon_\omega}} \right) = \frac{1}{2\omega_p\tau}$$

$$R = 1 - 4 \operatorname{Re} \left(\frac{1}{\sqrt{\epsilon}} \right) = 1 - \frac{2}{\omega_p\tau} \quad \checkmark$$

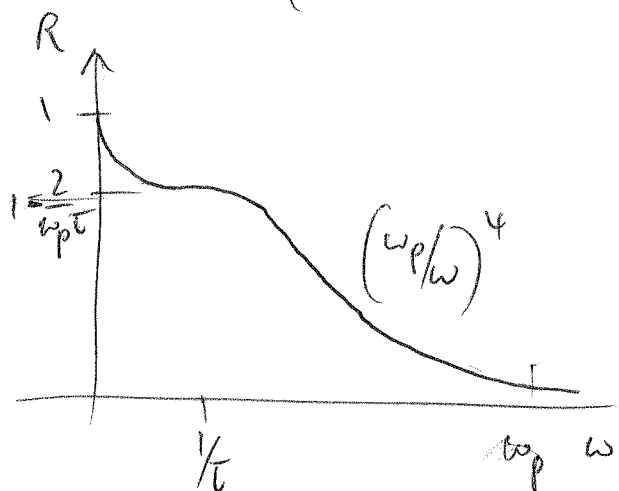
(c) $\omega\tau \gg \omega_p\tau$

$$\epsilon = 1 - \frac{(\omega_p\tau)^2}{(\omega\tau)^2}$$

$$\sqrt{\epsilon} = 1 - \frac{1}{2} \left(\frac{\omega_p}{\omega} \right)^2$$

$$\frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \approx \frac{1}{2} \frac{(\omega_p/\omega)^2}{2} = \frac{1}{4} \left(\frac{\omega_p}{\omega} \right)^2$$

$$R = \frac{1}{16} \left(\frac{\omega_p}{\omega} \right)^4$$



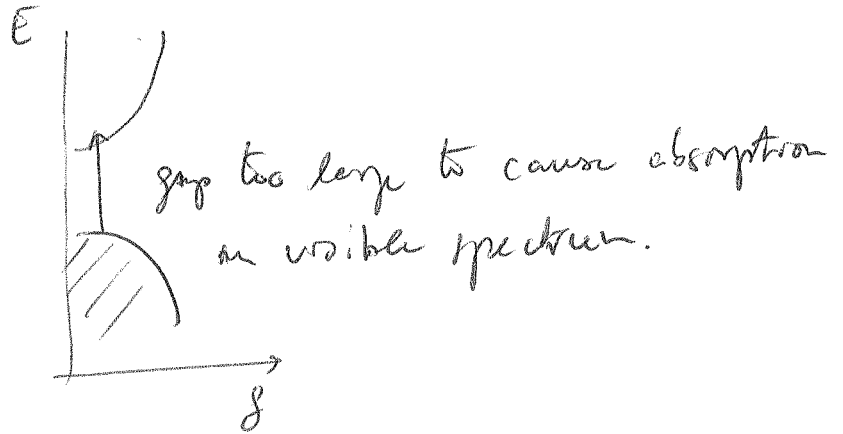
(4)

3. Optical properties of solids

Discuss why, at optical frequencies, glass is transparent, and silver is shiny, while graphite appears black, and powdered sugar is white.

Solution:

②

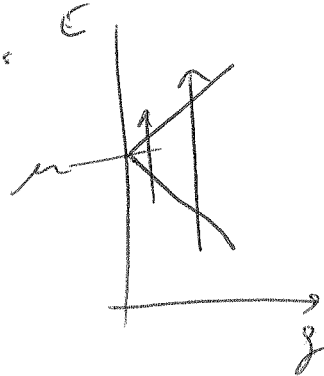
glass: insulator

Aluminum: metal. Drude theory explains that metals are highly reflective at frequencies well below the plasma freq., because $\epsilon \sim -\frac{\omega_p^2}{\omega^2}$ for $\omega \ll \omega_p$,

and $R^* \sim \left| \frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \right|^2 \rightarrow 1$ as $|\epsilon|$ diverges.

graphite: $g(E_F) \sim 0$, but conduction and valence bands just meet.

Absorption possible at all frequencies \rightarrow black.



sugar: insulator, and would be transparent if present as large single crystal. The little sugar grains, however, present many surfaces, which scatter light. This makes sugar appear white, like e.g. snow (although ice is transparent).

4. Static conductivity tensor

Show that in the presence of a magnetic field \mathbf{B} aligned along the z -axis, the electrical conductivity can be written as a tensor $\mathbf{j} = \sigma \cdot \mathbf{E}$, with

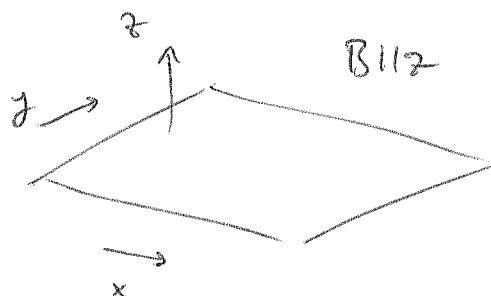
$$\sigma = \frac{\sigma_o}{1 + \beta^2} \begin{pmatrix} 1 & \beta & 0 \\ -\beta & 1 & 0 \\ 0 & 0 & 1 + \beta^2 \end{pmatrix} \quad (11)$$

Here $\omega_c = \frac{qB}{m^*}$, $\beta = \omega_c \tau$ and $\sigma_o = ne^2 \tau / m^*$. The carrier charge q can be $+e$ or $-e$.

In a high magnetic field ($\beta \gg 1$), show that $\sigma_{xy} = -\sigma_{yx} = nq/B$.

Solution:

(3)



$q = \text{electron charge} = -e$

$$m \frac{\underline{v}}{\tau} = q (\underline{E} + \underline{v} \times \underline{B}) \quad \left| \times \frac{nq\tau}{m} \right.$$

$$nq \underline{v} = \underline{j} = \underbrace{\frac{nq^2\tau}{m}}_{\sigma_0} (\underline{E} + \underline{v} \times \underline{B})$$

$\hookrightarrow (v_y, -v_x, 0)B$

$$j_x - \frac{q\tau B}{m} j_y = \sigma_0 E_x$$

$$j_y + \frac{q\tau B}{m} j_x = \sigma_0 E_y$$

$$j_z = \sigma_0 E_z$$

$$\omega_c = \frac{qB}{m}, \quad \beta = \omega_c \tau$$

(from $\omega_c^2 \tau m = qB\omega\tau$)
ⓐ

$$\underline{E} = \underline{\rho} \underline{j} = \frac{1}{\sigma_0} \begin{pmatrix} 1 & -\beta & 0 \\ \beta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix}$$

$$\underline{\sigma} = \underline{\rho}^{-1} = \frac{\sigma_0}{1+\beta^2} \begin{pmatrix} 1 & \beta & 0 \\ -\beta & 1 & 0 \\ 0 & 0 & 1+\beta^2 \end{pmatrix}$$

High B , $\beta \gg 1 \therefore \sigma_{xy} = -\frac{nq^2\tau}{m} \frac{1}{\beta} = -\frac{nq^2\tau}{m} \frac{1}{qB\tau} = -\frac{nq}{B} = -\frac{ne}{B}$

(as $q = -e$)

5. Density of states for free electrons

(a) What is the Fermi wavevector and Fermi energy as a function of particle density for a free electron gas in one and two dimensions (define density appropriately)?

(b) Calculate the density of states in energy for free electrons in one and two dimensions. [Answer: $(2m/\pi\hbar^2) \times (\hbar^2/2mE)^{\frac{1}{2}}$, (d=1); $(m/\pi\hbar^2)$, d=2; $(m/\pi^2\hbar^2) \times (2mE/\hbar^2)^{\frac{1}{2}}$, d=3 .]

(c) Show how the 3D density of states can be re-written as

$$(3/2)(n/E_F)(E/E_F)^{\frac{1}{2}}$$

with $n = N/V$.

Solution:

(4)

$$a) \textcircled{1D} \quad N = 2 \cdot (2k_F) \left(\frac{L}{2\pi} \right) \Rightarrow \underline{k_F = \frac{N}{L} \cdot \frac{\pi}{2}}$$

\uparrow \uparrow \uparrow
 2 spin states range of k-space density of allowed k-states, given periodic b.c.

$$E \propto k^2, \quad k \propto n \text{ (\# states bounded by } k)$$

$$\Rightarrow E \propto n^2 \quad \frac{d \ln E}{dE} = 2 \frac{d \ln n}{dE} \Rightarrow \frac{n}{E} \cdot \frac{1}{2} = \frac{dn}{dE} = g(E) \quad (*)$$

$$\Rightarrow g(E) \propto \frac{\sqrt{E}}{E} = \frac{1}{\sqrt{E}}$$

$$\underline{E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m} \left(\frac{\pi}{2} \right)^2 \left(\frac{N}{L} \right)^2}$$

$$b) \text{ From } (*): \quad g(E_F) = \frac{1}{2} \frac{N/L}{2E_F} = \alpha \frac{1}{\sqrt{E_F}}$$

$$\Rightarrow \alpha = \frac{1}{2} \frac{N/L}{\sqrt{E_F}} = \frac{1}{2} \frac{N/L}{N/L} \frac{\sqrt{2m}}{\hbar \pi/2}$$

$$\Rightarrow g(E) = \frac{\alpha}{\sqrt{E}} = \frac{\sqrt{2m}}{\pi \hbar} E^{-1/2}$$

$$a) \textcircled{2D} \quad N = 2 \pi k_F^2 \cdot \left(\frac{A}{(2\pi)^2} \right) \Rightarrow \underline{k_F^2 = 2\pi \frac{N}{A}}$$

$$\underline{E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m} \cdot 2\pi \frac{N}{A}}$$

$$b) \quad E \propto k^2, \quad k^2 \propto n \Rightarrow E \propto n$$

$$\frac{dn}{dE} = \text{const.} = \alpha \cdot E^0 = \frac{n}{E}$$

$$g(E_F) = \frac{N/A}{E_F} = \frac{n}{\pi \hbar^2} = \underline{g(E)}$$

$$c) \quad E \propto k^2, \quad k^3 \propto n \Rightarrow d \ln E = \frac{2}{3} d \ln n$$

$$\frac{1}{E} = \frac{2}{3} \frac{1}{n} \frac{dn}{dE}$$

$$\frac{3}{2} \frac{n}{E} = g(E) = \alpha \frac{E^{3/2}}{E} = \alpha \sqrt{E}$$

$$\text{At } E_F: g(E_F) = \frac{3}{2} \frac{N/V}{E_F} = \alpha \sqrt{E_F}$$

$$\Rightarrow \alpha = \frac{3}{2} \frac{N/V}{E_F^{3/2}}$$

$$\Rightarrow g(E) = \alpha \sqrt{E} = \frac{3}{2} \frac{N/V}{E_F} \cdot \sqrt{\frac{E}{E_F}}$$

6. Thomas-Fermi screening

Show that in a metal, a spatially modulated external potential with wavenumber q and amplitude $V_{ext}(q)$, induces a spatially oscillating number density n_{ind} with amplitude

$$n_{ind}(q) = \frac{\epsilon_0 q^2}{e} \frac{V_{ext}(q)}{[1 + q^2/q_{TF}^2]} ,$$

with $q_{TF}^2 = \frac{1}{\pi^2} \frac{m e^2}{\epsilon_0 \hbar^2} k_F = \frac{4}{\pi} \frac{k_F}{a_B} = (\frac{2.95}{\sqrt{r_s}} \text{\AA}^{-1})^2$, the Thomas-Fermi wavevector.

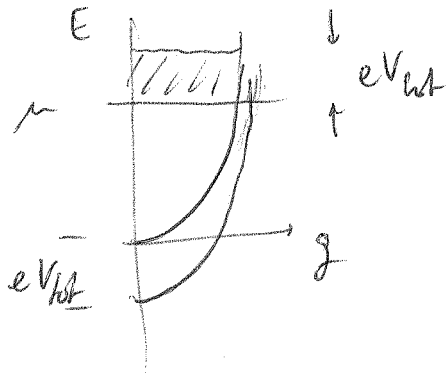
For the potential generated by a localised impurity of charge Q , $V_{ext} = Q/(4\pi\epsilon_0 r)$, show that the induced charge density is then of the form

$$n_{ind}(r) \propto \frac{e^{-r/\xi}}{r}$$

and identify the screening length ξ .

Solution:

(5)



$$n_{\text{mod}} = g(E_F) \cdot eV_{\text{ext}}$$

$$\nabla^2 \delta V = \frac{n_{\text{mod}} e}{\epsilon_0} = \frac{e^2 g}{\epsilon_0} V_{\text{ext}}$$

$$\nabla^2 \delta V = \frac{g e^2}{\epsilon_0} (V_{\text{ext}} + \delta V) \quad (*)$$

Define $g_{\text{TF}}^2 = \frac{g e^2}{\epsilon_0}$

Poisson decomposition of (*): $-g^2 \delta V_g = g_{\text{TF}}^2 V_g + g_{\text{TF}}^2 \delta V_g$

$$\delta V_g = - \frac{g_{\text{TF}}^2}{g^2 + g_{\text{TF}}^2} V_g^{(\text{ext})} \rightarrow n_g^{(\text{mod})} = + g^2 \frac{g_{\text{TF}}^2}{\epsilon_0} \frac{1}{g^2 + g_{\text{TF}}^2} V_g^{(\text{ext})}$$

$$V_{\text{ext}} = \left(1 - \frac{g_{\text{TF}}^2}{g^2 + g_{\text{TF}}^2} \right) V_g^{(\text{ext})} = \frac{g^2}{g^2 + g_{\text{TF}}^2} V_g^{(\text{ext})}$$

For $V_g^{(\text{ext})} = \frac{Q}{4\pi\epsilon_0 r}$, $V_g^{(\text{ext})} = \frac{Q}{\epsilon_0} \frac{1}{g^2}$

($\nabla^2 V_{\text{ext}} = - \frac{Q}{\epsilon_0} \delta(r)$, FT gives $g^2 V_g^{\text{ext}} = \frac{Q}{\epsilon_0}$)

$$\Rightarrow n_g^{(\text{mod})} = \frac{\epsilon_0}{e} g^2 \frac{g_{\text{TF}}^2}{g^2 + g_{\text{TF}}^2} \frac{Q}{\epsilon_0} \frac{1}{g^2} = \frac{Q}{e} \frac{g_{\text{TF}}^2}{g^2 + g_{\text{TF}}^2}$$

FT of $n_g^{(\text{mod})}$ is $n_{\text{mod}}(r) = \frac{Q}{e} \frac{g_{\text{TF}}^2}{4\pi r} e^{-g_{\text{TF}} r} \propto \frac{1}{r} e^{-r/\xi}$

with $\xi = \frac{1}{g_{\text{TF}}}$

①

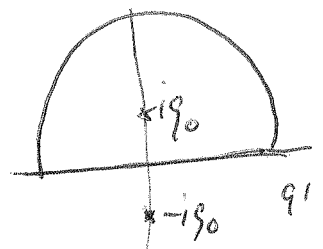
FT of $\frac{1}{q^2 + q_0^2}$ is not part of the exercise, but

here's how it could be done:

$$\int \frac{d^3q}{(2\pi)^3} \frac{1}{q^2 + q_0^2} e^{i\mathbf{q} \cdot \mathbf{r}} = 2\pi \int_{-1}^1 d(\cos\theta) \int_0^\infty \frac{q^2 dq}{(2\pi)^3} \frac{e^{iq\cos\theta r}}{q^2 + q_0^2} =$$

$$= \frac{1}{(2\pi)^2} \int_0^\infty \frac{q^2 dq}{q^2 + q_0^2} \frac{1}{ir} (e^{iqr} - e^{-iqr}) =$$

$$= \frac{1}{ir} \frac{1}{(2\pi)^2} \int_{-\infty}^\infty \frac{e^{iqr}}{(q+iq_0)(q-iq_0)} q dq =$$



$$= \frac{1}{ir} \frac{2\pi i}{(2\pi)^2} \cancel{iq_0} e^{-q_0 r} \frac{1}{2\cancel{iq_0}} = \frac{1}{4\pi r} e^{-q_0 r} \quad \checkmark$$

Total induced charge: $\int n_{\text{ind}}(\mathbf{r}) d^3r = n_{\text{ind}}(q=0)$

$$n_{\text{ind}}(q=0) = \frac{Q}{e} \frac{q_{\text{TF}}^2}{0^2 + q_{\text{TF}}^2} = \frac{Q}{e} \quad \text{exactly cancels}$$

introduced external charge Q .

7. Diatomic molecule

This is a simple problem to illustrate the physics of a diatomic molecule. It also provides an elementary example of the *Linear Combination of Atomic Orbitals* (LCAO), or tight binding method, which we shall be using later to describe extended solids.

We restrict the basis of states to just the ground state of each atom in isolation, whereas of course an accurate solution would require a complete set of states that of necessity would include all the excited states of the atoms. The basis set consists of two states $|a\rangle$ and $|b\rangle$ that satisfy

$$H_a|a\rangle = E_a|a\rangle \quad (12)$$

$$H_b|b\rangle = E_b|b\rangle \quad (13)$$

and we look for solutions

$$|\psi\rangle = \alpha|a\rangle + \beta|b\rangle \quad (14)$$

Neglecting the direct matrix elements $\langle a|b\rangle$ for simplicity (these are easily included if necessary), derive the matrix equation for the wavefunctions and eigenvalues

$$\begin{pmatrix} H_{aa} - E & H_{ab} \\ H_{ba} & H_{bb} - E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad (15)$$

where the matrix elements are of two kinds:

Onsite, or *crystal field* terms

$$H_{aa} = \langle a|T + V_a + V_b|a\rangle = E_a + \langle a|V_b|a\rangle = \tilde{E}_a \quad (16)$$

Offsite, or *hopping* terms

$$H_{ab} = \langle a|T + V_a + V_b|b\rangle = t \quad (17)$$

(Note that the sign of t depends on the symmetry of the orbitals: for s-states, with an attractive potential $V_i < 0$, then t is negative; but for p_x states t is positive for atoms aligned along x.)

Solve for the wavefunctions and eigenvalues, for $t < 0$.

Sketch the wavefunctions and charge densities for the lower and upper states, in the cases of (a) identical atoms $\tilde{E}_a = \tilde{E}_b$, and (b) the strongly ionic limit $\tilde{E}_a - \tilde{E}_b \gg |t|$

Solution:

⑦

$$H_{aa} = \langle a | H | a \rangle$$

$$H_{bb} = \langle b | H | b \rangle$$

$$H_{ab} = \langle a | H | b \rangle$$

$$H_{ba} = H_{ab}^* = \langle b | H | a \rangle$$

$$|\psi\rangle = \alpha |a\rangle + \beta |b\rangle \quad \text{eigenstate of } \hat{H}$$

Apply \hat{H} :

$$H|\psi\rangle = \alpha H|a\rangle + \beta H|b\rangle = \alpha E|a\rangle + \beta E|b\rangle$$

Left multiply $\langle a|$, $\langle b|$:

$$\alpha H_{aa} + \beta H_{ab} = \alpha E$$

$$\alpha H_{ab}^* + \beta H_{bb} = \beta E$$

$$\Rightarrow \begin{pmatrix} H_{aa} & H_{ab} \\ H_{ab}^* & H_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

non-trivial sol of $\begin{vmatrix} H_{aa} - E & H_{ab} \\ H_{ab}^* & H_{bb} - E \end{vmatrix} = 0$

$$E = \frac{H_{aa} + H_{bb}}{2} \pm \left(\left(\frac{H_{aa} - H_{bb}}{2} \right)^2 + |H_{ab}|^2 \right)^{1/2}$$

①

Or, using matⁿ on question sheet

$$H_{aa} = \tilde{E}_a, \quad H_{bb} = \tilde{E}_b, \quad H_{ab} = t$$

$$E = \frac{\tilde{E}_a + \tilde{E}_b}{2} \pm \left(\left(\frac{\tilde{E}_a - \tilde{E}_b}{2} \right)^2 + |t|^2 \right)^{1/2}$$

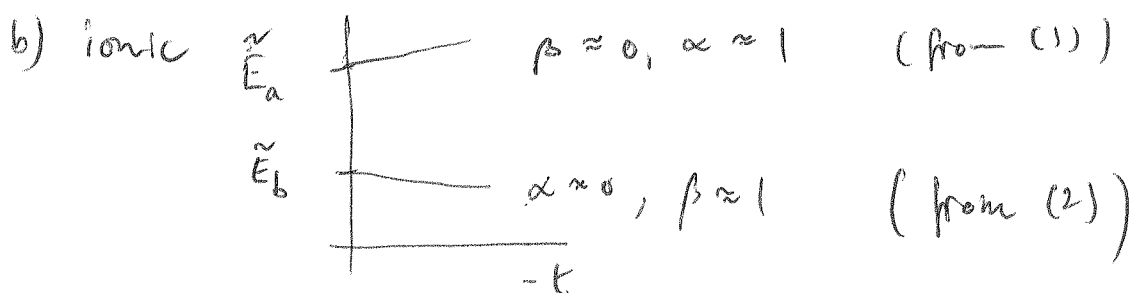
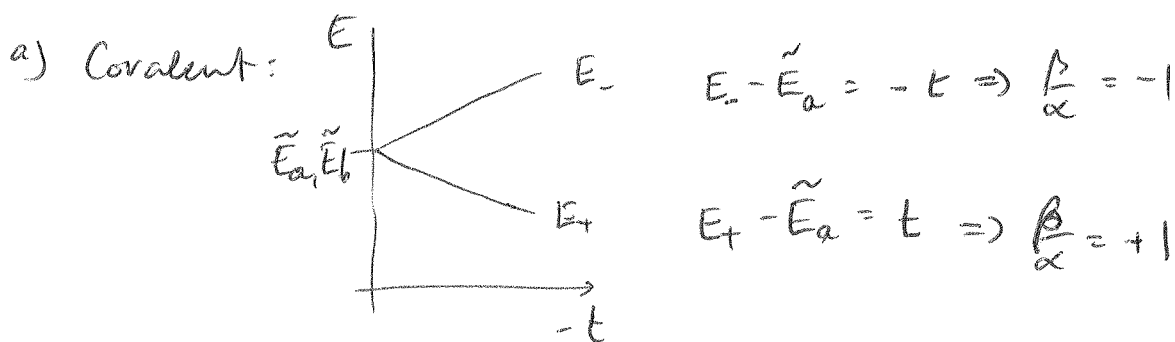
EI - vectors:

$$(\tilde{E}_a - E)\alpha = -t\beta \quad \text{---} \quad (1)$$

$$(\tilde{E}_b - E)\beta = -t^*\alpha \quad (2)$$

$$\Rightarrow (1): \quad \frac{\beta}{\alpha} = \frac{E - \tilde{E}_a}{t}$$

$$(2): \quad \frac{\alpha}{\beta} = \frac{E - \tilde{E}_b}{t^*}$$



8. BCC and FCC lattices

Show that the reciprocal lattice of a body centred cubic lattice (BCC) of spacing a is a face centred cubic (FCC) lattice of spacing $4\pi/a$; and that the reciprocal lattice of a FCC lattice of spacing a is a BCC lattice of spacing $4\pi/a$.

Solution: Apply

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

etc. ...

Note that $\mathbf{g} \cdot \mathbf{R} = 2\pi n$ with \mathbf{g} = reciprocal lattice vector and \mathbf{R} = real space lattice vector defines the reciprocal lattice. By relabelling, we can show that the reciprocal of the reciprocal will give back the original lattice.

9. Reciprocal lattice cell volume

Show that the volume of the primitive unit cell of the reciprocal lattice is $(2\pi)^3/\Omega_{\text{cell}}$, where Ω_{cell} is the volume of the primitive unit cell of the crystal.

$$\begin{aligned} \mathbf{a}_1^* (\mathbf{a}_2^* \times \mathbf{a}_3^*) &= \left(\frac{2\pi}{\Omega_{\text{cell}}} \right)^3 (\mathbf{a}_2 \times \mathbf{a}_3) ((\mathbf{a}_3 \times \mathbf{a}_1) \times (\mathbf{a}_1 \times \mathbf{a}_2)) = \\ &= \left(\frac{2\pi}{\Omega_{\text{cell}}} \right)^3 (\mathbf{a}_2 \times \mathbf{a}_3) \left[\underbrace{\mathbf{a}_1}_{\Omega_{\text{cell}}} \underbrace{((\mathbf{a}_3 \times \mathbf{a}_1) \cdot \mathbf{a}_2)}_{\Omega_{\text{cell}}} - \cancel{\mathbf{a}_2 ((\mathbf{a}_3 \times \mathbf{a}_1) \cdot \mathbf{a}_1)} \right] \\ &= \frac{(2\pi)^3}{\Omega_{\text{cell}}} \quad \checkmark \end{aligned}$$

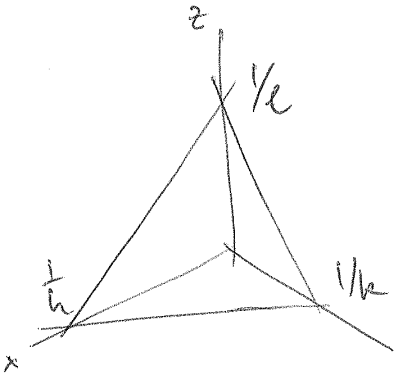
10. Bragg's law

- Show that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to the (hkl) plane of the crystal lattice.
- Show that the distance between two adjacent (hkl) planes is $2\pi/|\mathbf{G}|$.
- Show that the condition $\mathbf{k} \cdot \frac{\mathbf{G}}{2} = \left(\frac{G}{2}\right)^2$ may be written as

$$\frac{2\pi}{\lambda} \sin \theta = \frac{\pi}{d} \quad (18)$$

where $\lambda = 2\pi/k$, and θ is the angle between the incident beam and the crystal plane.

a)



plane \perp to $h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3$:

$$\left(\frac{1}{h}\underline{a}_1 - \frac{1}{k}\underline{a}_2\right)(h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3) = 0$$

because $\underline{a}_1 \perp \underline{b}_2, \underline{b}_3$
 $\underline{a}_1 \cdot \underline{b}_1 = 2\pi$ etc.

Similarly for a second vector.

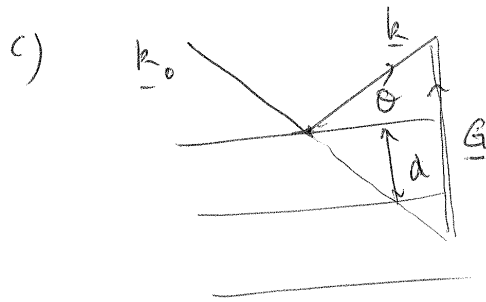
b) One plane goes through 0.

Distance of next plane to 0: $d = \frac{\hat{n} \cdot \underline{x}}{|\underline{n}|}$

\uparrow
any pt. on plane

here: $\underline{n} = \underline{G}$

$$\frac{\underline{G} \cdot \frac{\underline{a}_1}{h}}{|\underline{G}|} = \frac{2\pi}{|\underline{G}|} = d \quad \checkmark$$



$$|k| = |k_0|$$

$$\underline{k} - \underline{G} = \underline{k}_0$$

$$(\underline{k} - \underline{G})^2 = \underline{k}_0^2 = \underline{k}^2 - 2\underline{k} \cdot \underline{G} + \underline{G}^2$$

$$\Rightarrow \left(\frac{G}{2}\right)^2 = \underline{k} \cdot \underline{G} \cdot \frac{1}{2} \quad \checkmark$$

But also, from picture, $|G| = 2|k| \sin \theta$

From previous part of question: $|G| = n \frac{2\pi}{d}$

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

Bragg condition

G could be a multiple of G_0 , which defines the planes.

11. Acoustic phonon dispersion in the monatomic chain

The equation of motion for a chain of atoms of mass m , which are coupled together by springs with spring constant K , is $m\ddot{u}_n = K(u_{n+1} - u_n) + K(u_{n-1} - u_n)$. Use a plane wave trial function for the displacement of atom n , $u_n(t) = u_0 \cos(qr_n - \omega(q)t)$, to derive the dispersion relation for the one-dimensional monatomic chain:

$$m\omega^2(q) = 2K(1 - \cos(qa)) = 4K \sin^2\left(\frac{qa}{2}\right)$$

$$m \ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n)$$

$$\text{Try } u_n(t) = \text{Re} \left(u e^{i(qR_n - \omega_q t)} \right)$$

$$-m\omega_q^2 = K \left(e^{iqa} + e^{-iqa} - 2 \right)$$

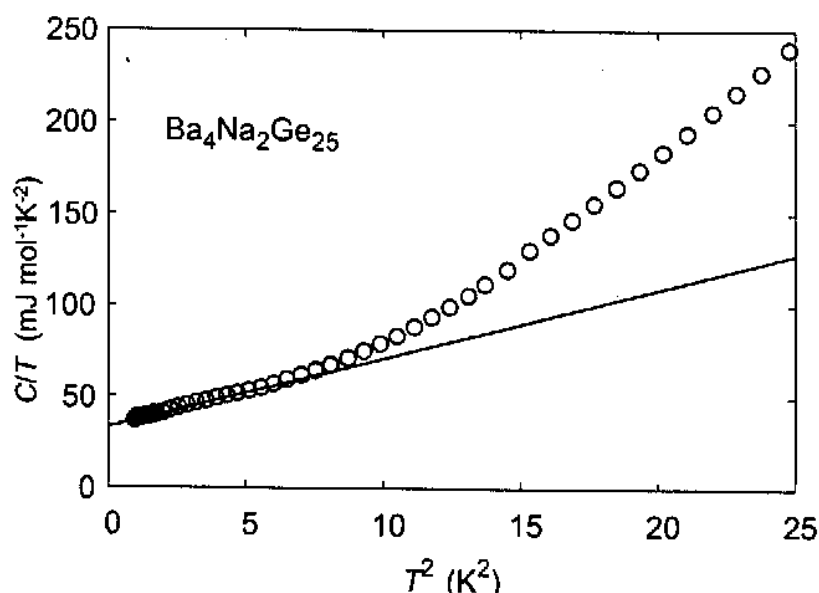
$$\omega_q^2 = 2 \frac{K}{m} (1 - \cos qa) = \frac{4K}{m} \sin^2 \left(\frac{qa}{2} \right)$$

12. Heat capacity of a metal

Show that the molar heat capacity C of metals at low temperature, T , takes the form

$$C = \gamma T + \beta T^3, \quad ,$$

where $\gamma = \frac{\pi^2}{3} k_B^2 g(E_F)$ and $\beta = \frac{12\pi^4}{5} N_A k_B \theta_D^{-3}$ are material dependent constants. $g(E_F)$ is the molar density of states at the Fermi energy, E_F , θ_D is the Debye temperature and N_A is Avogadro's number. [It is not necessary to deduce the precise form of the numerical prefactors.]



The graph above shows the heat capacity per mole of the metallic compound $\text{Ba}_4\text{Na}_2\text{Ge}_{25}$, measured to 5 K and plotted as C/T vs. T^2 . The line is a linear fit to the low-temperature region. The molar volume of $\text{Ba}_4\text{Na}_2\text{Ge}_{25}$ is $V_m = 4.6 \cdot 10^{-4} \text{ m}^3$.

From the measured data, extract the parameter γ and find $g(E_F)$. Assuming a free

electron model with a single, parabolic band and two conduction electrons per formula unit, estimate the Fermi energy and the Fermi wavevector, k_F . Would you expect the Fermi wavevector computed above to lie inside or outside the first Brillouin zone?

From the measured data, extract the parameter β and find θ_D . Estimate the Debye wavevector k_D and the speed of sound in this material.

Why does the measured heat capacity at temperatures $T^2 > 10 \text{ K}^2$ deviate significantly from the low temperature form discussed above? What form do you expect the molar heat capacity to take at even higher temperatures $T \gg \theta_D$?

Solution:

(12)

* $C_{el} = \gamma T$: # el within range $k_B T$ of μ

$$= g(E_F) k_B T. \Rightarrow U_{el} \approx \underbrace{\frac{3}{2} k_B T}_{\text{eq. ferm}} \cdot g(E_F) k_B T$$

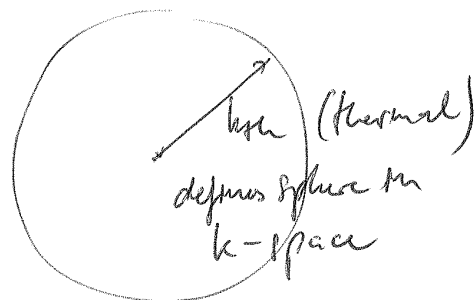
$$\frac{dU_{el}}{dT} = 3 k_B^2 T g(E_F) = C_{el} = \gamma T$$

$$\text{with } \gamma \sim 3 k_B^2 g(E_F) \xrightarrow{\text{exact}} \frac{\pi^2}{3} k_B^2 g(E_F)$$

* $C_{lat} = \beta T$: # phonon modes with energy $< k_B T$

$$= \frac{4\pi}{3} k_{th}^3 \cdot \frac{V}{(2\pi)^3}$$

$$\hbar(\omega_{th}) = \hbar \omega_{th} = k_B T$$



$$\Rightarrow U_{lat} \approx \underbrace{3}_{\text{polarizations}} \cdot \underbrace{\frac{V}{(2\pi)^3}}_{\text{polarizations}} \cdot \frac{4\pi}{3} \left(\frac{k_B T}{\hbar v} \right)^3 \cdot \underbrace{k_B T}_{\text{eq. ferm.}}$$

$$\Rightarrow C_{lat} \approx \cancel{3 k_B} \frac{V}{6\pi^2} \cdot 4 \left(\frac{k_B T}{\hbar v} \right)^3 = 3 k_B N \cdot 4 \left(\frac{k_B T}{\hbar v k_D} \right)^3$$

(Debye wavevector k_D s.t. $\frac{4\pi}{3} k_D^3 \frac{V}{(2\pi)^3} = N \Rightarrow k_D^3 = 6\pi^2 \frac{N}{V}$)

$$\Rightarrow C_{lat} = 12 R \left(\frac{T}{\Theta_D} \right)^3 \xrightarrow{\text{exact}} \frac{12\pi^4}{5} R \left(\frac{T}{\Theta_D} \right)^3$$

(per mole)

C

From the graph :

$$\gamma = 30 \frac{\text{mJ}}{\text{mol K}^2}, \quad \beta = 4 \frac{\text{mJ}}{\text{mol K}^4}$$

$$g(E_F) = \frac{3}{\pi^2 k_B^2} \gamma = 4.8 \cdot 10^{43} \frac{1}{\text{J}}$$

For parabolic band : $g(E_F) = \frac{3}{2} \frac{2N_A}{E_F} = 4.8 \cdot 10^{43} \frac{1}{\text{J}}$

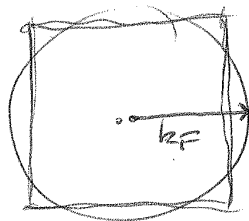
$$\underline{E_F = 0.24 \text{ eV}}$$

$$k_F^3 = 3\pi^2 \frac{N}{V} = 3\pi^2 \frac{2N_A}{V_m} = 7.7 \cdot 10^{28} \frac{1}{\text{m}^3}$$

$$\underline{k_F = 0.42 \text{ \AA}^{-1}}$$

$2e^-/\text{fu} \Rightarrow \text{Volume of BZ} = \text{Volume inside F.S.}$

$k_F > / \text{shortest vector from center of BZ to BZ boundary} /$



$$\beta = 4 \frac{\ln 2}{\ln k^4} = \frac{12.774}{5} R \frac{1}{\theta_D^3} \Rightarrow \theta_D = 81 \text{ K}$$

$$6\pi^2 \frac{N}{V} = k_D^3 = 6\pi^2 \frac{N_A}{V_m} \quad \alpha = K_F \quad \text{in this case}$$

$$k_D = 0.42 \text{ \AA}^{-1}$$

$$\hbar v k_D = k_B \theta_D \Rightarrow v = \frac{k_B}{\hbar k_D} \quad 81 \text{ K} = \underline{\underline{2400 \frac{\text{m}}{\text{s}}}}$$

For $T^2 > 10 \text{ K}^2$, $\frac{C}{T}$ exceeds ρT^2 significantly.

This could be caused by increasing activation of optic modes, which appear to have very low oscillation frequency in this material. Actually, this is due to rattling motion of heavy Ba atoms in the cages. Optic modes can be treated in Einstein model $\rightarrow C \sim e^{-\Delta/k_B T}$, this gives upturn.
 $T \gg \theta_D: C_m \rightarrow 3R \times \# \text{ atoms per f.u.}, \text{ constant.} \quad (3)$

Note: Starred questions are challenge problems; they will do you good, but they go beyond the minimum requirements of the course.