

UNOFFICIAL SOLUTIONS BY TheLongCat

C3: CONDENSED MATTER PHYSICS

TRINITY TERM 2023

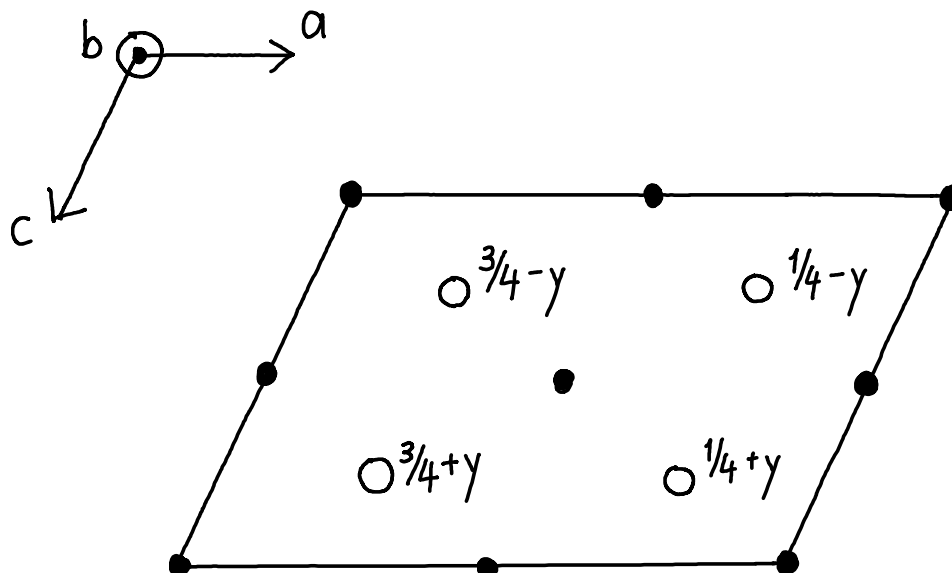
Last updated: 11th February 2025

Disclaimer: due to its unofficial nature, the author does not warrant the accuracy of the presented solutions in any form. However, the author is happy to discuss the typos and errors should one arises.

Turn over as you please – we are NOT under exam conditions here.

1. Symmetry elements in a crystal and the corresponding extinction conditions. If you are comfortable with spotting them under exam conditions then this question can be quite straightforward to solve.¹

(a) Sketch of the crystal:



- i. Inversion points exist at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and all Cu atoms.
 - ii. There exists no mirror plane.
 - iii. We see that there are 2_b about the O atoms. In ac coordinates, they are $(\frac{1}{4}, \frac{1}{4})$, $(\frac{1}{4}, \frac{3}{4})$, $(\frac{3}{4}, \frac{1}{4})$, and $(\frac{3}{4}, \frac{3}{4})$.
 - iv. A diagonal n-glide plane at $b = \frac{1}{4}$.
- (b) From the diagram above, we see that the basis of 2 O's and 1 Cu may be replicated via the translation $a = \frac{1}{2}$, $b = \frac{1}{2} \Rightarrow C$ centering.
- (c) We know that structure factor $S_{hkl} = S_{\text{lattice}} \times S_{\text{basis}}$.

From the C-centering, we have $S_{\text{lattice}} \propto (1 + e^{2\pi i(h/2+k/2)})$. Thus we have $h + k = \text{odd}$ for extinction.

We also have the following symmetry equivalent positions due to the glide: $x, y, z \xrightarrow{\text{glide}} \frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$.

So the structure factor will always have a common factor of:

$$[e^{2\pi i(hx+ky+lz)} + e^{2\pi i(h(1/2+x)+k(1/2-y)+l(1/2+z))}] = e^{2\pi i(hx+ky+lz)} [1 + e^{\pi i(h+l+k-4ky)}]$$

Thus another extinction condition is $k = 0$ and $h + l = \text{odd}$.²

¹That being said, CuO is a monoclinic crystal with space group C2/c. <http://pd.chem.ucl.ac.uk/pdnn/symm3/centred.htm> is an excellent webpage describing it. Apologies if I have missed any symmetry elements in the answer!

²This webpage from UCL is fantastic on summarising glide-derived *reflection* conditions: <http://pd.chem.ucl.ac.uk/pdnn/symm4/glide.htm>

2. A rather rare $\mathbf{k} \cdot \mathbf{p}$ question! Still pretty doable if you stick to the basic principles of perturbation theory.

(a) From Bloch's theorem,

$$\begin{aligned} \psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) &= \psi_{n\mathbf{k}}(\mathbf{r}) \\ \Rightarrow \underbrace{u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R})}_{u_{n\mathbf{k}}(\mathbf{r}) \text{ by definition}} e^{i\mathbf{k} \cdot \mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{R}} &= \underbrace{u_{n\mathbf{k}}(\mathbf{r})}_{u_{n\mathbf{k}}(\mathbf{r})} e^{i\mathbf{k} \cdot \mathbf{r}} \\ \Rightarrow e^{i\mathbf{k} \cdot \mathbf{R}} &= 1 \end{aligned}$$

Hence \mathbf{k} must be a reciprocal lattice vector.

(b) From the Hamiltonian $\mathcal{H} = p^2/2m + V(\mathbf{r})$, we have by TISE:

$$\begin{aligned} \frac{1}{2m} (-i\hbar\nabla) [(-i\hbar\nabla) (u_{n\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}})] + V(\mathbf{r}) u_{n\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} &= E_{n\mathbf{k}} u_{n\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \\ \frac{-i\hbar\nabla}{2m} [-i\hbar\nabla u_{n\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} + \hbar u_{n\mathbf{k}} \mathbf{k} e^{i\mathbf{k} \cdot \mathbf{r}}] + \dots &= \dots \\ \frac{1}{2m} [(-i\hbar\nabla)^2 u_{n\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} + 2\hbar u_{n\mathbf{k}} \mathbf{k} e^{i\mathbf{k} \cdot \mathbf{r}} + \hbar u_{n\mathbf{k}} k^2 e^{i\mathbf{k} \cdot \mathbf{r}}] + \dots &= \dots \\ \Rightarrow \left[\frac{(\mathbf{p} + \hbar\mathbf{k})^2}{2m} + V(\mathbf{r}) \right] u_{n\mathbf{k}} &= E_{n\mathbf{k}} u_{n\mathbf{k}} \end{aligned}$$

(c) We want perturbation so we recast the Hamiltonian in the following form:

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + \lambda \Delta\mathcal{H} \\ &= \left[\frac{p^2}{2m} + V(\mathbf{r}) \right] + \frac{\lambda}{2m} [2\hbar\mathbf{k} \cdot \mathbf{p} + \hbar^2 k^2] \end{aligned}$$

(d) From perturbation theory we have the 1st order energy shift as:

$$\begin{aligned} \Delta E^{(1)} &= \langle u_{20} | \Delta\mathcal{H} | u_{20} \rangle \\ &= \langle u_{20} | \frac{\hbar\mathbf{k} \cdot \mathbf{p}}{m} | u_{20} \rangle + \langle u_{20} | \frac{\hbar^2 k^2}{2m} | u_{20} \rangle \\ &= \frac{\hbar^2 k^2}{2m} \end{aligned}$$

2nd order energy shift:

$$\begin{aligned} \Delta E^{(2)} &= \sum_{n \neq 2} \frac{|\langle u_{n0} | \Delta\mathcal{H} | u_{20} \rangle|^2}{E_{20} - E_{n0}} \\ &= \frac{|\langle u_{10} | \Delta\mathcal{H} | u_{20} \rangle|^2}{E_{20} - E_{10}} \quad \text{for a 2-band, isotropic semiconductor} \\ &= \frac{\left| \langle u_{10} | \frac{\hbar\mathbf{k} \cdot \mathbf{p}}{m} | u_{20} \rangle \right|^2}{E_g} \quad \text{where } E_g \text{ is the band gap} \\ &= \frac{\hbar^2 k^2}{m^2} \cdot \frac{1}{E_g} \cdot P_{12} \end{aligned}$$

So to 2nd order,

$$\begin{aligned} E_{2\mathbf{k}} &= E_{20} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k^2}{m^2} \cdot \frac{P_{12}}{E_g} \\ &= E_{20} + \frac{\hbar^2 k^2}{2m} \left[1 + 2 \frac{P_{12}}{m E_g} \right] \end{aligned}$$

(e) From above,

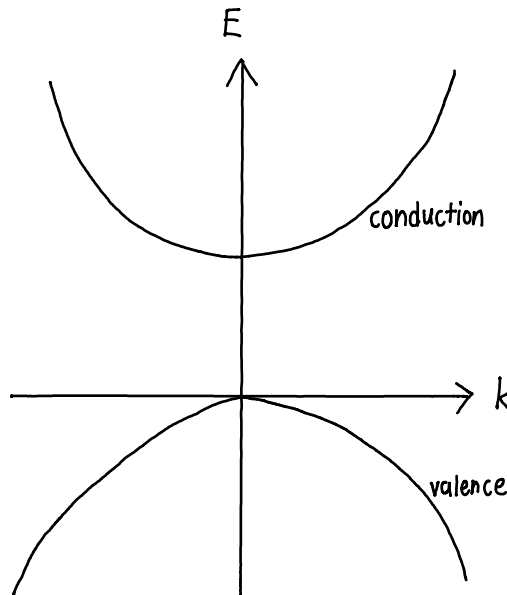
$$\begin{aligned} \frac{\partial^2 E}{\partial k^2} &= \frac{\hbar^2}{m} \left[1 + 2 \frac{P_{12}}{E_g} \right] = \frac{\hbar^2}{m^*} \\ \Rightarrow \frac{1}{m^*} &\propto \frac{1}{E_g} \end{aligned}$$

For holes, we repeat the perturbation from u_{10} instead so we have $\Delta E^{(2)} \rightarrow -\Delta E^{(2)}$.

Hence:

$$\begin{aligned} \frac{1}{m_h^*} &= \frac{1}{m} \left[1 - 2 \frac{P_{12}}{E_g} \right] \\ &\propto -\frac{1}{E_g} \end{aligned}$$

We may illustrate the difference in sign by inspecting the structure of an isotropic quadratic band:



Since the effective mass is defined with respect to the 2nd derivative of a band, it is clear that the only difference between the conduction and valence band here is the sign of the slope, hence the sign difference in effective mass.

3. A classic optical properties question. In fact most of this question is a rehash of Q7 2016!

(a) Substitute $x = x_0 e^{i\omega t}$ into the ODE gives:

$$\begin{aligned} (-\omega^2 - i\gamma\omega + \omega_{\text{TO}}^2) x &= \frac{q}{\mu} E \\ x &= \frac{qE}{\mu} \cdot \frac{1}{(\omega_{\text{TO}}^2 - \omega^2) - i\gamma\omega} \end{aligned}$$

The displacement field D is given as:

$$\begin{aligned} D &= \epsilon_0 E + P + P_{\text{bg}} \\ &= \epsilon_0 \epsilon_r E \end{aligned}$$

where P_{bg} is the background polarisation.

Since polarisation $P = nqx$, we then have:

$$\begin{aligned} \epsilon_r &= 1 + \chi_{\text{bg}} + \frac{nq}{\epsilon_0 E} \cdot \frac{qE}{\mu} \cdot \frac{1}{(\omega_{\text{TO}}^2 - \omega^2) - i\gamma\omega} \\ &= \underbrace{1 + \chi_{\text{bg}}}_{\epsilon_\infty} + \frac{nq^2}{\epsilon_0 \mu \omega_{\text{TO}}^2} \cdot \frac{1}{(\omega_{\text{TO}}^2 - \omega^2) - i\gamma\omega} \\ &= \epsilon_\infty + \underbrace{\frac{nq^2}{\epsilon_0 \mu \omega_{\text{TO}}^2}}_{\epsilon_s} \cdot \frac{1}{(1 - \omega^2/\omega_{\text{TO}}^2) - i\gamma\omega/\omega_{\text{TO}}^2} \\ &= \epsilon_\infty + (\epsilon_s - \epsilon_\infty) \cdot \frac{1}{(1 - \omega^2/\omega_{\text{TO}}^2) - i\gamma\omega/\omega_{\text{TO}}^2} \end{aligned}$$

(b) Note that reflectivity $R = \left| \frac{\tilde{n} - 1}{\tilde{n} + 1} \right|^2$ where complex $\tilde{n} = \sqrt{\epsilon_r}$.

As $\omega \rightarrow \omega_{\text{TO}}$, $\epsilon_r \rightarrow \epsilon_\infty + (\epsilon_s - \epsilon_\infty) \cdot \frac{1}{-i\gamma/\omega_{\text{TO}}} \rightarrow \infty$ for small γ , hence we enter the Reststrahlen regime where EM wave no longer propagates.

At $\epsilon_r = 0$, we enter the LO mode where the polarisation oscillates longitudinally. ($R = 1$ but immediately drops afterwards)

From the graph, we immediately see that:

$$\begin{aligned} \omega_{\text{TO}} &\simeq \frac{30 \text{ meV}}{\hbar} = 4.56 \times 10^{13} \text{ rad s}^{-1} \\ \omega_{\text{LO}} &\simeq \frac{38 \text{ meV}}{\hbar} = 5.77 \times 10^{13} \text{ rad s}^{-1} \end{aligned}$$

Thus:

$$\begin{aligned}
 R &= \left| \frac{\tilde{n} - 1}{\tilde{n} + 1} \right|^2 \\
 \Rightarrow \sqrt{\epsilon_r} - 1 &= (\sqrt{\epsilon_r} + 1) \sqrt{R} \\
 (1 - \sqrt{R}) \sqrt{\epsilon_r} &= \sqrt{R} + 1 \\
 \epsilon_r &= \left(\frac{1 + \sqrt{R}}{1 - \sqrt{R}} \right)^2 \quad \text{assuming real } \epsilon_r
 \end{aligned}$$

So:

$$\begin{aligned}
 \epsilon_\infty &\simeq \left(\frac{1 + \sqrt{0.1}}{1 - \sqrt{0.1}} \right)^2 = 3.71 \\
 \epsilon_s &\simeq \left(\frac{1 + \sqrt{0.3}}{1 - \sqrt{0.3}} \right)^2 = 11.7
 \end{aligned}$$

(c) For $\gamma \ll \omega_{\text{TO}}$, $\epsilon_r \simeq i\omega_{\text{TO}}/\gamma (\epsilon_s - \epsilon_\infty)$ at $\omega = \omega_{\text{TO}}$:

$$\begin{aligned}
 R_{\text{TO}} &= \left| \frac{\sqrt{\omega_{\text{TO}}/\gamma (\epsilon_s - \epsilon_\infty)} e^{i\pi/4} - 1}{\sqrt{\omega_{\text{TO}}/\gamma (\epsilon_s - \epsilon_\infty)} e^{i\pi/4} + 1} \right|^2 \\
 &= \frac{\Omega^2 + 1 - \Omega \cdot 2 \cos \frac{\pi}{4}}{\Omega^2 + 1 + \Omega \cdot 2 \cos \frac{\pi}{4}} \quad \text{where } \Omega = \sqrt{\frac{\omega_{\text{TO}}}{\gamma} (\epsilon_s - \epsilon_\infty)} \\
 &\Rightarrow R_{\text{TO}} (\Omega^2 + \sqrt{2}\Omega + 1) = \Omega^2 - \sqrt{2}\Omega + 1 \\
 &\Rightarrow (1 - R_{\text{TO}}) \Omega^2 + (-\sqrt{2} - \sqrt{2}R_{\text{TO}}) \Omega + (1 - R_{\text{TO}}) = 0 \\
 \Omega &= \frac{\sqrt{2}(1 + R_{\text{TO}}) \pm \sqrt{2(1 + R_{\text{TO}})^2 - 4(1 - R_{\text{TO}})^2}}{2(1 - R_{\text{TO}})} \\
 &\simeq \sqrt{2} \frac{1 + R_{\text{TO}}}{1 - R_{\text{TO}}} \quad \text{picking positive root} \\
 &\Rightarrow \frac{\gamma}{\omega_{\text{TO}}} = \frac{1}{2} (\epsilon_s - \epsilon_\infty) \left(\frac{1 - R_{\text{TO}}}{1 + R_{\text{TO}}} \right)^2
 \end{aligned}$$

(d) From c, we have $\gamma \simeq 7.90 \times 10^9 \text{ s}^{-1} = 1/\tau \Rightarrow \tau \sim 10^{-12} \text{ s}$.

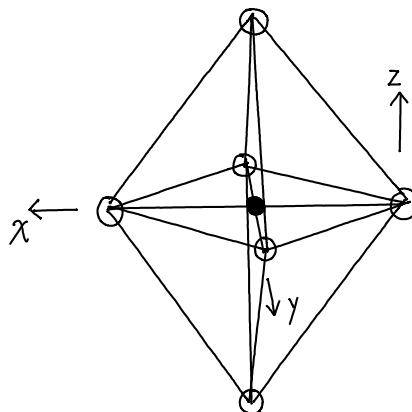
Raman broadening: $\Gamma = \hbar/\tau_{\text{ph}} \Rightarrow \tau_{\text{ph}} \simeq \hbar/2.5 \text{ meV} = 0.4 \text{ ps}$.

The difference between the two can be attributed to the limited resolution of the graphs.

Finite lifetime is due to the higher order process of phonon-phonon scattering (anharmonic term).

4. Another year, another classic magnetism question. Though there is some sprinkles of symmetry breaking this year.

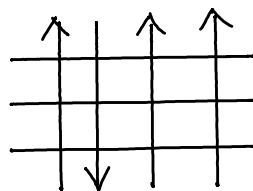
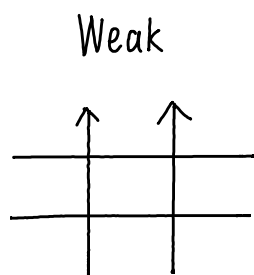
- (a) Orbital quenching: the presence of crystal field perturbs the electrons such that the orbital angular momentum is forced to 0.



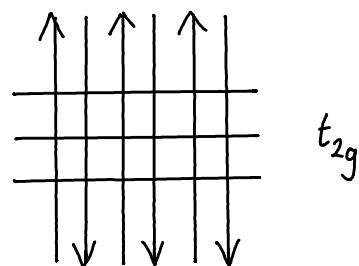
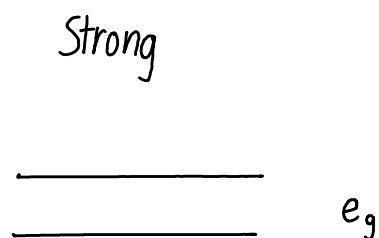
In an octahedral of O^{2-} ions, as the 3d orbitals are subject to different crystal fields:

- e_g : higher energy due to O^{2-} along the Cartesian axes
- t_{2g} : lower energy

So we have the orbital splitting below:



$$S=2 \Rightarrow M=g\mu_B S \simeq 4\mu_B$$



$$S=0 \Rightarrow M=0$$

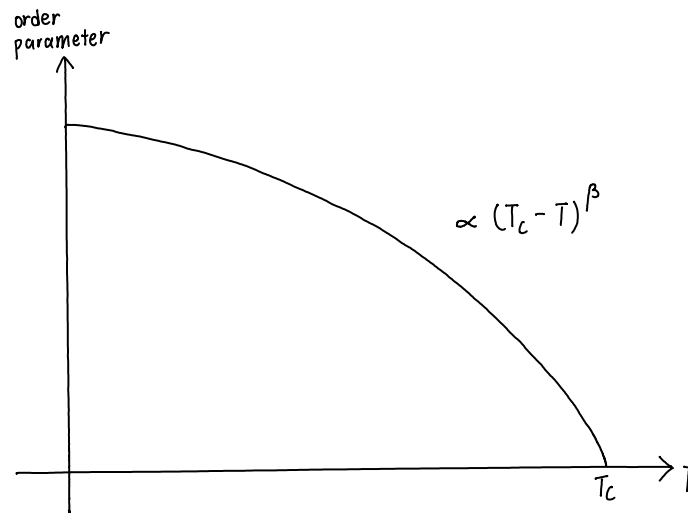
Hund's Rule broken
 \Rightarrow orbital quenching

This leads to the Jahn-Teller effect where the crystal spontaneously deforms to save energy with $\Delta E = E_{\text{elastic}} - E_{\text{static}}$.

- (b) At T_N , as the ordered magnetic state breaks down, time inversion symmetry is no longer present in the system and thus we have a breaking of time inversion symmetry.

The universality class of the transition is *3D Ising*, another example of the same order phase transition is *3D Heisenberg*.

To measure the order parameter in either case, one may perform a neutron diffraction experiment and obtain the intensity I , and the order parameter shall be proportional to its square root: $\phi \propto \sqrt{I}$:

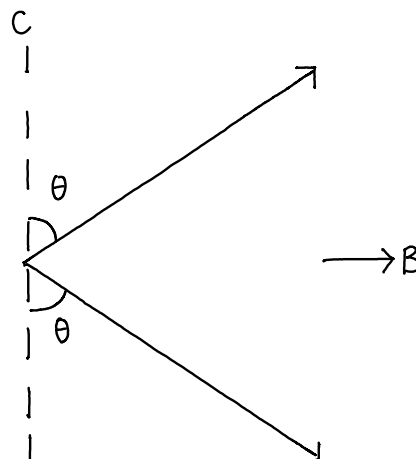


The principle of universality states that for two phase transitions in the same universality class, they should bear the same critical parameters, e.g. β .

Hence by measuring and fitting the temperature dependence of the order parameter against $(T_c - T)^\beta$, we may compare the critical parameters of the two phase transitions and verify if they are of the same universality class.

- (c) Unpacking the nearest-neighbour sum into sum over lattice gives $J \rightarrow J/2$:

$$\mathcal{H} = \sum_{i,j} \frac{J}{2} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i D (S_i^z)^2$$



So:

$$\begin{aligned}\mathbf{S}_i \cdot \mathbf{S}_j &\rightarrow S^2 \sin^2 \theta - S^2 \cos^2 \theta \\ &= -S^2 \cos 2\theta \\ S_i^z &\rightarrow \pm S \cos \theta\end{aligned}$$

Hence spin energy per site is:

$$E_s = -\frac{n}{2}JS^2 \cos 2\theta - DS^2 \cos^2 \theta$$

where $n = 8$ is the number of neighbours.

Adding dipole energy:

$$\begin{aligned}E_d &= \boldsymbol{\mu} \cdot \mathbf{B} \\ &= -g\mu_B S \sin \theta \cdot B \quad \text{due to electron having negative charge}\end{aligned}$$

So total energy per site is:

$$E = -\frac{n}{2}JS^2 \cos 2\theta - g\mu_B SB \sin \theta - DS^2 \cos^2 \theta$$

At stationary state:

$$\begin{aligned}\frac{\partial E}{\partial \theta} &= 0 \\ \Rightarrow nJS^2 \sin 2\theta - g\mu_B BS \cos \theta + 2DS^2 \cos \theta &= 0 \\ \cos \theta [2nJS^2 \sin \theta - g\mu_B BS + 2DS^2 \sin \theta] &= 0 \\ \cos \theta = 0 \quad \text{or} \quad \sin \theta &= \frac{g\mu_B BS}{2nJS^2 + 2DS^2} \\ \sin \theta &= \frac{g\mu_B B}{2S(nJ + D)}\end{aligned}$$

So magnetisation along field per spin:

$$\begin{aligned}M &= -g\mu_B S \sin \theta \\ &= -\frac{(g\mu_B)^2}{2(nJ + D)} \cdot B\end{aligned}$$

(d) Antiferromagnetic: $B = 0$ and $\theta = 0 \Rightarrow E_{\text{AFM}} = -n/2JS^2 - DS^2$.

Equating this to the flip energy at equilibrium:

$$\begin{aligned}E_{\text{sf}} &= \frac{n}{2}JS^2 - DS^2 - g\mu_B BS \\ \Rightarrow B_{\text{sf}} &= \frac{nJS}{g\mu_B}\end{aligned}$$

(e) We know that the slope of the graph for the case $B \perp c$ is:

$$\frac{(g\mu_B)^2}{2(nJ + D)} = \frac{1 \cdot \mu_B}{8 \text{ T}}$$

Also $B_{\text{sf}} \simeq 8 \text{ T}$ gives $g = 2.35$. Combining these equations then gives:

$$J = 0.07 \text{ meV}$$

$$D = 0.72 \text{ meV}$$

Note that $D > J$, this indicates that the Ising model fits the magnet well.

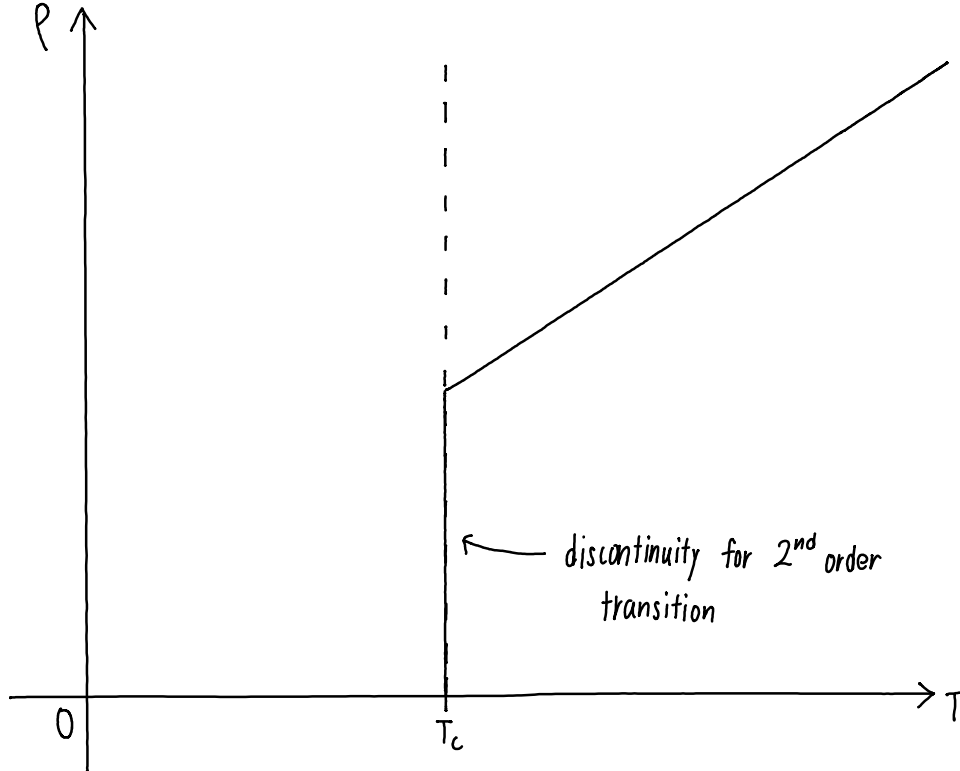
Method: SQUID magnetometer. I shall leave the explanation as an exercise for the reader.

5. Inverse AC Josephson effect and some BCS questions.

(a) Properties of SC:

1. Zero resistivity under critical temperature T_c .
2. Meissner effect: $\chi = -1$ and SC repels all applied field less than the critical field.

Sketch of resistivity ρ against temperature T :



For BCS SC, below $T < T_c$, the Fermi surface destabilises into a gap due to the electrons forming a BCS condensate in terms of Cooper pairs via the electron-phonon interaction.

(b) 1st Josephson equation: $I(\phi) = I_J \sin \phi$

2nd Josephson equation: $V = \frac{\hbar}{2e} \frac{\partial \phi}{\partial t}$

For an AC current,

$$\begin{aligned}
 V &= V_0 + V_{\text{rf}} \cos \omega t \\
 \phi(t) &= \phi_0 + \frac{2eV_0}{\hbar} t + \frac{2eV_{\text{rf}}}{\hbar \omega} \sin \omega t \\
 \Rightarrow I(t) &= I_J \sin \left[\phi_0 + \frac{2eV_0}{\hbar} t + \frac{2eV_{\text{rf}}}{\hbar \omega} \sin \omega t \right] \\
 &= I_J \sum_{n=-\infty}^{\infty} (-1)^n J_n \left(\frac{2eV_{\text{rf}}}{\hbar \omega} \right) \sin \left[\phi_0 + \underbrace{\frac{2eV_0}{\hbar} t - n\omega t}_{(2eV_0/\hbar - n\omega)t} \right]
 \end{aligned}$$

For every $n\omega = \frac{2eV_0}{\hbar}$, the time dependence of I vanishes \Rightarrow DC spikes (Shapiro steps) develop. This is called the inverse AC Josephson effect.

In the presence of microwaves, due to the inverse AC effect, we have a series of Shapiro steps. For the graph without microwaves, we have a voltage biased JJ: the jump in the middle is due to the breakdown of Cooper pairs and voltage develops as a consequence of the presence of normal state electrons \Rightarrow finite R .

The reason why the jump in current is different is due to the RF voltage reducing I_J via the Bessel sum.

We have $I_J \simeq 0.1 \text{ mA}$ and $\omega \simeq 2eV_0/\hbar = 2e/\hbar (2.05 \text{ mV}) = 6.23 \times 10^{12} \text{ rad s}^{-1}$.

- (c) Condensation energy: $E_{\text{cond}} = \frac{B_c^2}{2\mu_0} = g_n - g_s$ where g_n and g_s are the Gibbs free energy per unit volume associated to the normal and SC phases.

Noting that $g = u - Ts + mB$, we have:

$$\begin{aligned} dg &= -s dT + B dm \\ \Rightarrow \text{Entropy} \quad s &= - \left(\frac{\partial g}{\partial T} \right)_B \\ \Rightarrow \text{Heat capacity} \quad c &= \left(\frac{\partial u}{\partial T} \right)_B \\ &= T \left(\frac{\partial s}{\partial T} \right)_B \quad \text{for } du = T ds - m dB \\ &= -T \left(\frac{\partial}{\partial T} \left(\frac{\partial g}{\partial T} \right)_B \right)_B \end{aligned}$$

Hence the jump in heat capacity:

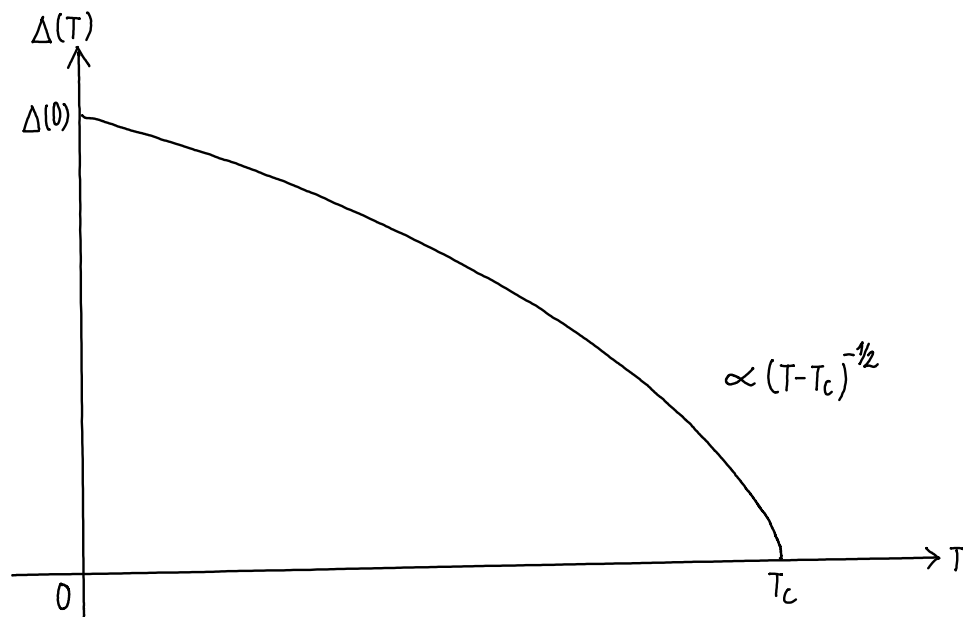
$$\begin{aligned} \Delta c &= -T \left[\frac{\partial}{\partial T} \left(\frac{\partial(\Delta g)}{\partial T} \right)_B \right]_B \\ &= -\frac{TB_0^2}{2\mu_0} \left[\frac{\partial}{\partial T} \left(\frac{\partial}{\partial T} (1 - \alpha t^2 + \beta t^3)^2 \right)_B \right]_B \quad \text{where } \alpha = 1.211, \beta = 0.211, t = T/T_c \\ &= -\frac{TB_0^2}{T_c^2 \mu_0} \left[(1 - \alpha t^2 + \beta t^3) (-2\alpha + 6\beta t) + (-2\alpha t^2 + 3\beta t^2)^2 \right] \\ &= -616 \text{ J K}^{-1} \text{ m}^{-3} \quad \text{at } T = T_c \Rightarrow t = 1 \end{aligned}$$

- (d) From BCS, $\Delta C = 1.43C_n$, and $C_n = \gamma T = 317 \text{ J K}^{-1} \text{ m}^{-3}$, thus $\Delta C = 450 \text{ J K}^{-1} \text{ m}^{-3}$.

- (e) From BCS, $|\Delta(0)| = 2\hbar\omega_{\text{De}}^{-1/\lambda}$ and $k_B T_c \simeq 1.13\hbar\omega_{\text{De}}^{-1/\lambda}$:

$$\begin{aligned} k_B T_c &\simeq 1.13 \frac{\Delta}{2} \\ \Delta &\simeq \frac{k_B T_c}{2.26} \\ &= 1.42 \times 10^{-4} \text{ eV} \end{aligned}$$

Sketch of SC gap against temperature:



As the gap is the result of the electrons at the Fermi surface delocalising to join the Cooper pair condensate, higher density should lead to larger gap.

6. Perhaps the most straightforward question in this paper.

(a) From the question we have:

$$\mathbf{j}_h = - \underset{\kappa_{ij}}{\underset{\square}{\kappa}} \nabla T$$

We also know the tensor transformation law:

$$\kappa'_{ij} = \frac{\partial x'_i}{\partial x_a} \frac{\partial x'_j}{\partial x_b} \kappa_{ab}$$

By Neumann's Principle, the bulk properties of a crystal should reflect its symmetries. In an orthorhombic crystal, we have symmetry elements $2_x, 2_y, 2_z$.

Hence about an axis we have the following 2-fold rotation matrix (about the subspace of its normal plane):

$$\Rightarrow 2_z = \begin{pmatrix} -1 & 0 \\ 0 & -1 \\ & & 1 \end{pmatrix} \quad \text{for example}$$

Now we need the rotated matrix to be invariant \Rightarrow observe that off-diagonal terms have odd parity under a general rotation and must vanish by symmetry.

Hence $\kappa_{ij} = \text{diag}(\kappa_{xx}, \kappa_{yy}, \kappa_{zz})$.

(b) Evaluate $\kappa_{\mathbf{u}}$ as follows:

$$\begin{aligned} \kappa_{\mathbf{u}} &\equiv \frac{\mathbf{j}_h \cdot \hat{\mathbf{u}}}{|\nabla T|} \\ &= \frac{-\kappa \nabla T \cdot \hat{\mathbf{u}}}{|\nabla T|} \\ &= \frac{[\kappa |\nabla T| \hat{\mathbf{u}}] \cdot \hat{\mathbf{u}}}{|\nabla T|} \\ &= \begin{pmatrix} \kappa_{xx} u_x & \kappa_{yy} u_y & \kappa_{zz} u_z \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} \\ &= u_x^2 \kappa_{xx} + u_y^2 \kappa_{yy} + u_z^2 \kappa_{zz} \quad \text{in orthorhombic crystal} \end{aligned}$$

(c) We know $a = 0.575 \text{ nm}$, $b = 0.587 \text{ nm}$, $c = 0.769 \text{ nm}$, and that $\widehat{\mathbf{a} + \mathbf{b}} = \frac{a\hat{\mathbf{x}} + b\hat{\mathbf{y}}}{\sqrt{a^2 + b^2}}$:

$$\begin{aligned} \kappa_{[110]} &= \left(\frac{a}{\sqrt{a^2 + b^2}} \right)^2 \kappa_{xx} + \left(\frac{b}{\sqrt{a^2 + b^2}} \right)^2 \kappa_{yy} + 0 \\ &= 24.2 \text{ W m}^{-1} \text{ K}^{-1} = \frac{a^2 \kappa_{xx} + b^2 \kappa_{yy}}{a^2 + b^2} \end{aligned} \quad (1)$$

Similarly,

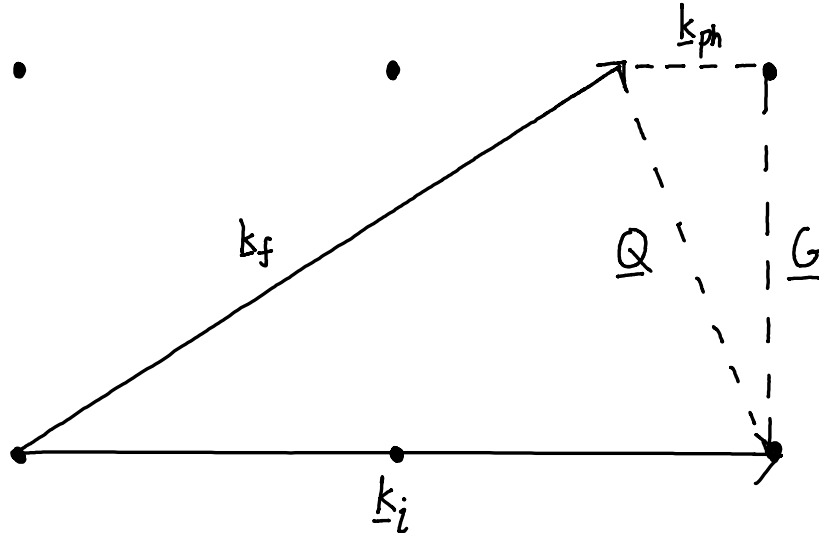
$$\begin{aligned}\kappa_{[1\bar{2}0]} &= \left(\frac{a}{\sqrt{a^2 + 4b^2}} \right)^2 \kappa_{xx} + \left(\frac{2b}{\sqrt{a^2 + 4b^2}} \right)^2 \kappa_{yy} + 0 \\ &= 28.1 \text{ W m}^{-1} \text{ K}^{-1} = \frac{a^2 \kappa_{xx} + 4b^2 \kappa_{yy}}{a^2 + 4b^2}\end{aligned}\quad (2)$$

$$\begin{aligned}\kappa_{[001]} &= 0 + 0 + \left(\frac{c}{\sqrt{c^2}} \right) \kappa_{zz} \\ &= 5.4 \text{ W m}^{-1} \text{ K}^{-1} = \kappa_{zz}\end{aligned}\quad (3)$$

Combining (1) and (2) gives:

$$\begin{aligned}\kappa_{xx} &= 17.5 \text{ W m}^{-1} \text{ K}^{-1} \\ \kappa_{yy} &= 30.6 \text{ W m}^{-1} \text{ K}^{-1}\end{aligned}$$

(d) Momentum transfer triangle in a reciprocal lattice:



We know that phase velocity $v = \omega/k$ and $\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i = \mathbf{G} + \mathbf{k}_{ph}$ where \mathbf{k}_{ph} is a wavevector in the 1st BZ by the periodicity in the reciprocal lattice.

We then find the wavevector of the phonons ($q_1 = 0.13$, $q_2 = 0.10$):

$$\begin{aligned}k_1 &= q_1 \times \frac{2\pi}{a} \\ &= 1.42 \times 10^9 \text{ m}^{-1} \\ k_2 &= q_2 \times \frac{2\pi}{b} \\ &= 1.07 \times 10^9 \text{ m}^{-1}\end{aligned}$$

Hence the velocity of sound along each principal axis is ($\omega = 2\pi (1.0 \times 10^{12} \text{ Hz}) = 6.28 \times 10^{12} \text{ rad s}^{-1}$):

$$\begin{aligned} v_1 &= \frac{\omega}{k_1} \\ &= 4420 \text{ m s}^{-1} \\ v_2 &= \frac{\omega}{k_2} \\ &= 5870 \text{ m s}^{-1} \end{aligned}$$

Note that phonon propagation has an anisotropy in the ab plane, since thermal conduction in a solid largely stems from phonon propagation, this physically leads to the anisotropy in heat conduction. Also larger $v \rightarrow$ larger κ .