

UNOFFICIAL SOLUTIONS BY TheLongCat

C3: CONDENSED MATTER PHYSICS

TRINITY TERM 2024

Last updated: 11th July 2024

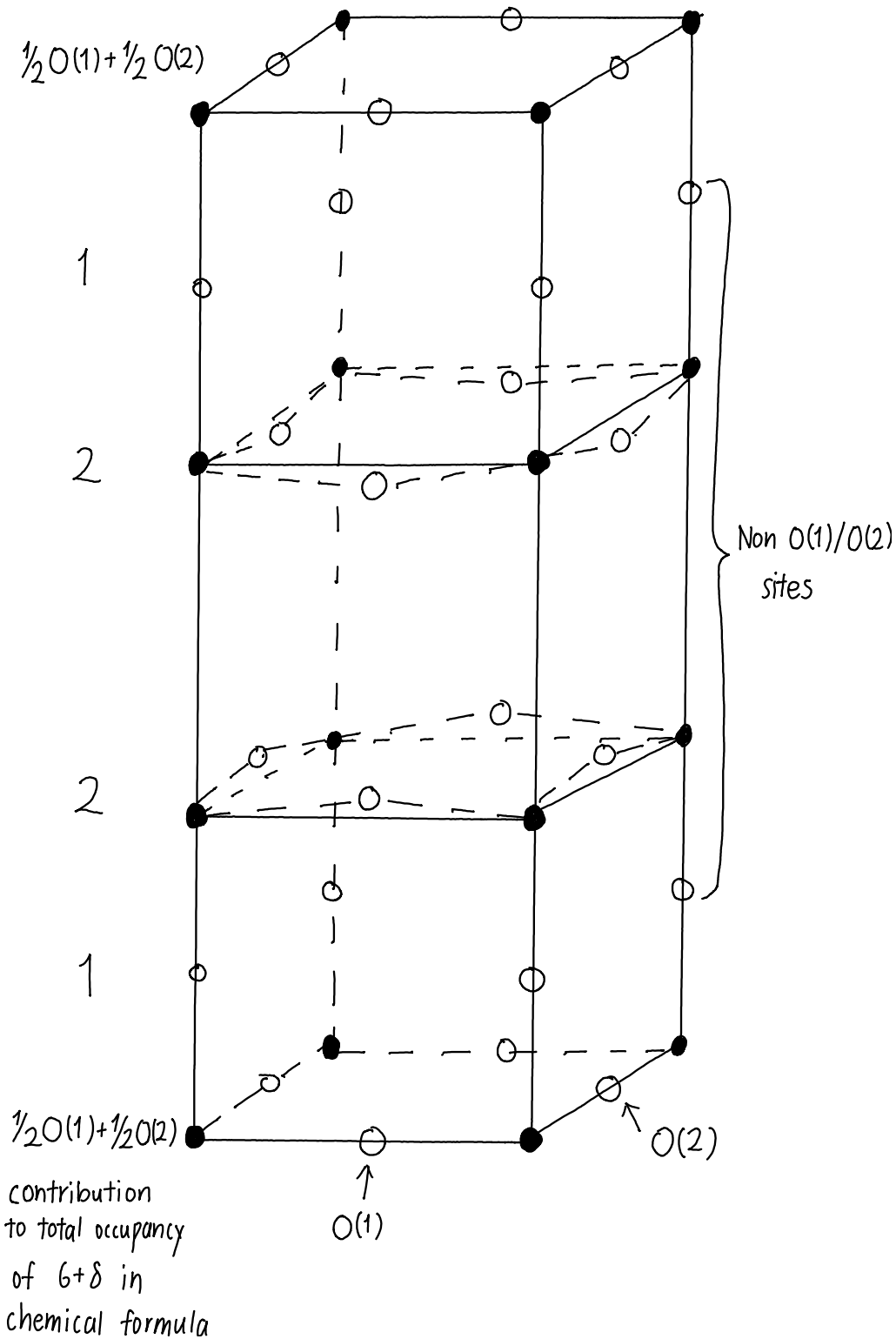
Disclaimer: due to its unofficial nature, the author does not warrant the accuracy of the presented solutions in any form. However, the author is happy to discuss the typos and errors should one arises.

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

1. (DRAFT) Crystallography question on a YBCO¹ crystal.

(a) If all oxygen sites are fully occupied, we have an occupancy of 8.

However for $\delta = 0.5$, the occupancy would be $6 + 0.5 = 6.5$.



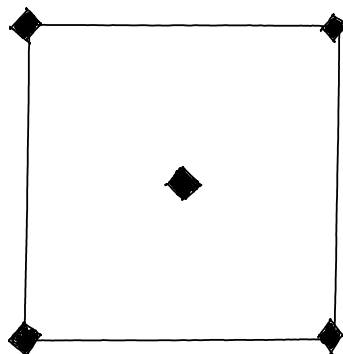
¹Speaking of which, my friend has recently recommended me this awesome video of someone growing a YBCO superconductor *by himself*: <https://www.youtube.com/watch?v=sLFaa6RPJIU>

With the sketch as aid (ignoring Y and Ba atoms), we proceed to find the average fractional occupancy f of the degenerate O(1)/O(2) sites:

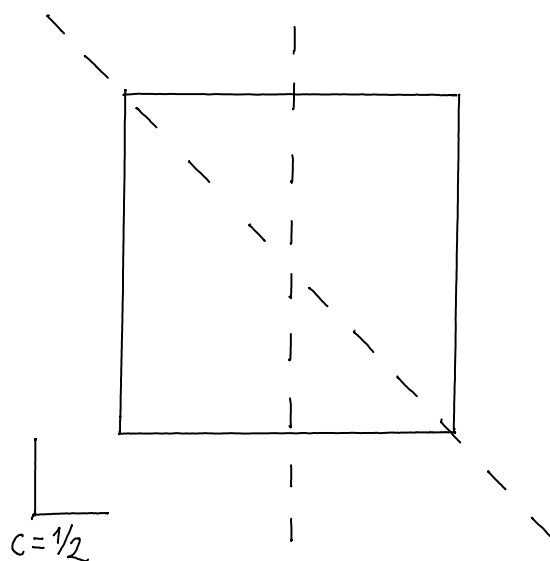
$$\begin{aligned} 2f &= 0.5 \\ \Rightarrow f &= 0.25 \end{aligned}$$

(b) Drawing out tetragonal symmetry elements should do the job.

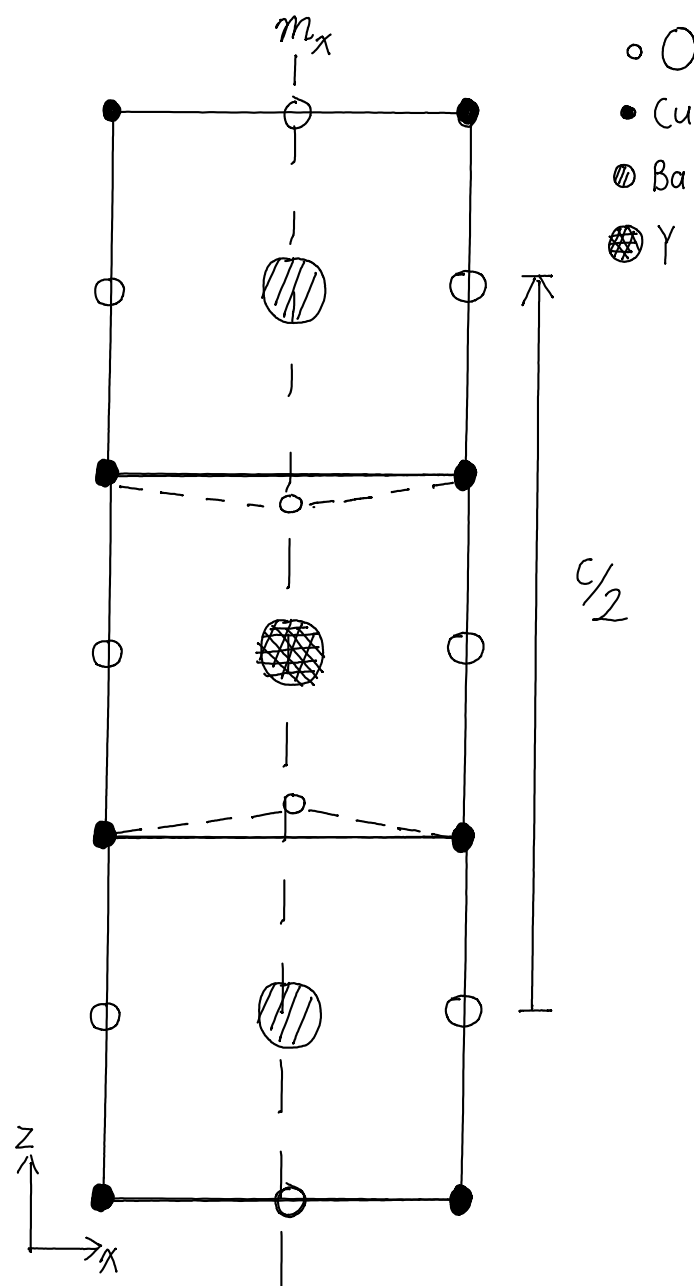
i. **(TO BE VERIFIED)** Naturally we have a 4-fold axis about the c-axis about $(\frac{1}{2}, \frac{1}{2})$.



ii. Mirror planes along a/b axes and the diagonals, and a m_z at $c = \frac{1}{2}$.



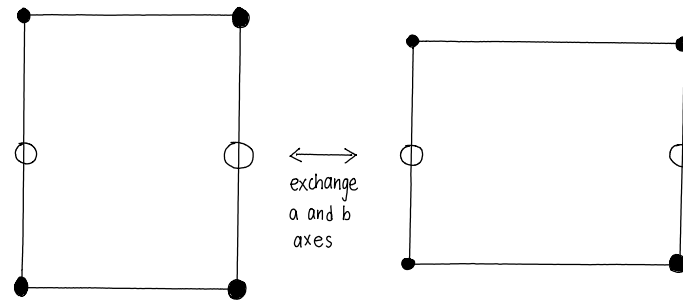
iii. Glide plane of m_x with translation of $\frac{1}{2}$ along the c-axis.



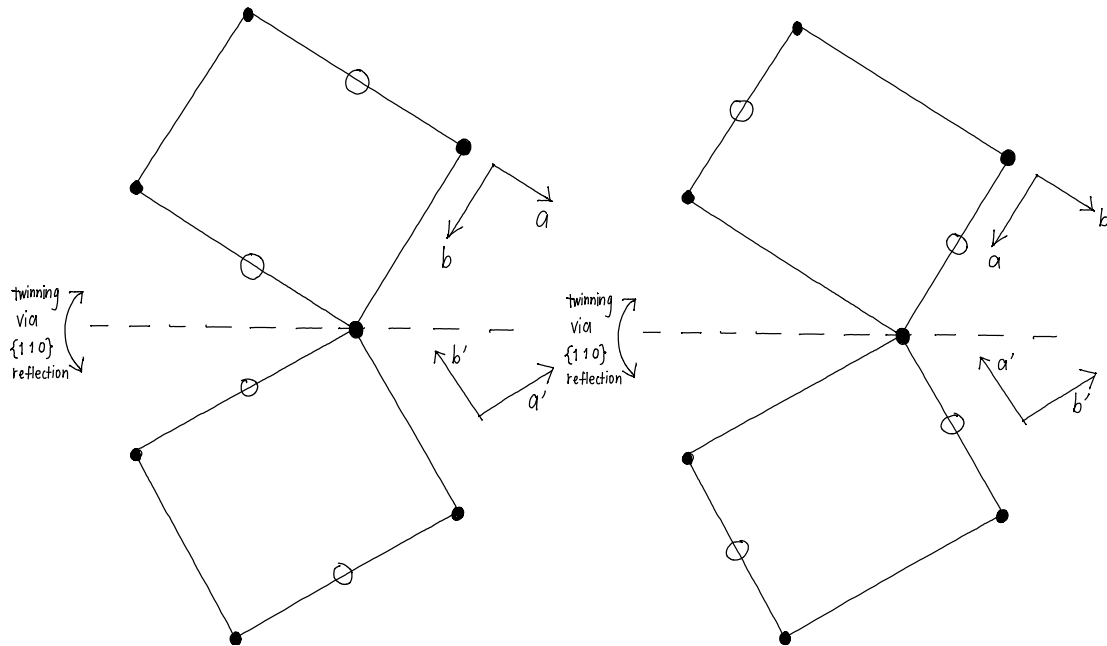
(c) As the crystal undergoes transition from tetragonal to orthorhombic structure, the symmetry between a and b axes is lost.

Therefore of all the symmetry elements listed in part b, the 4-fold rotation axes and the diagonal mirror plane are no longer present.

(d) Sketches of $z = 0$ layer illustrating the domains:



Sketches illustrating twinning structures:



(e) **(TO BE VERIFIED)** As mentioned above, when the YBCO undergoes transition from the tetrahedral to the orthorhombic structure, it loses the symmetry between the a and b axes. This gives rise to the splitting of the $(h00)$ and the $(0k0)$ peaks.

In addition, a crystal may also possess structural defects such as domains and micro-twins as described above. This introduces the asymmetry in the crystal, thereby causing further splits in the peaks – there should be 3 split peaks for each orthorhombic sub-peak from the reflection in the (110) and $(\bar{1}10)$ planes.

In total we then may have up to 6 split peaks.

2. Density of states of a non-parabolic dispersion relation.

Despite the seeming difficulty, it is perfectly doable with the hints given².

(a) Straightforward calculation from the fact that we have an *isotropic* band, thus

$$\begin{aligned} A(k_{||}) &= \pi k^2 \\ \Rightarrow \frac{\partial A}{\partial k} &= 2\pi k \end{aligned}$$

By chain rule, we have $\frac{\partial A}{\partial \epsilon} = \frac{\partial A}{\partial k} \frac{dk}{d\epsilon}$:

$$\begin{aligned} \omega_c &= \frac{2\pi eB}{\hbar^2} \times \frac{d\epsilon}{dk} \times \frac{1}{2\pi k} \\ &= \frac{eB}{\hbar^2} \frac{d\epsilon/dk}{k} \end{aligned} \quad (1)$$

(b) Implicitly differentiating the given dispersion gives (here $\epsilon' = d\epsilon/dk$):

$$\begin{aligned} \epsilon' + \frac{2\epsilon\epsilon'}{E_g} &= \frac{\hbar^2 k}{m_0^*} \\ \Rightarrow \epsilon' &= \frac{\hbar^2 k}{m_0^*} \left[1 + \frac{2\epsilon}{E_g} \right]^{-1} \end{aligned} \quad (2)$$

Plugging (2) into (1) then gives:

$$\begin{aligned} \omega_c &= \frac{eB}{\hbar^2 k} \frac{\hbar^2 k}{m_0^*} \left[1 + \frac{2\epsilon}{E_g} \right]^{-1} \\ &= \frac{eB}{m_0^*} \frac{1}{1 + 2\epsilon/E_g} \end{aligned}$$

(c) Here we need to use the definition of cyclotron frequency $\omega_c = \frac{eB}{m_c}$, where m_c is the cyclotron mass. Comparing the two expression then gives:

$$m_c = m_0^* \left[1 + \frac{2\epsilon}{E_g} \right]$$

(d) Following the hints and taking care that we have a **3D** (see footnote ☺) integral:

$$\begin{aligned} g(E) &= \frac{2}{V} \sum_{\mathbf{k}} \delta[E - \epsilon(\mathbf{k})] \\ &\rightarrow \frac{2}{V} \times \frac{V}{(2\pi)^3} \int d^3\mathbf{k} \delta[E - \epsilon(\mathbf{k})] \quad \text{by continuum approximation} \\ &= \frac{2}{(2\pi)^3} \int dk \, 4\pi k^2 \delta[E - \epsilon(\mathbf{k})] \end{aligned}$$

²Though sadly the author rolled a 1 in perception and failed to spot the boldface \mathbf{k} in the hint given and lost 7 easy marks in part d...

From (2) we have $k dk = \frac{m_0^*}{\hbar^2} \left[1 + \frac{2\epsilon}{E_g} \right] d\epsilon$, combining this together with k from the dispersion then gives:

$$\begin{aligned} g(E) &= \frac{1}{\pi^2} \int d\epsilon \frac{\sqrt{2}m_0^{*3/2}}{\hbar^3} \left(1 + \frac{2\epsilon}{E_g} \right) \sqrt{\epsilon \left[1 + \frac{\epsilon}{E_g} \right]} \delta[E - \epsilon] \\ &= \underbrace{\frac{\sqrt{2}m_0^{*3/2}}{\pi^2 \hbar^3}}_{\alpha} \left(1 + \frac{2E}{E_g} \right) \sqrt{E \left[1 + \frac{E}{E_g} \right]} \end{aligned}$$

as per the properties of the delta function.

- (e) In the limit of $E/E_g \ll 1$, we may drop the ϵ/E_g term in the dispersion to get the parabolic dispersion immediately. Similar result follows for the cyclotron mass.

For d.o.s., we may drop higher order terms in the following expansion:

$$\begin{aligned} \lim_{E/E_g \rightarrow 0} g(E) &= \lim_{E/E_g \rightarrow 0} \alpha \sqrt{E} \left(1 + \frac{2E}{E_g} \right) \left[1 + \frac{E}{2E_g} + \dots \right] \\ &= \lim_{E/E_g \rightarrow 0} \alpha \sqrt{E} \left(1 + \frac{5}{2} \frac{E}{E_g} + \dots \right) \\ &= \alpha \sqrt{E} \end{aligned}$$

And we have now recovered the parabolic d.o.s.!

- (f) For the parabolic approximation to fit within the dispersion above with an accuracy of 10%, we construct the following ratio (for that $g(E)$ determines almost all properties of a material):

$$\begin{aligned} \frac{\alpha \left(1 + \frac{2E}{E_g} \right) \sqrt{E \left[1 + \frac{E}{E_g} \right]}}{\alpha \sqrt{E}} &= 110\% \\ \Rightarrow \left(1 + \frac{2E}{E_g} \right) \sqrt{1 + \frac{E}{E_g}} &= 1.1 \end{aligned} \quad (3)$$

From here we could meticulously solve the cubic equation, however we can binomial expand (3) in hopes of the results being small³:

$$\begin{aligned} \left(1 + \frac{2E}{E_g} \right) \left[1 + \frac{E}{2E_g} \right] &= 1.1 \\ \left(\frac{E}{E_g} \right)^2 + \frac{5}{2} \frac{E}{E_g} - 0.1 &= 0 \\ \frac{E}{E_g} &= \frac{-5/2 \pm \sqrt{25/4 + 0.4}}{2} \\ &= 0.0394 \end{aligned}$$

where the unphysical negative root is dropped.

³As reassurance, the actual roots are pretty small: 0.03946 and the unphysical roots of $-1.01973 \pm 0.53910i$.

For the final part of this question, we simply plug in the value of the band gap for each semiconductor.

InAs:

$$\begin{aligned} E &= 0.0394 \times 0.35 \text{ eV} \\ &= 0.0138 \text{ eV} \end{aligned}$$

GaSb:

$$\begin{aligned} E &= 0.0394 \times 0.73 \text{ eV} \\ &= 0.0287 \text{ eV} \end{aligned}$$

GaAs:

$$\begin{aligned} E &= 0.0394 \times 1.42 \text{ eV} \\ &= 0.0559 \text{ eV} \end{aligned}$$

3. Classic optical properties question.

- (a) Standard derivation. You really should know how to do this off your head by the time you read this.

Anyway standard answers below:

As usual, to find relative permittivity ϵ_r we shall imagine the system as a collection of electric dipoles \rightarrow *find displacement \mathbf{x} first!*

Plugging in Ansatz $\mathbf{x} = \mathbf{x}_0 \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]$ gives

$$\begin{aligned} -m\omega^2 \mathbf{x}_0 - im\gamma\omega \mathbf{x}_0 &= q\mathbf{E}_0 \\ \Rightarrow \mathbf{x}_0 &= \frac{q\mathbf{E}_0}{-m\omega^2 - im\gamma\omega} \end{aligned}$$

where $\gamma = \tau^{-1}$.

Next we find polarisation $\mathbf{P} = Nq\mathbf{x}$, combining this together with the definition of the displacement field $\mathbf{D} = \epsilon_0\mathbf{E} + \mathbf{P} + \mathbf{P}_{\text{bg}} = \epsilon_0\epsilon_r\mathbf{E}$, where \mathbf{P}_{bg} is the background polarisation, then gives

$$\begin{aligned} \epsilon_r &= 1 + \chi_{\text{bg}} + \frac{Nq\mathbf{x}}{\epsilon_0\mathbf{E}} \\ &= 1 + \chi_{\text{bg}} + \frac{Nq\mathbf{x}_0}{\epsilon_0\mathbf{E}_0} \\ &= \underbrace{1 + \chi_{\text{bg}}}_{\epsilon_\infty} + \frac{Nq^2}{\epsilon_0(-m\omega^2 - im\gamma\omega)} \\ &= \epsilon_\infty + \frac{\epsilon_\infty\omega_p^2}{-\omega^2 - i\gamma\omega} \\ &= \epsilon_\infty \left(1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} \right) \end{aligned}$$

where $\omega_p^2 = \frac{Nq^2}{m\epsilon_0\epsilon_\infty}$ is the plasma frequency.

- (b) Lookup from the graph to get N . I picked the high-frequency limit so $\epsilon_r \rightarrow \epsilon_\infty (1 - \omega_p^2/\omega^2)$.

Then we have reflectivity R with the complex refractive index $\tilde{n} = \sqrt{\epsilon_r}$:

$$R = \left| \frac{\tilde{n} - 1}{\tilde{n} + 1} \right| \quad (4)$$

Rearranging (4) gives

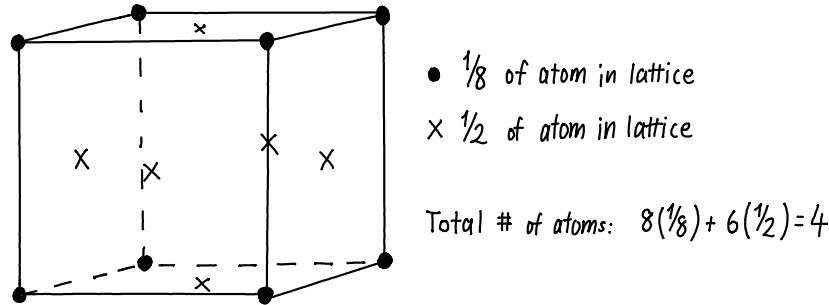
$$|\epsilon_r| = \left| \frac{1 + R}{1 - R} \right|^2 \quad (5)$$

Plugging in $R = 0.05$, $\hbar\omega = 21 \text{ eV}$, and $\epsilon_\infty = 1$ due to aluminium being metal (or from the graph $R(\omega \rightarrow \infty) = 0$) gives

$$\begin{aligned} \left| 1 - \frac{\omega_p^2}{\omega^2} \right| &= \left| \frac{1+R}{1-R} \right|^2 \\ \Rightarrow \frac{\omega_p^2}{\omega^2} &= \left| \frac{1+R}{1-R} \right|^2 + 1 \quad \text{by inspection} \\ \omega_p^2 &= 2.26 \times 10^{33} \text{ rad s}^{-1} \end{aligned}$$

Further plugging in $q = e$, $m = m_e$ into the definition of ω_p then give

$$N = \omega_p^2 \times \frac{m_e \epsilon_0}{e^2} = 7.11 \times 10^{29} \text{ m}^{-3}$$



Then we realise that in an FCC lattice, the carrier density is

$$N = \frac{4x}{a^3} \quad (6)$$

where x is the valency⁴ of aluminium.

Solving (6) then gives $x = 11.8$.

(c) The magnitude of the energy suggests that the dip is due to a band transition⁵.

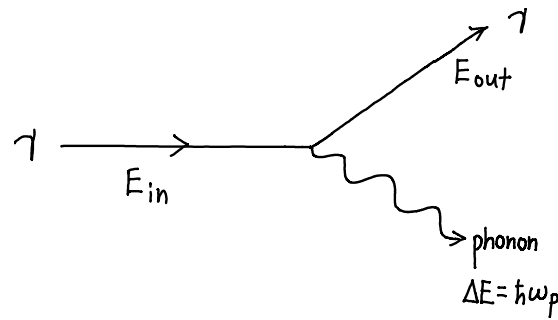
In fact measurement with ARPES⁶ shows that the band gap of aluminium at the X point is about 1.68 eV.

⁴Is this really valency though? I think my chemist friends would fill my inbox with friendly reminders that aluminium has a valency +3, the x I calculated here is the atomic number I believe.

⁵For those who tend to confuse between this and excitons, note that the energies involved in exciton formation are of order meV.

⁶Experimental band structure of aluminum: <https://link.aps.org/doi/10.1103/PhysRevB.27.727>

(d) Raman scattering so we are probing plasmons here.



From before we have $\omega_p \propto N^{1/2}$. Therefore a plot of $\hbar\omega_p$ against $N^{1/2}$ will be a straight line with gradient $\frac{\hbar q}{\sqrt{m\epsilon_0\epsilon_\infty}}$.

From the graph we then have gradient of $\frac{18 - 7}{3.1 - 1.2} = 5.789 \times 10^{-11} \text{ meV m}^{3/2}$.

Equating the two expressions then gives

$$\begin{aligned} m &= \frac{\hbar^2 q^2}{\epsilon_0 \epsilon_\infty \text{gradient}^2} \\ &= 3.023 \times 10^{-32} \text{ kg} \\ &= 0.033 m_e \end{aligned}$$

4. Magnetism with a spin at spin wave (pun totally intended).

(a) Standard derivation similar to Q5 2021.

B_{mf} is the molecular mean field of the lattice – this is the effective average magnetic field experienced by a spin as a result of the exchange interaction.

Next we examine the Heisenberg exchange Hamiltonian for each spin in the magnetic structure from the question:

$$\begin{aligned}\mathcal{H}_i &= \sum_{ij} \frac{J}{2} \mathbf{S}_i \cdot \mathbf{S}_j \\ &= 6 \times \frac{J}{2} \times (-S^2) \\ &= -3JS^2\end{aligned}\tag{7}$$

where the factor of $\frac{1}{2}$ comes from the over-counting in unfolding the sum $\langle ij \rangle \rightarrow ij$.

Equating (7) with $g\mu_B B_{\text{mf}} S_i$ then gives

$$B_{\text{mf}} = -\frac{3JS}{g\mu_B}\tag{8}$$

Now recall magnetisation $M = \mu_{\text{total}}/V$ where μ_{total} is the total magnetic moment in a magnetic unit cell of volume V :

$$\begin{aligned}M &= \frac{4g\mu_B S}{(2a)^3} \\ &= \frac{g\mu_B S}{2a^3}\end{aligned}\tag{9}$$

since each sublattice in the question is an FCC lattice with lattice parameter $2a$.

Comparing (8) and (9) then gives

$$\lambda = \frac{6Ja^3}{(g\mu_B)^2}$$

We then substitute from left to right to get T_N , noting that M_s follows from (9) and invoking the small y approximation gives:

$$\begin{aligned}M_A &\approx \frac{g\mu_B S}{2a^3} \frac{S+1}{3S} y \\ &= \frac{g\mu_B S}{2a^3} \frac{S+1}{3S} \frac{g\mu_B S}{k_B T_N} \left(\frac{6Ja^3}{(g\mu_B)^2} M_A \right) \\ \Rightarrow T_N &= \frac{JS(S+1)}{k_B}\end{aligned}\tag{10}$$

- (b) From the graph, we see that the maximum energy occurs at $(\frac{1}{2}, \frac{1}{2}, 0)$. This corresponds to $\gamma_{\mathbf{k}} = [-1 - 1 + 1]/3 = -1/3$. Hence

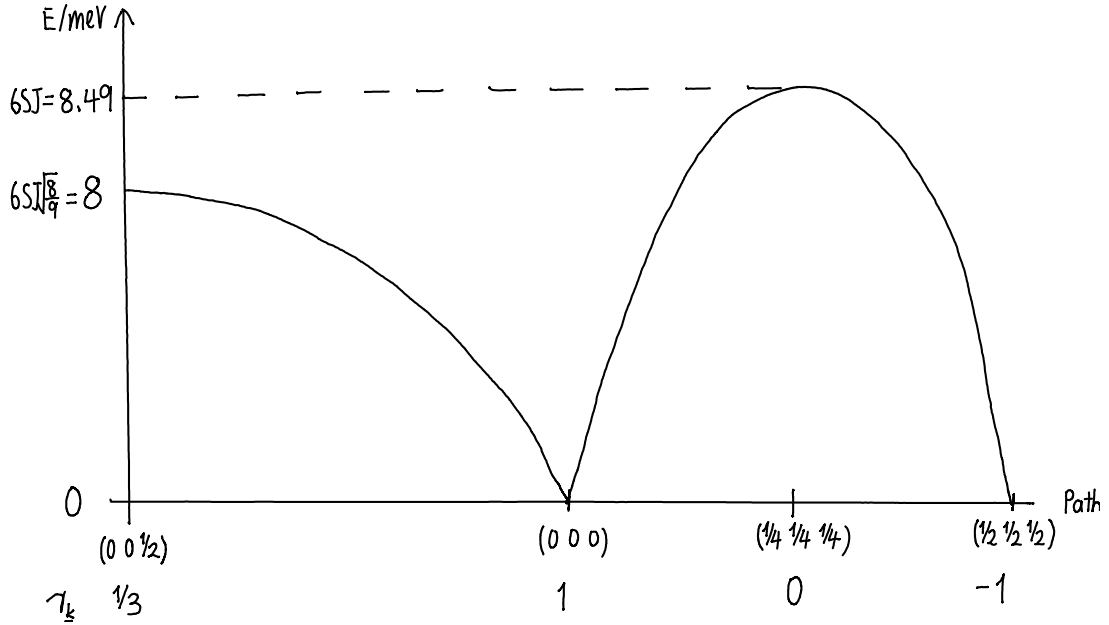
$$E_{\max} = 6SJ\sqrt{1 - \frac{1}{9}}$$

$$J = \frac{E_{\max}}{4\sqrt{2}S} = 0.566 \text{ meV} \quad (11)$$

for $E_{\max} \approx 8 \text{ meV}$, $S = \frac{5}{2}$.

Sketch of dispersion for path $(0, 0, \frac{1}{2}) \rightarrow (0, 0, 0) \rightarrow (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ by tracing out the cosine term:

$$\gamma_{\mathbf{k}} = \begin{cases} \frac{1}{3} & @ (0, 0, \frac{1}{2}) \\ 1 & @ (0, 0, 0) \\ -\frac{1}{3} & @ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \\ 0 & @ (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) \end{cases}$$



Gapless spin-wave spectrum suggests that we have a *spontaneous symmetry breaking* and the universality class of the transition is *3D Heisenberg*.

Substituting (11) into (10) gives $T_N = 57 \text{ K}$. This is lower than the measured value $T_N^{\text{exp}} = 83 \text{ K}$ as the mean-field theory ignores fluctuations in the exchange interactions, which then lead to it underestimating the interaction energy.

- (c) For small wavevector, we first rewrite $\gamma_{\mathbf{k}}$ as

$$\begin{aligned} \gamma_{\mathbf{k}} &= \frac{\cos(k_x a) + \cos(k_y a) + \cos(k_z a)}{3} \\ &\approx \frac{(1 - k_x^2 a^2/2) + (1 - k_y^2 a^2/2) + (1 - k_z^2 a^2/2)}{3} \\ &= 1 - \frac{|\mathbf{k}|^2 a^2}{6} \end{aligned}$$

Therefore the dispersion may be approximated as

$$\begin{aligned}
 \hbar\omega_{\mathbf{k}} &= 6SJ\sqrt{1 - \gamma_{\mathbf{k}}^2} \\
 &\approx 6SJ\sqrt{1 - \left(1 - \frac{|\mathbf{k}|^2 a^2}{3}\right)} \quad \text{ignoring higher order terms} \\
 &= 6SJ\frac{|\mathbf{k}|a}{\sqrt{3}} \\
 \Rightarrow \omega_{\mathbf{k}} &\approx \underbrace{\frac{6SJa}{\sqrt{3}\hbar}}_c |\mathbf{k}|
 \end{aligned}$$

Energy of an ensemble of spin waves, with $n_B = [\exp(E/k_B T) - 1]^{-1}$ being the Bose occupation factor:

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

Assuming isotropy, we then have the following d.o.s. due to the linear dispersion:

$$\begin{aligned}
 g(k) \, dk &= \frac{2}{(2\pi)^3} 4\pi k^2 \, dk \\
 &= \frac{2}{(2\pi)^3} 4\pi \left(\frac{E}{\hbar c}\right)^2 \frac{dE}{\hbar c} \\
 &= \frac{1}{\pi^2 \hbar^3 c^3} E^2 \, dE \\
 &= g(E) \, dE
 \end{aligned}$$

Thus the total energy is

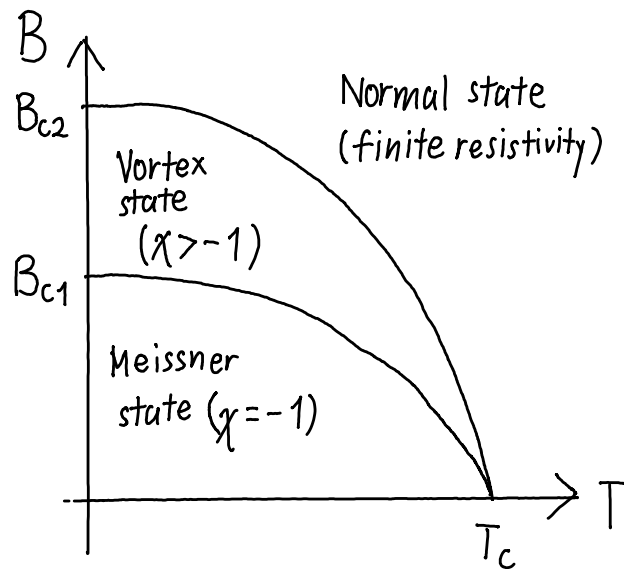
$$\begin{aligned}
 E &= \int_0^\infty dE \frac{1}{\pi^2 \hbar^3 c^3} E^2 \frac{1}{\exp(E/k_B T) - 1} E \\
 &= \frac{1}{\pi^2 \hbar^3 c^3} \int_0^\infty \frac{E^3}{\exp(E/k_B T) - 1} dE \\
 &= \frac{1}{\pi^2 \hbar^3 c^3} \int_0^\infty (k_B T)^4 \frac{x^3}{\exp(x) - 1} dx \quad \text{where } x = E/k_B T \\
 &= \frac{k_B^4}{\pi^2 \hbar^3 c^3} T^4
 \end{aligned} \tag{12}$$

Differentiating (12) w.r.t. T yields the heat capacity per volume due to spin waves in the low temperature limit:

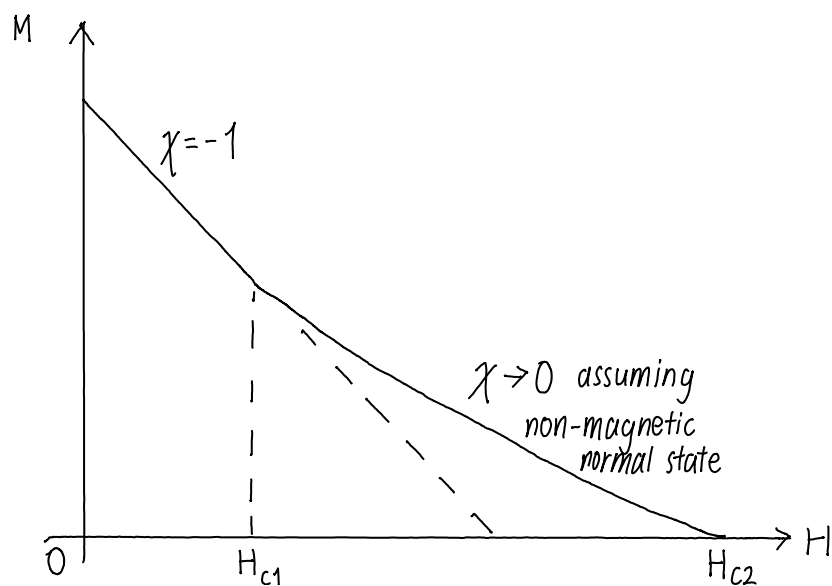
$$\begin{aligned}
 C_m &= \left(\frac{\partial E}{\partial T}\right)_V \\
 &= \frac{4k_B^4}{\pi^2 \hbar^3 c^3} T^3
 \end{aligned}$$

5. Ye olde superconductors.

(a) Standard sketches.

i. Heed that we have a type II SC here \rightarrow vortex state!

ii. See Q5 2018 for reference.

(b) A rather strange part. I'd say that it tests more on Ampere's Law⁷ than SC!

i. By Silsbee's Rule (fancy name for Ampere's Law under critical conditions), we have:

$$B_c \cdot 2\pi r = \mu_0 I_c \quad (13)$$

where B_c is the critical/upper-critical B field for type I/II SC, I_c is the critical current.

⁷As an anecdote, the author bombed this part by creating a new universe in which Ampere's Law took the form of $\oint \mathbf{B} \cdot d\mathbf{A} \dots$

Plugging in the dimensions of the Ta and Nb wires given in the question then gives:

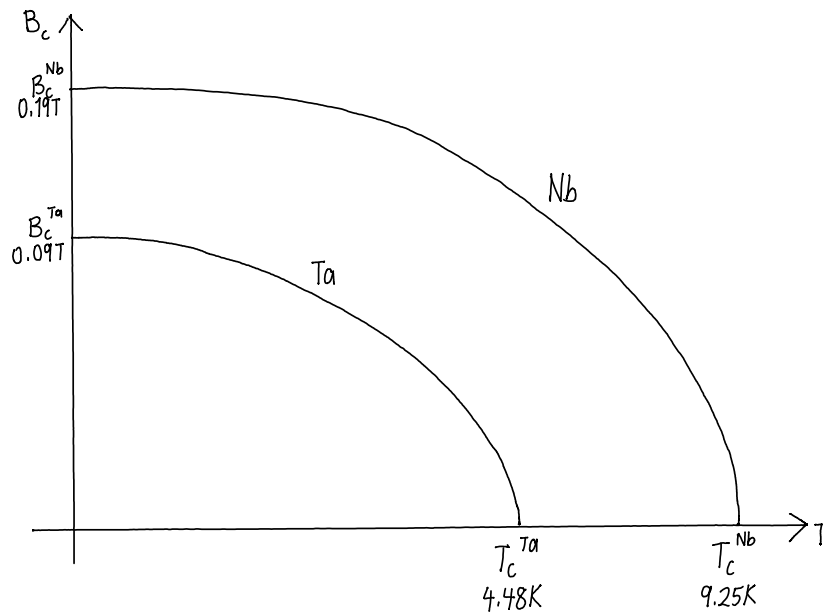
$$I_c^{\text{Ta}} = \frac{(0.09 \text{ T})2\pi(0.1 \text{ mm})}{\mu_0} = 45 \text{ A}$$

$$\Rightarrow J_c^{\text{Ta}} = \frac{I_c^{\text{Ta}}}{\pi(0.1 \text{ mm})^2} = 1.43 \times 10^9 \text{ A m}^{-2}$$

$$I_c^{\text{Nb}} = \frac{(0.19 \text{ T})2\pi(0.025 \text{ mm})}{\mu_0} = 23.75 \text{ A}$$

$$\Rightarrow J_c^{\text{Nb}} = \frac{I_c^{\text{Nb}}}{\pi(0.025 \text{ mm})^2} = 1.21 \times 10^{10} \text{ A m}^{-2}$$

ii. The temperature dependence is already given so sketch it!



Note that Nb is superconducting in larger range of B and T .

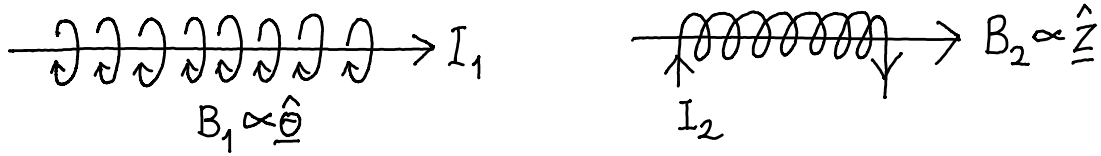
iii. At T_1 we have the critical B field as:

$$B_c(T_1) = B_c \left[1 - \left(\frac{T_1}{T_c} \right)^2 \right] \quad (14)$$

Then by Silsbee's Rule we have the critical current at T_1 :

$$\begin{aligned} I_c^{\text{Ta}}(T_1) &= \frac{B_c(T_1) \cdot 2\pi r_1}{\mu_0} \\ &= I_c^{\text{Ta}} \left[1 - \left(\frac{T_1}{T_c} \right)^2 \right] \\ &= (45 \text{ A}) \left[1 - \left(\frac{4.15 \text{ K}}{4.48 \text{ K}} \right)^2 \right] \\ &= 6.39 \text{ A} \end{aligned}$$

iv. Nothing to do with SC since we are only at the surface with no screening!



From the sketch we see that the B field contributions from each wire are perpendicular to each other ($\hat{\theta}$ and \hat{z} in cylindrical coordinates), hence the magnitude of the net B field would be:

$$B = \sqrt{B_1^2 + B_2^2} \quad (15)$$

where $B_{1/2}$ is the B field due to $I_{1/2}$.

By Ampere's Law we then have:

$$B_1 = \frac{\mu_0 I_1}{2\pi r_1} \quad (16)$$

$$B_2 = \mu_0 \frac{N}{L} I_2 \quad (17)$$

$$\text{So } \alpha = \left(\frac{\mu_0}{2\pi r_1} \right)^2, \beta = \left(\frac{\mu_0 N}{L} \right)^2.$$

v. Equating B with $B_c^{\text{Ta}}(T_1)$ and therefore (15) becomes:

$$\begin{aligned} B_c^{\text{Ta}}(T_1) &= \sqrt{\alpha I_1^2 + \beta I_2^2} \\ \Rightarrow \beta &= \frac{1}{I_2^2} \left[(B_c^{\text{Ta}}(T_1))^2 - \alpha I_1^2 \right] = (\mu_0 n_c)^2 \\ \Rightarrow n_c &= \frac{1}{\mu_0 I_2} \sqrt{(B_c^{\text{Ta}}(T_1))^2 - \alpha I_1^2} = 1.02 \times 10^5 \text{ m}^{-1} = 102 \text{ mm}^{-1} \end{aligned}$$

where $n_c = (N/L)_c$ is the critical number of turns per unit length beyond which the Ta wire becomes resistive.

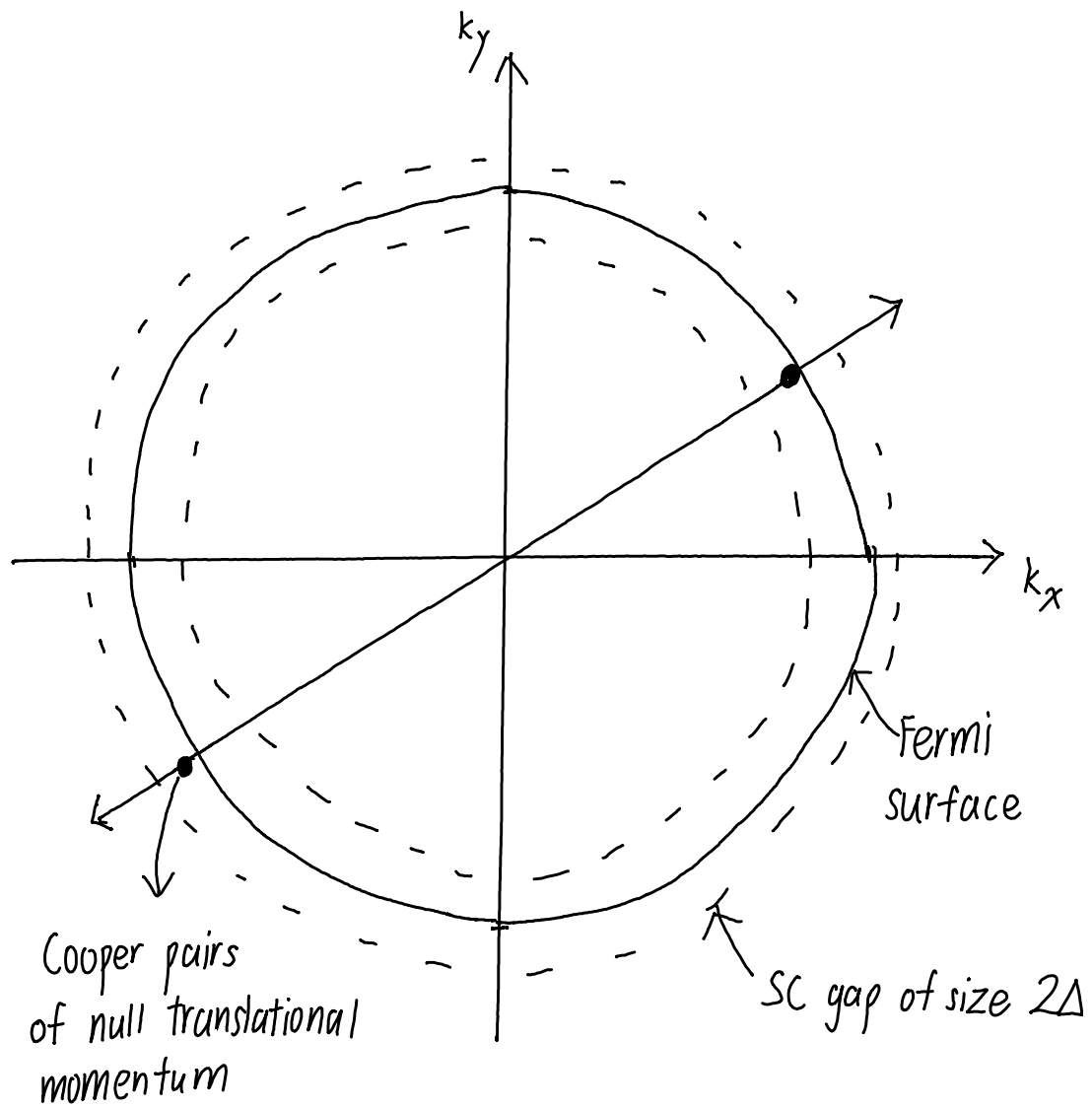
(c) Simple question on BCS theory.

- i. Recall from BCS theory that $\lambda = g(E_F) |g_{\text{eff}}|^2$ is the phonon-electron coupling parameter – it encodes the interaction between phonon and electron near the Fermi surface and has been shown to be attractive by Cooper.

$\hbar\omega_D$ is the energy at Debye frequency – in Cooper's theory this is the upper energy limit for which the electron-phonon interaction remains attractive.

Both parameters suggest that an electron pair may form under low temperature, this is called the Cooper pair.

- ii. Usual sketch from lecture notes, note that the Cooper pair I have drawn corresponds to the ground state where there is no centre-of-mass motion.



$\frac{1}{\sqrt{2}} [|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$ as spin wavefunction due to Pauli exclusion

iii. From the given gap equation,

$$\lambda \int_0^{\hbar\omega_D} d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} = 1 \quad (18)$$

Taking the limit of $\Delta \ll \hbar\omega_D \Rightarrow \hbar\omega_D/\Delta \gg 1$ yields:

$$\begin{aligned} & \lambda \int_0^{\hbar\omega_D} \frac{d\epsilon/\Delta}{\sqrt{1 + (\epsilon/\Delta)^2}} = 1 \\ \Rightarrow & \lambda \int_0^{\hbar\omega_D/\Delta} \frac{dx}{\sqrt{1 + x^2}} = 1 \quad \text{where } x = \epsilon/\Delta \\ & \sinh^{-1} \left(\frac{\hbar\omega_D}{\Delta} \right) - \sinh^{-1} 0 = \frac{1}{\lambda} \\ \Rightarrow & \ln \left(\sqrt{\left(\frac{\hbar\omega_D}{\Delta} \right)^2 + 1} + \left(\frac{\hbar\omega_D}{\Delta} \right) \right) - 0 = \frac{1}{\lambda} \\ \Rightarrow & \ln \left[2 \left(\frac{\hbar\omega_D}{\Delta} \right) \right] = \frac{1}{\lambda} \quad \text{since } \hbar\omega_D/\Delta \gg 1 \\ & \Delta = 2\hbar\omega_D e^{-1/\lambda} \end{aligned} \quad (19)$$

iv. Substituting $\hbar\omega_D = k_B T_D$, $T_D \approx 276 \text{ K}$ and $\lambda \approx 0.1$ into (19) gives:

$$\begin{aligned} \Delta &= 2k_B T_D e^{-1/\lambda} \\ &= 3.46 \times 10^{-25} \text{ J} \\ &= 2.16 \times 10^{-6} \text{ eV} \end{aligned}$$

Aside: It doesn't fit the measured value of $2\Delta = 3.8 \text{ meV}$? This paper⁸ suggests that $\lambda \approx 1.1$ eV for the magnitude to match.

⁸Superconductivity in Nb: Impact of Temperature, Dimensionality and Cooper-Pairing: <https://doi.org/10.3390/nano14030254>

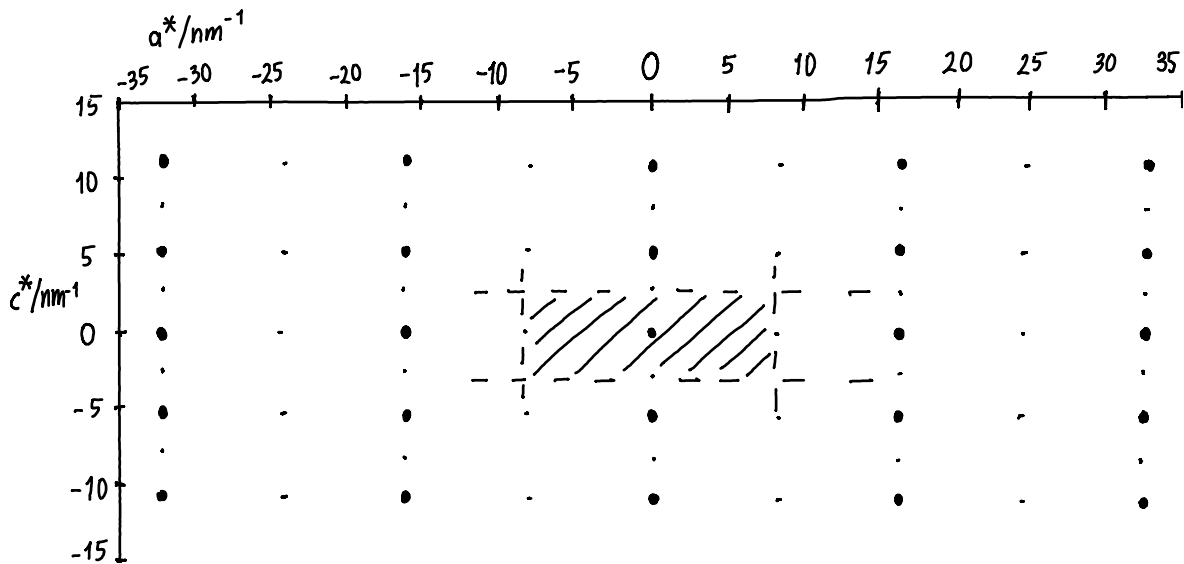
6. (DRAFT) Phonon dispersion and the practical bits of inelastic neutron scattering.

(a) BC tetragonal direct lattice \rightarrow FC tetragonal reciprocal lattice⁹.

Also by definition of reciprocal lattice vector, we have:

$$\begin{aligned} \mathbf{a}^* &= \frac{2\pi(\mathbf{b} \times \mathbf{c})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \\ \Rightarrow a^* &= \frac{2\pi}{a} = 16.2 \text{ nm}^{-1} \\ \mathbf{c}^* &= \frac{2\pi(\mathbf{a} \times \mathbf{b})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \\ \Rightarrow c^* &= \frac{2\pi}{c} = 5.39 \text{ nm}^{-1} \end{aligned}$$

Taking care of the scaling, we should have the following sketch for $-2 \leq h \leq 2$ and $-2 \leq l \leq 2$, together with the 1st BZ shaded:



(b) Questions on phonon dispersion and reciprocal lattice.

i. For a 3D crystal of N lattice points and p atoms, we have a total of $3Np$ phonon modes.

For CaFe_2As_2 , $p = 5$. Hence for a given wavevector, there should be $3p = 15$ phonon modes in total.

ii. (TO BE VERIFIED) Note that the positions $(1, 0, 0)$ and $(0, 0, 1)$ are Γ points that are symmetry-equivalent by translation. Therefore the dispersion curve must meet at those points, i.e. phonon frequencies must be identical.

iii. Being a tetragonal lattice, the symmetry element 4_z must be present, hence there will be degenerate transverse modes along the c axis.

Further note that by the definition of acoustic mode in which all atoms oscillate in phase, we'd only have 2 transverse acoustic (TA) modes which corresponds to vibrations in a and b axes.

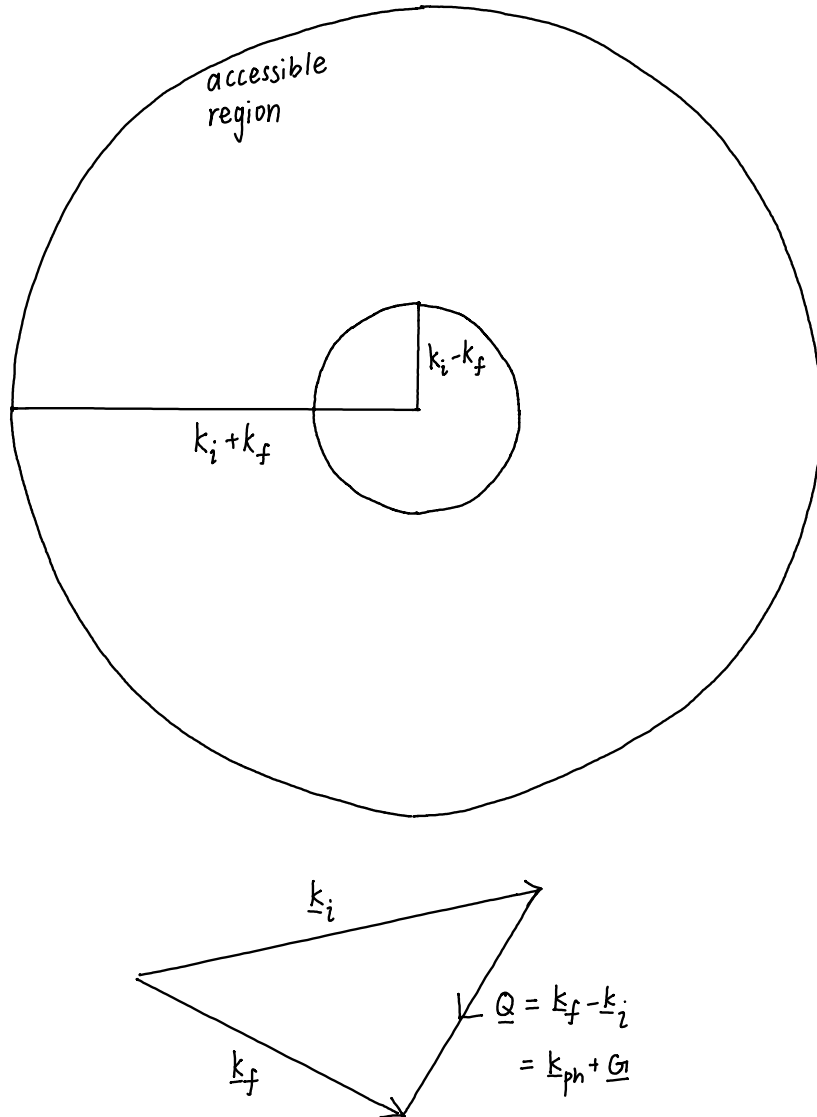
⁹Proof is similar to the cubic case – the direct and reciprocal bases no longer share the same length, but they cancel out upon taking $\mathbf{G} \cdot \mathbf{R}$!

Now since the TA modes are degenerate, only 2 acoustic modes will be observable, with the other one being the longitudinal acoustic (LA) mode.

There is no four-fold rotation symmetry about the a axis, hence all 3 acoustic modes are non-degenerate.

- (c) i. Definition of scattering vector: $\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i = \mathbf{k}_{ph} + \mathbf{G}$ where \mathbf{k}_{ph} is the wavevector in the 1st BZ¹⁰.

For inelastic neutron scattering, we have the following accessible Ewald sphere by the conservation of momentum:



It is clear that there exists a forbidden zone near the zone centre. Therefore to probe the forbidden zone, one must use the periodicity of reciprocal lattice to measure such zone in higher BZs. This may be done for \mathbf{Q} with non-zero \mathbf{G} .

¹⁰It is as if $\mathbf{Q} = \mathbf{k}_{ph} \pmod{\mathbf{G}}$ at a slight abuse of notation.

- ii. **(TO BE VERIFIED)** Calculate $S(\mathbf{G})$ for 1st, 2nd and 3rd BZs. Then compare to see which yields the largest structure factor.

By definition, we have the structure factor:

$$\begin{aligned}
 S(\mathbf{G}) &= \sum_{x \in \text{UC}} b_x e^{i\mathbf{G} \cdot \mathbf{R}_x} \\
 &= S_{\text{lattice}} \times S_{\text{basis}} \\
 &= (1 + e^{i\pi(h+k+l)}) [b_{\text{Ca}} + b_{\text{Fe}} (e^{i\pi(h+l/2)} - e^{i\pi(h-l/2)}) + b_{\text{As}} (e^{i\pi lz} - e^{-i\pi lz})] \\
 &= (1 + e^{i\pi(h+k+l)}) \left[b_{\text{Ca}} + 2ib_{\text{Fe}} e^{i\pi h} \sin\left(\frac{l}{2}\right) + 2ib_{\text{As}} \sin(lz) \right]
 \end{aligned}$$

where h , k and l are the usual Miller indices.

Enforcing $k = 0$ and calculating the structure factor for each possible \mathbf{G} then gives:

$$\begin{aligned}
 S(\mathbf{G}) &= \begin{cases} 0 & \text{for } h+l \text{ odd} \\ 2b_{\text{Ca}} & l = 0 \\ 2[b_{\text{Ca}} + 2ib_{\text{Fe}} \sin \frac{1}{2} + 2ib_{\text{As}} \sin z] & (1, 0, 1) \\ 2[b_{\text{Ca}} + 2ib_{\text{Fe}} \sin 1 + 2ib_{\text{As}} \sin(2z)] & (0, 0, 2) \end{cases} \\
 |S(\mathbf{G})|^2 &= \begin{cases} 0 & \text{for } h+l \text{ odd} \\ 88.36 \text{ fm}^2 & l = 0 \\ 88.61 \text{ fm}^2 & (1, 0, 1) \\ 89.34 \text{ fm}^2 & (0, 0, 2) \end{cases}
 \end{aligned}$$

Therefore to maximise the scattering intensity, one should probe the 3rd BZ.