

UNOFFICIAL SOLUTIONS BY TheLongCat

B6: CONDENSED-MATTER PHYSICS

TRINITY TERM 2018

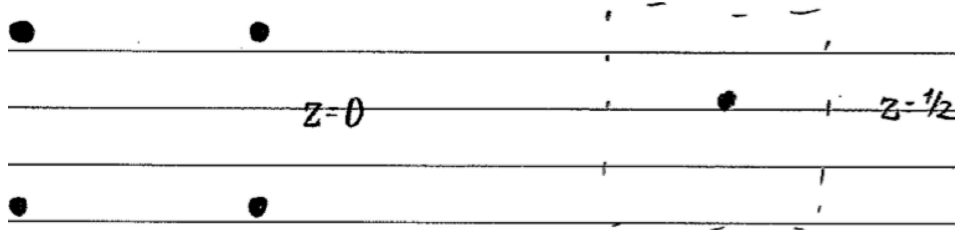
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Disclaimer: due to its unofficial nature, the author does not warrant the accuracy of the presented solutions in any form. However, the author is happy to discuss the typos and errors should one arises.

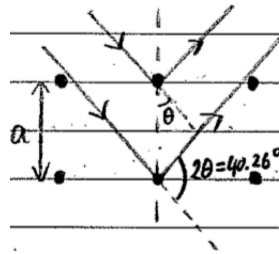
Turn over as you please – we are NOT under exam conditions here.

1. (DRAFT)

- (a) A lattice is an infinite set of linearly independent primitive lattice vectors (PLVs) in the real space. When combined with a basis in a crystal system, a crystal structure that precisely address the location of each atom is formed.



Therefore α -tungsten is a body-centred cubic lattice (BCC).



- (b) Bragg's condition:

$$\begin{aligned}
 2d_{hkl} \sin \theta &= \lambda \quad \text{for 1st peak} \\
 \Rightarrow d_{hkl} &= \frac{1}{2} \frac{\lambda}{\sin \theta} \\
 &= \frac{1}{2} \frac{0.1542 \text{ nm}}{\sin 20.13^\circ} \\
 &= 0.224 \text{ nm}
 \end{aligned}$$

For cubic lattice,

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (1)$$

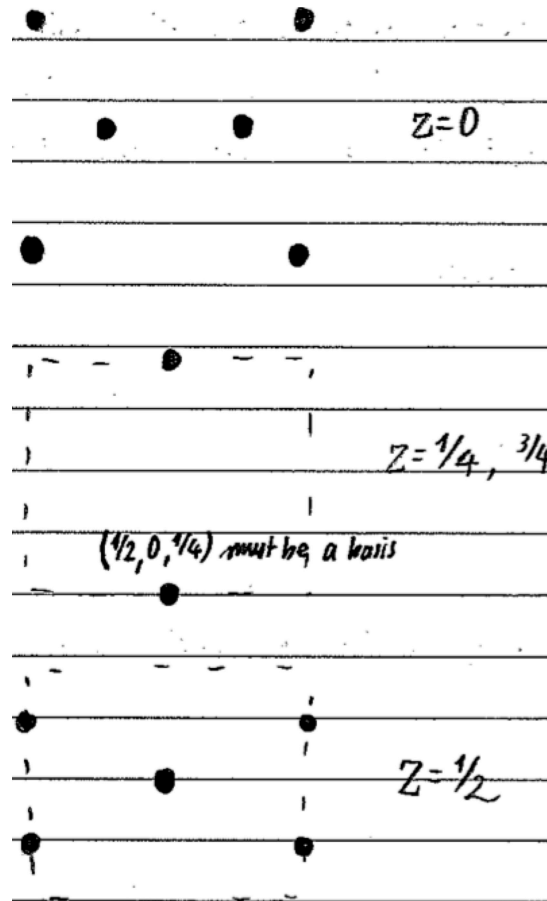
BCC selection rule: $h + k + l$ even:

$$\begin{aligned}
 S_{hkl} &= \sum_{\mathbf{x} \in \text{UC}} e^{i\mathbf{k} \cdot \mathbf{x}} \\
 &= 1 + e^{\pi i(h+k+l)} \\
 &= \begin{cases} 0 & h + k + l \text{ odd} \\ 2 & h + k + l \text{ even} \end{cases}
 \end{aligned}$$

So we know the smallest possible combination that yield the d_{hkl} above is (110):

$$\begin{aligned}
 N &= \sqrt{h^2 + k^2 + l^2} \\
 &= \sqrt{2}
 \end{aligned}$$

$$\stackrel{(1)}{\Rightarrow} a = \sqrt{2}d = 0.317 \text{ nm}$$



- (c) β -tungsten is a simple cubic crystal with basis $[0, 0, 0]$, $[0, \frac{1}{4}, \frac{1}{2}]$, $[0, \frac{\bar{1}}{4}, \frac{1}{2}]$, $[\frac{1}{2}, 0, \frac{1}{4}]$, $[\frac{1}{2}, 0, \frac{\bar{1}}{4}]$, $[\frac{1}{4}, \frac{1}{2}, 0]$, $[\frac{\bar{1}}{4}, \frac{1}{2}, 0]$, $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$.

So try:

$$\begin{aligned} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) + \left(\frac{1}{2}, 0, \frac{1}{4}\right) &= \left(1, \frac{1}{2}, \frac{3}{4}\right) \\ &\rightarrow \left(0, \frac{1}{2}, \frac{3}{4}\right) \end{aligned}$$

This does not lead to an atom!

So not BCC.

- (d) Laue condition:

$$\begin{aligned} e^{\mathbf{a} \cdot \mathbf{G}} &= 1 \\ \Rightarrow \mathbf{a} \cdot \mathbf{G} &= 2n\pi \end{aligned}$$

where \mathbf{a} is direct lattice vector, \mathbf{G} is reciprocal lattice vector.

Since β -tungsten is simple cubic, $S_{\text{UC}} = 1 \forall (hkl)$, hence any extinction has to come from the basis:

$$\begin{aligned} S_{\text{basis}}(hkl) &= 1 + e^{\pi i(h+k+l)} + 2e^{\pi i k} \cos\left(\frac{\pi h}{2}\right) \\ &\quad + 2e^{\pi i l} \cos\left(\frac{\pi k}{2}\right) + 2e^{\pi i h} \cos\left(\frac{\pi l}{2}\right) \end{aligned}$$

Trial and error then gives:

- $N = 1$: (100)

$$S_{\text{basis}}(100) = 1 - 1 + 2 \cos\left(\frac{\pi}{2}\right) + 2 \cos(0) - 2 \cos(0) = 0$$

- $N = 2$: (110)

$$S_{\text{basis}}(110) = 1 + 1 - 2 \cos\left(\frac{\pi}{2}\right) + 2 \cos\left(\frac{\pi}{2}\right) - 2 \cos(0) = 0$$

- $N = 3$: (111)

$$S_{\text{basis}}(111) = 1 - 1 - 2 \cos\left(\frac{\pi}{2}\right) - 2 \cos\left(\frac{\pi}{2}\right) - 2 \cos\left(\frac{\pi}{2}\right) = 0$$

- $N = 4$: (200)

$$S_{\text{basis}}(200) = 1 + 1 + 2 \cos(\pi) + 2 \cos(0) + 2 \cos(0) = 4$$

We also have multiplicity $M_{200} = 6$.

- $N = 5$: (210)

$$S_{\text{basis}}(210) = 1 - 1 - 2 \cos(\pi) + 2 \cos\left(\frac{\pi}{2}\right) + 2 \cos(0) = 4$$

We also have multiplicity $M_{210} = 24$.

Therefore ratio of intensities:

$$\begin{aligned} I_{hkl} &= |S_{hkl}|^2 M_{hkl} \\ \Rightarrow \frac{I_{200}}{I_{210}} &= \frac{4^2}{4^2} \times \frac{6}{24} \\ &= \frac{1}{4} \end{aligned}$$

(e) Lower angles $\Rightarrow N < 4$.

In the last part, we assumed that $f(\mathbf{k})$ is constant \forall atoms. But note that $(\frac{1}{2}, \frac{1}{4}, 0)$ and $(0, 0, \frac{1}{2})$ have different distances from the origin \Rightarrow different orbital overlaps. So we would actually have a separate structure factor: $f_1(1 + e^{\pi i(h+k+l)}) + f_2(\dots)$

For example, for $N = 2$:

$$\begin{aligned} S_{\text{basis}} &= f_1(1 + 1) + f_2\left(-2 \cos\left(\frac{\pi}{2}\right) + 2 \cos\left(\frac{\pi}{2}\right) - 2 \cos(0)\right) \\ &\neq 0 \end{aligned}$$

for $f_1 \neq f_2$. In fact $f_1 \simeq f_2$, hence the faint diffraction ring.

2. (DRAFT)

- (a) Chemical potential: energy required to add a particle into a system under thermal equilibrium at constant entropy and volume.

Fermi energy: chemical potential at temperature $T = 0$ K. Also in the context of CMP, halfway point before the highest filled state and lowest unfilled state if state distribution discontinuous.

- (b) TISE gives $\hat{H}|\psi\rangle = E|\psi\rangle$

System wavefunction $|\psi\rangle = \dots + |n\rangle + |n+1\rangle + \dots$

Try $\hat{H}(|n\rangle) = \varepsilon_0 |n\rangle + (-t) |n-1\rangle + (-t) |n+1\rangle$

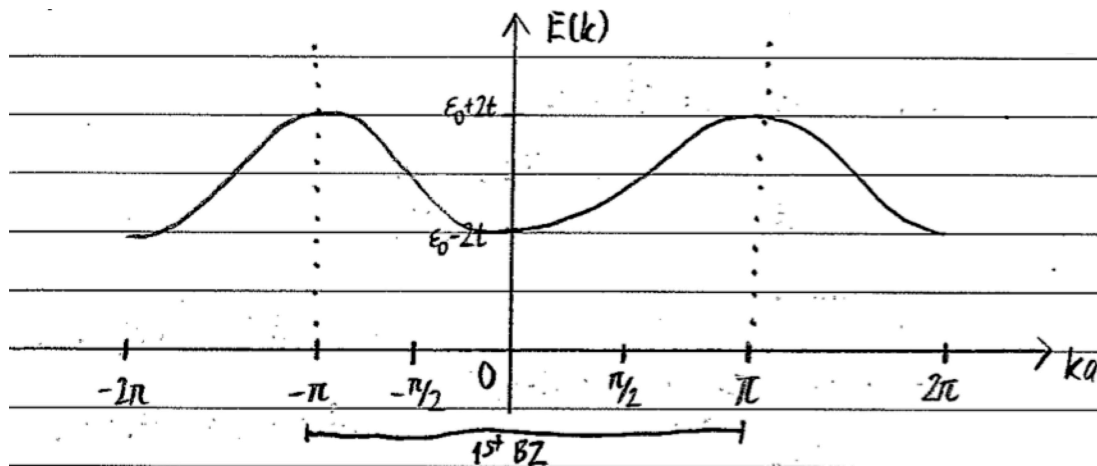
For plane wave,

$$\begin{aligned}\langle \mathbf{r} | n \rangle &= A e^{ikna} \\ \Rightarrow \hat{H} | n \rangle &= E_n | n \rangle \\ \Rightarrow E_n A e^{ikna} &= \varepsilon_0 A e^{ikna} - t A e^{ik(n-1)a} - t A e^{ik(n+1)a} \\ \Rightarrow E_n &= \varepsilon_0 - t (e^{ika} + e^{-ika}) \\ &= \varepsilon_0 - 2t \cos(ka)\end{aligned}$$

Born-von Karman boundary condition:

$$\begin{aligned}e^{ikna} &= e^{ik(n+1)a} \\ \Rightarrow e^{ika} &= 1 \\ \Rightarrow k &= \frac{2\pi}{a}\end{aligned}$$

Dispersion relation in the 1st Brillouin Zone¹:



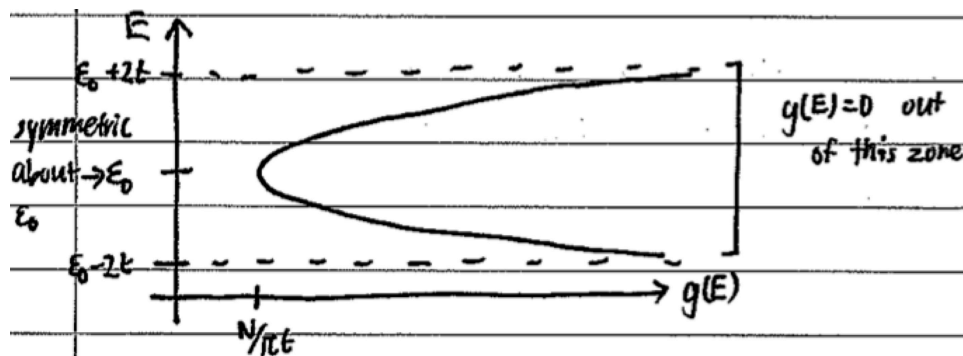
Also we have:

$$\begin{aligned}\frac{dE}{dk} &= 2ta \sin(ka) \\ &= a \sqrt{4t^2 - (\varepsilon_0 - E)^2}\end{aligned}$$

¹Tip: trace the curve and check you have repeated within a zone

Density of states:

$$\begin{aligned}
 \frac{dN}{dE} &= \frac{dN}{dk} \cdot \frac{dk}{dE} \\
 &= \frac{Na}{2\pi} \cdot \underbrace{2}_{\text{spin}} \cdot \underbrace{2}_{\text{dk degeneracy}} \cdot \frac{dk}{dE} \quad \text{assuming "isotropy" in 1D} \\
 &= \frac{2Na}{\pi} \cdot \frac{1}{a\sqrt{4t^2 - (\varepsilon_0 - E)^2}} \\
 \Rightarrow g(E) dE &= \frac{2N}{\pi} \frac{1}{\sqrt{4t^2 - (\varepsilon_0 - E)^2}} dE
 \end{aligned}$$

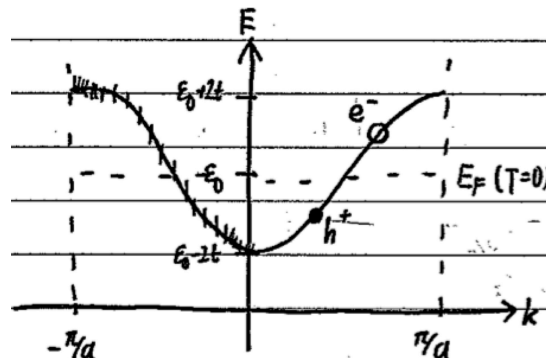


(c) Assuming monovalent atoms, the Fermi energy is simply:

$$E\left(ka = \frac{\pi}{2}\right) = \varepsilon_0$$

Chemical potential:

$$\begin{aligned}
 \mu &= \frac{dE}{dN} = \frac{1}{g(E)} \\
 &= \frac{\pi}{2N} \sqrt{4t^2 - (\varepsilon_0 - E)^2} \propto T
 \end{aligned}$$



Since E is symmetric about E_0 :

$$|\langle E_e - \varepsilon_0 \rangle| = |\langle E_h - \varepsilon_0 \rangle|$$

So μ remains constant (ε_0).

Or:

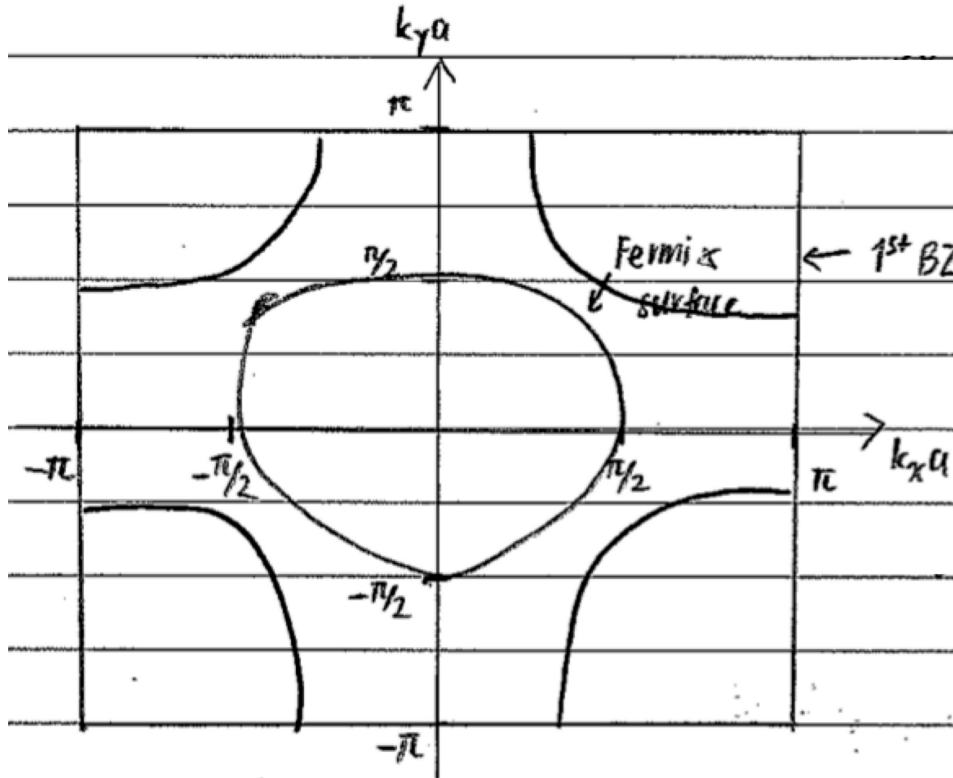
$$N = \int_{\varepsilon_0-2t}^{\varepsilon_0+2t} g(E) \frac{1}{e^{\beta(E-\mu)} + 1} dE \quad (2)$$

$$\begin{aligned} &= \int_{\varepsilon_0-2t}^{\varepsilon_0+2t} g(E) \left[1 - \frac{1}{e^{\beta(\mu-E)} + 1} \right] dE \\ &= \underbrace{\int_{\varepsilon_0-2t}^{\varepsilon_0+2t} g(E) dE}_{\text{total \# of states} = 2N} - \int \frac{g(E)}{e^{\beta(\mu-E)} + 1} dE \\ \Rightarrow N &= \int \frac{g(E)}{e^{\beta(\mu-E)} + 1} dE \quad (3) \end{aligned}$$

Comparing (2) and (3):

$$\int g(E) \frac{1}{e^{\beta(E-\mu)} + 1} dE = \int \frac{g(E)}{e^{\beta(\mu-E)} + 1} dE$$

Nothing that this must be true for all T , this implies that μ must be independent of T .



(d) Monovalent $\Rightarrow \frac{1}{2}$ of BZ area occupied by spin degeneracy.

By symmetry, (noting that the previous part has no dependence on dimensions)

$$\mu = E_F = \varepsilon_0 \quad \text{independent of } T$$

(e) Now:

$$E(k_x, k_y) = \varepsilon_0 - 2t_x \cos(k_x a_x) - 2t_y \cos(k_y a_y)$$

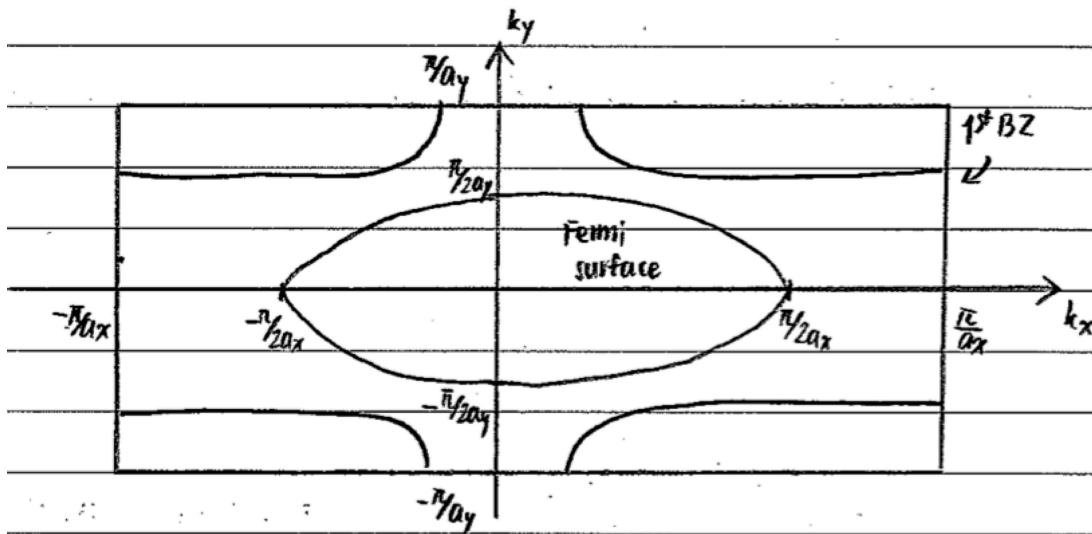
Also:

$$k_x^{\max} = \pm \frac{\pi}{a_x}$$

$$k_y^{\max} = \pm \frac{\pi}{a_y}$$

$$a_x < a_y \Rightarrow k_x^{\max} > k_y^{\max}$$

We expect BZ and Fermi surface to be squashed towards x axis as $t_x > t_y$.



3. (DRAFT)

- (a) A phonon is a quantum of lattice vibrations, similar to photons, a phonon is a boson and may occupy a non-empty state with others.

A Brillouin zone is a primitive unit cell of reciprocal lattice.

- (b) With $\xi = 0.084 \text{ nm}$, $A = 1600 \text{ eV}$, $B = 40 \text{ eV}$:

$$V(r) = Ae^{-\frac{2r}{\xi}} - Be^{-\frac{r}{\xi}}$$

At equilibrium,

$$\begin{aligned} \frac{dV}{dr} &= 0 \\ \Rightarrow -\frac{2A}{\xi}e^{-\frac{2r}{\xi}} + \frac{B}{\xi}e^{-\frac{r}{\xi}} &= 0 \\ \Rightarrow \frac{2A}{\cancel{\xi}}e^{-\frac{2r}{\xi}} &= \frac{B}{\cancel{\xi}}e^{-\frac{r}{\xi}} \\ e^{-\frac{r}{\xi}} &= \frac{B}{2A} \\ \Rightarrow r_0 &= \xi \left[\ln \left(\frac{2A}{B} \right) \right] \\ &= 0.3681 \text{ nm} \end{aligned}$$

Bonding energy:

$$V(a) - \underbrace{V(\infty)}_0 = -0.25 \text{ eV}$$

Around r_0 ,

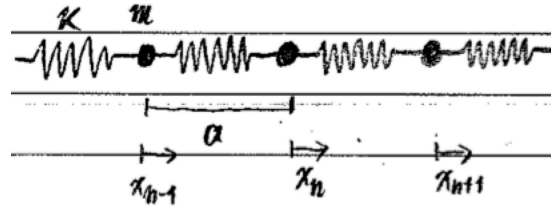
$$V(r) \simeq V(r_0) + (r - r_0) \frac{dV}{dr} \Big|_{r_0} + \frac{1}{2}(r - r_0)^2 \frac{d^2V}{dr^2} \Big|_{r_0} + \dots$$

$$\begin{aligned} \frac{d^2V}{dr^2} &= +\frac{4A}{\xi^2}e^{-\frac{2r}{\xi}} - \frac{B}{\xi^2}e^{-\frac{r}{\xi}} \\ \xrightarrow{r=r_0} &= \frac{\cancel{4A}}{\xi^2} \cdot \frac{B^2}{\cancel{4A^2}} - \frac{B}{\xi^2} \cdot \frac{B}{2A} \\ &= \frac{B^2}{\xi^2 A} \left(1 - \frac{1}{2} \right) = \frac{B^2}{2\xi^2 A} \end{aligned}$$

$$\Rightarrow V(r) \simeq V(r_0) + \frac{B^2}{4\xi^2 A}(r - r_0)^2$$

$$\begin{aligned} F(r - r_0) &= \frac{dV(r - r_0)}{d(r - r_0)} \\ &= -\frac{B^2}{2\xi^2 A}(r - r_0) \\ &= -\kappa(r - r_0) \end{aligned}$$

where $\kappa = \frac{B^2}{2\xi^2 A} = 70.8617 \text{ eV nm}^{-2} = 11 \text{ N m}^{-1}$.



(c) Newton's 2nd law:

$$\begin{aligned} m\ddot{x}_n &= \kappa(x_{n+1} - x_n) - \kappa(x_n - x_{n-1}) \\ &= \kappa(x_{n+1} - 2x_n + x_{n-1}) \end{aligned}$$

Insert Ansatz $x_n = Ae^{i\omega t - ikan}$:

$$\begin{aligned} \Rightarrow -m\omega^2 &= \kappa(e^{-ika} - 2 + e^{ika}) \\ \omega^2 &= \frac{2\kappa}{m}(1 - \cos(ka)) \end{aligned}$$

Group velocity:

$$\begin{aligned} v_g(k) &= \frac{\partial \omega}{\partial k} \\ \Rightarrow 2\omega \frac{\partial \omega}{\partial k} &= \frac{2\kappa a}{m} \sin(ka) \\ \frac{\partial \omega}{\partial k} &= \frac{\kappa a}{m\omega} \sin(ka) \\ \Rightarrow v_g(k) &= \frac{\kappa a}{m} \sin(ka) \cdot \sqrt{\frac{m}{2\kappa}} [1 - \cos(ka)]^{-1/2} \end{aligned}$$

Speed of sound:

$$\begin{aligned} v_s &= \lim_{k \rightarrow 0} v_g(k) \\ &= \frac{\kappa a}{m} \cdot \sqrt{\frac{m}{2\kappa}} \cdot (ka) \cdot \left[1 - 1 + \frac{1}{2}(ka)^2\right]^{-1/2} \\ &= \sqrt{\frac{\kappa a^2}{m} \cdot \frac{m}{2\kappa} \cdot \frac{1}{2} \cdot \frac{1}{(ka)^2}} = \sqrt{\frac{\kappa a^2}{m}} \\ &= 2100 \text{ m s}^{-1} \end{aligned}$$

Alternative way – consider the definition of speed of sound in a material:

$$v_s = \sqrt{\frac{1}{\rho\beta}}$$

where

$$\begin{aligned}\beta &= -\frac{1}{L} \sqrt{\frac{dL}{dF}} \\ &= -\frac{1}{a - \kappa \Delta x} \frac{\Delta x}{a} \\ &= \frac{1}{a\kappa}\end{aligned}$$

is the linear expansion coefficient, and

$$\rho = \frac{m}{a}$$

is the density of the chain.

Thus:

$$v_s = \sqrt{\frac{\kappa a^2}{m}}$$

(d) Third order term of $V(r)$:

$$\frac{1}{6} (r - r_0)^3 \left. \frac{d^3V}{dr^3} \right|_{r=r_0}$$

And:

$$\begin{aligned}\frac{d^3V}{dr^3} &= -\frac{8A}{\xi^3} \cdot \frac{B^2}{4A^2} + \frac{B}{\xi^3} \cdot \frac{B}{2A} \\ &= \frac{B^2}{\xi^3 A} \left[-2 + \frac{1}{2} \right] \\ &= -\frac{3B^2}{2\xi^3 A} \\ &= -2.5308 \times 10^{30} \text{ eV m}^{-3} = -4.0548 \times 10^{11} \text{ J m}^{-3}\end{aligned}$$

To estimate the thermal expansion coefficient, we shall consider the dimensions of the relevant terms:

$$\alpha = \frac{1}{L} \frac{\partial L}{\partial T} \Rightarrow [\alpha] = \text{T}^{-1}$$

We know that $L = a$, and only κ , κ_3 and k_B can enter $\frac{\partial L}{\partial T}$, so to arrange for the appropriate dimensions, we try:

$$\begin{aligned}\frac{\partial L}{\partial T} &= \frac{\kappa_3 k_B}{\kappa^2} \\ \Rightarrow \left(\frac{\partial L}{\partial t} \right) &= \frac{[\kappa_3] [k_B]}{[\kappa]^2} \\ &= \frac{[\text{E L}^{-3}] [\text{E T}^{-1}]}{[\text{E L}^{-2}]^2} \\ &= [\text{L T}^{-1}]\end{aligned}$$

which matches the expectation.

Hence:

$$\alpha = \frac{\kappa_3 k_B}{a \kappa^2}$$

(e) i. For higher orders to be negligible,

$$(\Delta x)^3 \kappa_3 \ll (\Delta x)^4 \kappa_4$$

From the previous part we also know,

$$\begin{aligned} \Delta x &= \frac{k_B \kappa_3}{\kappa^2} \Delta T \\ \Rightarrow \Delta T &\ll \frac{\kappa_3}{\kappa_4} \left(\frac{\kappa^2}{k_B \kappa_3} \right) \\ &= \frac{\kappa^2}{\kappa + k_B} \\ &= 650 \text{ K} \end{aligned}$$

ii. Consider a quantum harmonic oscillator,

$$\begin{aligned} E_n &= \left(n + \frac{1}{2} \right) \hbar \omega \\ \Delta E &\sim \hbar \omega \end{aligned}$$

So for QM effect to diminish, we require

$$\begin{aligned} k_B T &\gg \frac{\hbar \omega}{2 \sqrt{\frac{\kappa}{m}}} \quad \text{for estimation} \sin(ka) \\ \Rightarrow T &\gg 90 \text{ K} \end{aligned}$$

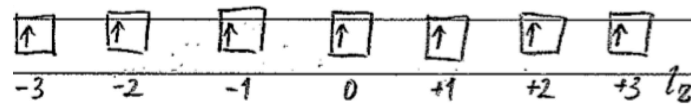
4. (DRAFT)

- (a) Paramagnet: matter whose magnetisation aligns with an externally applied B field. Most metals with $J \neq 0$ exhibits this, e.g. steel. $\chi > 0$, $M = 0$ when $B = 0$.

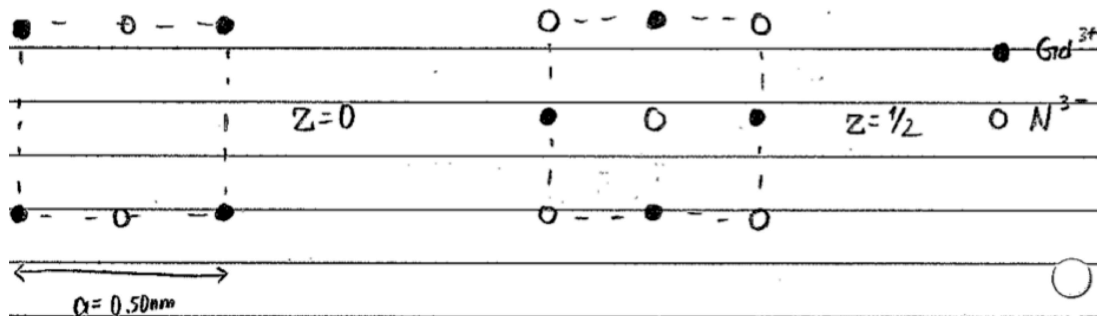
Diamagnet: matter whose magnetisation anti-aligns with the external B field. All atoms exhibit this to some extent, e.g. xenon gas. $\chi < 0$, $M = 0$ when $B = 0$.

Ferromagnet: matter whose magnetisation occurs spontaneously and may retain even after an external B field is removed, e.g. iron. $\chi > 0$, $M \neq 0$ when $B = 0$.

- (b) Hund's Rules give:



So every e^- in the f shell has their spins aligned, so Gd^{3+} has $S = \frac{7}{2}$.



- (c) Paramagnetic Hamiltonian:

$$\hat{H} = \tilde{g}\mu_B \mathbf{B} \cdot \mathbf{J}$$

where

$$\tilde{g} = \frac{1}{2}(g+1) + \frac{1}{2}(g-1) \underbrace{\left[\frac{S(S+1) - L(L+1)}{J(J+1)} \right]}_{1 \text{ since } L=0}$$

$$= 2$$

Single particle partition function:

$$Z = \sum_{J=-\frac{7}{2}}^{J=+\frac{7}{2}} \exp[-\beta(\tilde{g}\mu_B B J)]$$

$$= 2 \cosh \left[2\beta\mu_B B \left(\frac{7}{2} \right) \right]$$

$$= 2 \cosh(7\beta\mu_B B)$$

since only $\pm \hat{z}$ is only allowed.

Total partition function for N independent particles:

$$\begin{aligned}\mathcal{Z} &= \mathcal{Z}^N \\ &= [2 \cosh(7\beta\mu_B B)]^N\end{aligned}$$

Magnetic moment:

$$\begin{aligned}m &= -\frac{\partial F}{\partial B} \\ &= -\frac{\partial}{\partial B} [-k_B T \ln \mathcal{Z}] \\ &= k_B T \cdot \frac{1}{\mathcal{Z}} \cdot \frac{\partial \mathcal{Z}}{\partial B} \\ &= k_B T \cdot \frac{N [2 \cosh(7\beta\mu_B B)]^{N-1} (2 \sinh(7\beta\mu_B B) \cdot 7\beta\mu_B)}{[2 \cosh(7\beta\mu_B B)]^N} \\ &= \frac{2N \sinh(7\beta\mu_B B) \cdot 7\mu_B}{2 \cosh(7\beta\mu_B B)} \\ &= 7N \tanh(7\beta\mu_B B)\end{aligned}$$

Number density of Gd^{3+} :

$$\begin{aligned}n &= \frac{\frac{1}{8} \cdot 8 + 4 \cdot \frac{1}{2}}{(0.50 \text{ nm})^3} \\ &= 3.20 \times 10^{28} \text{ m}^{-3}\end{aligned}$$

Magnetisation:

$$\begin{aligned}M &= \frac{m}{V} \\ &= 7 \frac{N}{V} \tanh(7\beta\mu_B B) \\ &= 7n \tanh(7\beta\mu_B B) \\ &\approx \frac{n (7\mu_B)^2}{k_B T} B\end{aligned}$$

for $\mu_B B \ll k_B T$.

Also magnetic susceptibility $\chi = \lim_{B \rightarrow 0} \frac{\partial M}{\partial H}$.

Assuming $\chi \ll 1$,

$$\begin{aligned}H &\simeq \frac{B}{\mu_0} \\ \Rightarrow \chi &= \mu_0 \frac{\partial M}{\partial B} \\ &= \frac{\mu_0 n (7\mu_B)^2}{k_B T}\end{aligned}$$

Hence:

$$C = \frac{\mu_0 n (7\mu_B)^2}{k_B}$$

$$= 12.3 \text{ K}$$

(d) For ferromagnetism, there exists the exchange interaction in the Hamiltonian:

$$\hat{H}_{\text{exchange}} = \sum_{j \neq i} A_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

So the denominator should have an additional term that lets $\chi \rightarrow \infty$ as $T \rightarrow T_c$.

At the transition temperature T_c , χ should diverge, hence it should be of form:

$$\chi = \frac{C}{T - T_c}$$

At $T = 0$, entropy is null. Therefore all magnetic moments align, hence:

$$\lim_{\beta \rightarrow \infty} M = 7n\mu_B \underbrace{\lim_{\beta \rightarrow \infty} \tanh(7\beta\mu_B B)}_1$$

$$= 7n\mu_B$$

