FSK 324 Test 2 - 2011
Memorandum

Section A

Q 1. (i) Show that

$$\bar{\varepsilon} = \frac{\hbar\omega}{e^{\hbar\omega/KT} - 1}.$$

Soln.

Let $x = e^{-\hbar\omega/KT}$

$$\Rightarrow \bar{\varepsilon} = \frac{\sum_{n=0}^{\infty} \varepsilon_n e^{-\frac{\varepsilon_n}{KT}}}{\sum_{n=0}^{\infty} e^{-\frac{\varepsilon_n}{KT}}} = \frac{\sum_{n=0}^{\infty} n\hbar\omega e^{-\frac{n\hbar\omega}{KT}}}{\sum_{n=0}^{\infty} e^{-\frac{n\hbar\omega}{KT}}}$$

$$= \frac{\hbar\omega \sum_{n=0}^{\infty} n x^n}{\sum_{n=0}^{\infty} x^n} \quad -(1)$$

But

$$\frac{d}{dx} \sum_{n=0}^{\infty} x^n = \sum_{n=0}^{\infty} \frac{d}{dx} x^n = \sum_{n=0}^{\infty} n x^{n-1}$$

$$= x^{-1} \sum_{n=0}^{\infty} n x^n \quad -(2)$$

Then since

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad -(3)$$

it follows that

$$\frac{d}{dx} \sum_{n=0}^{\infty} x^n = \frac{d}{dx}\left(\frac{1}{1-x}\right)$$

②

$$\Rightarrow \frac{d}{dx}\sum_{n=0}^{\infty} x^n = \frac{d}{d(1-x)}(1-x)^{-1}\frac{d(1-x)}{dx}$$

$$= -\frac{1}{(1-x)^2}(-1)$$

$$= \frac{1}{(1-x)^2} \qquad — (4)$$

Equating (2) and (4) ~~(3) and (4)~~

$$\Rightarrow \frac{1}{(1-x)^2} = x^{-1}\sum_{n=0}^{\infty} n x^n$$

$$\Rightarrow \sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2} \qquad -(5)$$

Finally substitute (5) and (3) into (1)

$$\Rightarrow \bar{\varepsilon} = \frac{\hbar\omega \dfrac{x}{(1-x)^2}}{\dfrac{1}{(1-x)}}$$

$$= \hbar\omega \frac{x}{1-x}$$

$$= \hbar\omega \frac{e^{-\frac{\hbar\omega}{KT}}}{1-e^{-\frac{\hbar\omega}{KT}}}$$

$$\therefore \boxed{\bar{\varepsilon} = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{KT}}-1}}$$

Q.E.D.

(ii) Derive C_V

$$C_V = \left.\frac{\partial E}{\partial T}\right|_V$$

Since $\bar{\varepsilon} = \dfrac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$ (per oscillator, per degree of freedom)

It follows that

$\bar{\varepsilon} = N_A \dfrac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$ (per mole, per degree of freedom)

and $E = 3\bar{\varepsilon} = \dfrac{3N_A\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$ (per mole, for all 3 degrees of freedom)

$$\therefore \quad \frac{\partial E}{\partial T} = 3N_A\hbar\omega \frac{\partial}{\partial T}\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^{-1}$$

$$= 3N_A\hbar\omega \frac{\partial\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^{-1}}{\partial\left(e^{\frac{\hbar\omega}{kT}} - 1\right)} \frac{\partial\left(e^{\frac{\hbar\omega}{kT}} - 1\right)}{\partial T}$$

$$= -3N_A\hbar\omega \left(e^{\frac{\hbar\omega}{kT}} - 1\right)^{-2} \frac{\partial e^{\frac{\hbar\omega}{kT}}}{\partial\left(\frac{\hbar\omega}{kT}\right)} \frac{\partial}{\partial T}\left(\frac{\hbar\omega}{k} \cdot T^{-1}\right)$$

$$= -3N_A\hbar\omega \cdot \frac{1}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2} \cdot e^{\frac{\hbar\omega}{kT}} \cdot \left(\frac{\hbar\omega}{k}\right)\left(-\frac{1}{T^2}\right)$$

$$\Rightarrow \frac{\partial E}{\partial T} = 3N_A \frac{(\hbar\omega)^2}{kT^2} \frac{e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}}-1\right)^2}$$

$$= \underbrace{3kN_A}_{R} \cdot \left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}}-1\right)^2}$$

$$= 3R\left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}}-1\right)^2}$$

Putting $\omega = \omega_E$, the Einstein frequency gives

$$\boxed{C_V = 3R\left(\frac{\hbar\omega_E}{kT}\right)^2 \frac{e^{\hbar\omega_E/kT}}{\left(e^{\hbar\omega_E/kT}-1\right)^2}}$$

Question 2

(i) $u(x) = A e^{ikx}$ (wave equation in 1-D)

The BVK condition is

$$u(0) = u(L) \quad \text{where} \quad 0 \leq x \leq L$$

$$\Rightarrow \quad A e^{ik(0)} = A e^{ikL}$$

$$\Rightarrow \quad e^{ikL} = 1 \quad \text{for } A \neq 0 \qquad -(1)$$

Then since $e^{i\phi} = \cos\phi + i\sin\phi$,

equation (1) becomes

$$\cos(KL) + i\sin(KL) = 1 + i\cdot 0$$

where $\cos KL = 1$ and $\sin KL = 0$

which are valid when

$$KL = 2\pi n \quad , \quad n = 0, \pm 1, \pm 2, \ldots$$

$$\therefore \quad \boxed{K = \frac{2\pi n}{L}} \quad \text{for } n \in \mathbb{Z}$$

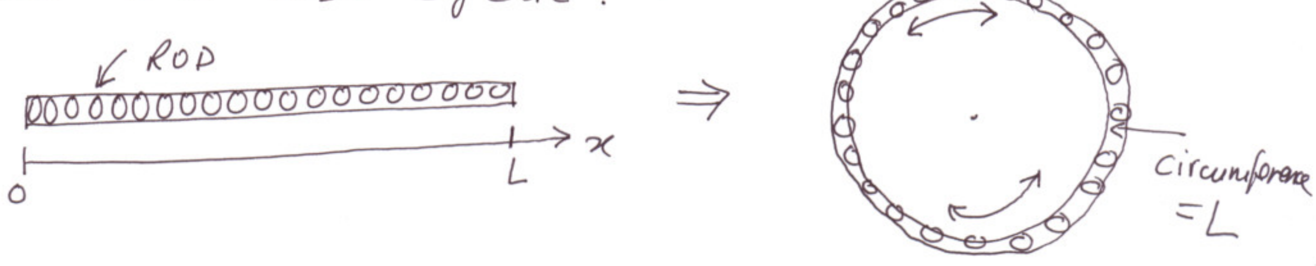
The integer n represents the <u>nth vibrational mode</u>

(ii) The number of vibration modes is

$$n = \frac{L}{2\pi} K$$

$$\Rightarrow \quad \frac{dn}{dK} = \frac{L}{2\pi} \quad \Rightarrow \quad \boxed{dn = \frac{L}{2\pi} dK}$$

(iii) The Physical significance of the BLK condition is that the ends of the rod in which the vibrations occur are restricted in such a way that the energy propagation is also cyclic.



Question 3.

Silicon, $M = 28.09 g/mol$; $\theta_D = 647K$; $R = 8.314 J/K mol$

(i) $m = 400g$

$T_i = 300K$

$T_f = 10K$

Note that both T_i and T_f << θ_D, hence the low-temperature approximation can be used reasonably well:

$$C_V = \frac{12}{5}\pi^4 R \left(\frac{T}{\theta_D}\right)^3$$

But $C_V = \left.\frac{\partial E}{\partial T}\right|_V \Rightarrow E = \int_{T_i}^{T_f} C_V \, dT$ { amount of heat that should be removed to effect the cooling

Hence

$$E = \frac{12}{5}\pi^4 \frac{R}{\theta_D^3} \int_{300}^{10} T^3 \, dT$$

$$= \frac{12}{5}\pi^4 \frac{R}{\theta_D^3} \cdot \frac{1}{4} T^3 . T \Big|_{300}^{10}$$

$$= \frac{3}{5}\pi^4 R \left[T \left(\frac{T}{\theta_D}\right)^3 \Big|_{300}^{10} \right]$$

$$= \frac{3}{5}\pi^4 R \left[10 \left(\frac{10}{647}\right)^3 - 300 \left(\frac{300}{647}\right)^3 \right] \text{ joules/mol}$$

$$= 485.9155 \left(3.69222 \times 10^{-5} - 29.9069536\right) J/mol$$

$$= -14532.2347 \, J/mol$$

But

$$n = \frac{m}{M} \quad \text{(number of moles)}$$

$$= \frac{400}{28.09}$$

$$= 14.24 \text{ mol}$$

$$\therefore E = -14532.2347 \frac{J}{mol} \times 14.24 mol$$

$$E = -206.94 \text{ KJ}$$

(ii) Amount of helium ?

$$L = 2.7 \text{ KJ}/l$$

$$\underset{\text{(Heat flow)}}{Q = -E} = \cancel{V}_{He} L \quad \text{where } V_{He} = \text{volume of helium required}$$

$$\therefore V_{He} = \frac{Q}{L} = \frac{+206.94 \text{ KJ}}{2.7 \text{ KJ}/l}$$

$$\boxed{V_{He} = 76.64 l}$$

(iii) $\omega_D = ?$

$$\hbar \omega_D = K \theta_D \Rightarrow \omega_D = \frac{K}{\hbar} \theta_D$$

$$= \frac{1.38 \times 10^{-23} \times 647}{\frac{6.626 \times 10^{-34}}{2\pi}} \text{ rad/s}$$

$$\therefore \boxed{\omega_D = 8.467 \times 10^{13} \text{ rad/s}}$$

Question 4

(1) The aim is to first show that

$$u(x,t) = Ae^{i(kx-\omega t)}$$

can, after repeated differentiation be written as

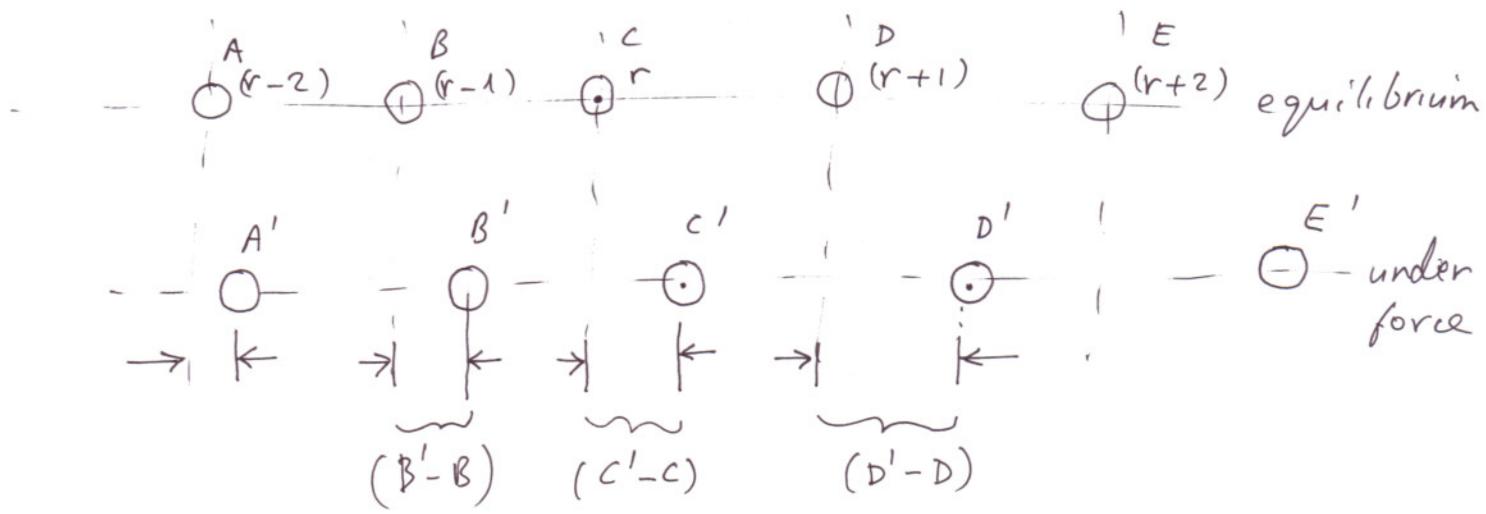
$$\ddot{u} = -\omega^2 u \qquad \text{(all such motions are said to be simple harmonic)}$$

OR, in terms of a restorative force

$$F_r = m\ddot{u} \qquad \text{(Newton's second law)}$$

$$\Rightarrow \quad F_r = -m\omega^2 u \qquad — (1)$$

Since the coupled atoms oscillate elastically



Considering the r-th atom and its immediate adjacent atoms, the net displacement of the r-th atom is

$$\Delta u = (u_{r+1} - u_r) - (u_r - u_{r-1})$$

and if the elastic medium of elasticity μ experiences this displacement then from Hooke's Law

$$F = \mu \Delta u$$

$$= \mu\left[(u_{r+1} - u_r) - (u_r - u_{r-1})\right] \quad — (2)$$

9.

Equating (1) and (2)

$$\Rightarrow \quad -m\omega^2 u_r = \mu\left[u_{r+1} - 2u_r + u_{r-1}\right] \quad -(3)$$

Since $u_r = A e^{ikra} e^{-i\omega t}$

$\therefore \quad u_{r+1} = A e^{ikra} e^{ika} e^{-i\omega t}$

$u_{r-1} = A e^{ikra} e^{-ika} e^{-i\omega t}$

with $x = ra$

$(ra + a) = (r+1)a$

$(ra - a) = (r-1)a$

$$\Rightarrow \quad -m\omega^2 u_r = \mu\left[u_r e^{ika} - 2u_r + u_r e^{-ika}\right]$$

(notice how $e^{-i\omega t}$ is eliminated from the equation)

$$\Rightarrow \quad \omega^2 = \frac{\mu}{m}\left[2 - e^{ika} - e^{-ika}\right] \quad -(4)$$

But $e^{\pm i\phi} = \cos\phi \pm i\sin\phi$

$\therefore \quad e^{i\phi} + e^{-i\phi} = 2\cos\phi$

Hence $e^{ika} + e^{-ika} = 2\cos(ka)$

$$\Rightarrow \quad \omega^2 = \frac{\mu}{m}\left[2 - 2\cos(ka)\right]$$

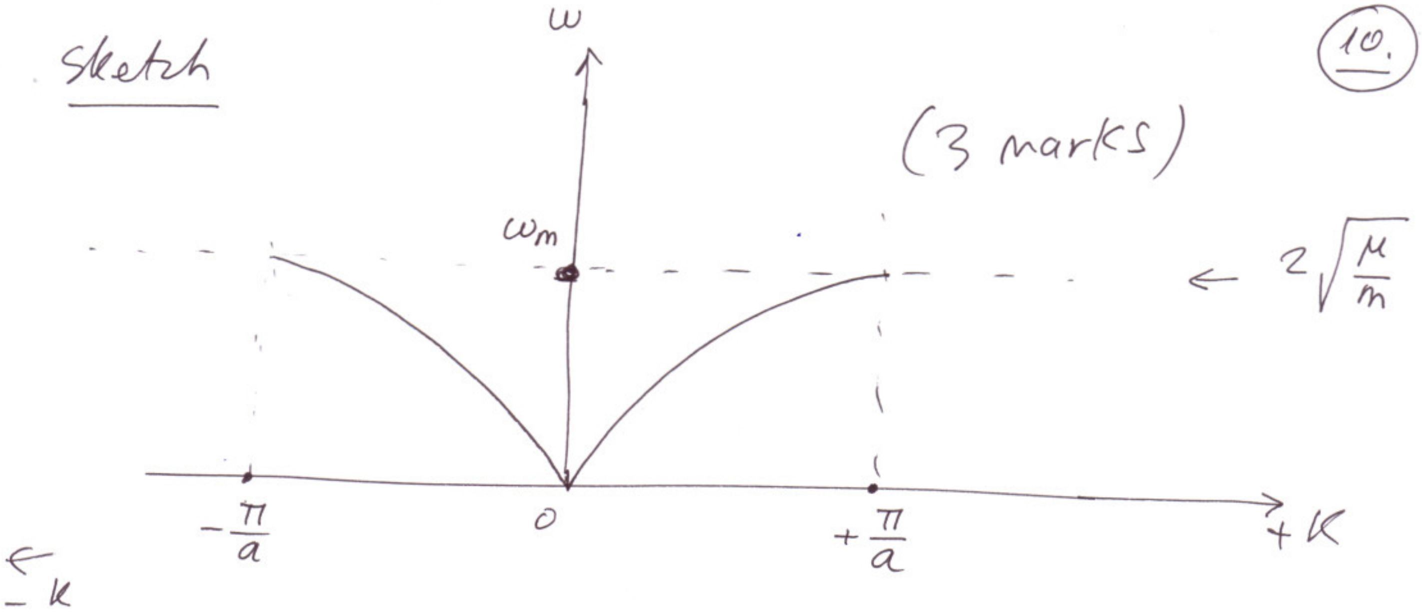
$$= \frac{2\mu}{m}\left[1 - \cos(ka)\right]$$

$$= \frac{4\mu}{m}\sin^2\left(\frac{ka}{2}\right) \quad \Rightarrow \quad \boxed{\omega = \pm\,\omega_m \sin\left(\frac{ka}{2}\right)}$$

where $\boxed{\omega_m = 2\sqrt{\frac{\mu}{m}}}$

(ii) Sketch

(3 marks)



ω has a maximum value when $\sin\left(\frac{Ka}{2}\right) = 1$

$$\Rightarrow \frac{Ka}{2} = \pm\frac{\pi}{2} \quad \therefore \quad K = \pm\frac{\pi}{a} \qquad \text{1 mark}$$

Question 5

(i) $\omega^2 = a \pm b(K)$ where $a = \mu\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$

$$b = \mu\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2 Ka}{M_1 M_2}}$$

The two branches $\omega_1(K)$ and $\omega_2(K)$ are

$$\omega_1(K) = \sqrt{a + b(K)} \quad \Leftarrow \text{optical branch}$$

$$\omega_2(K) = \sqrt{a - b(K)} \quad \Leftarrow \text{acoustic branch}$$

~~(ii)~~

(ii) sketch

Optical

when $k=0$

$$b(0) = \mu\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2}$$

$$= \mu\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

$$\therefore \omega_1^2(0) = a + b(0)$$

$$= 2\mu\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

Acoustic

when $k=0$

$$b = \mu\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

$$\therefore \omega_2^2(0) = a - b(0)$$

$$= 0$$

Limiting values of k

when $\sin^2(ka) = 1$, $ka = \pm\frac{\pi}{2}$ $\therefore$ $k = \frac{\pm\pi}{2a}$

Optical

$$\Rightarrow \omega_1^2\left(\pm\frac{\pi}{2a}\right) = a + b\left(\pm\frac{\pi}{2a}\right)$$

$$= \mu\left(\frac{1}{M_1}+\frac{1}{M_2}\right) + \mu\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1M_2}}$$

$$= \mu\left(\frac{1}{M_1}+\frac{1}{M_2}\right) + \mu\underbrace{\sqrt{\frac{(M_1+M_2)^2}{(M_1M_2)^2} - \frac{4M_1M_2}{(M_1M_2)^2}}}_{\underbrace{\frac{1}{M_1M_2}\sqrt{M_1^2+2M_1M_2+M_2^2-4M_1M_2}}_{\underbrace{\frac{1}{M_1M_2}\sqrt{(M_1-M_2)^2}}_{\frac{M_1-M_2}{M_1M_2} = \frac{1}{M_2}-\frac{1}{M_1}}}}$$

$$\therefore \omega_1^2\left(\pm\frac{\pi}{2a}\right)$$

$$= \mu\left(\frac{1}{M_1}+\frac{1}{M_2}+\frac{1}{M_2}-\frac{1}{M_1}\right)$$

$$= \frac{2\mu}{M_2} \Rightarrow \omega_1\left(\pm\frac{\pi}{2a}\right) = \sqrt{\frac{2\mu}{M_2}}$$

Acoustic

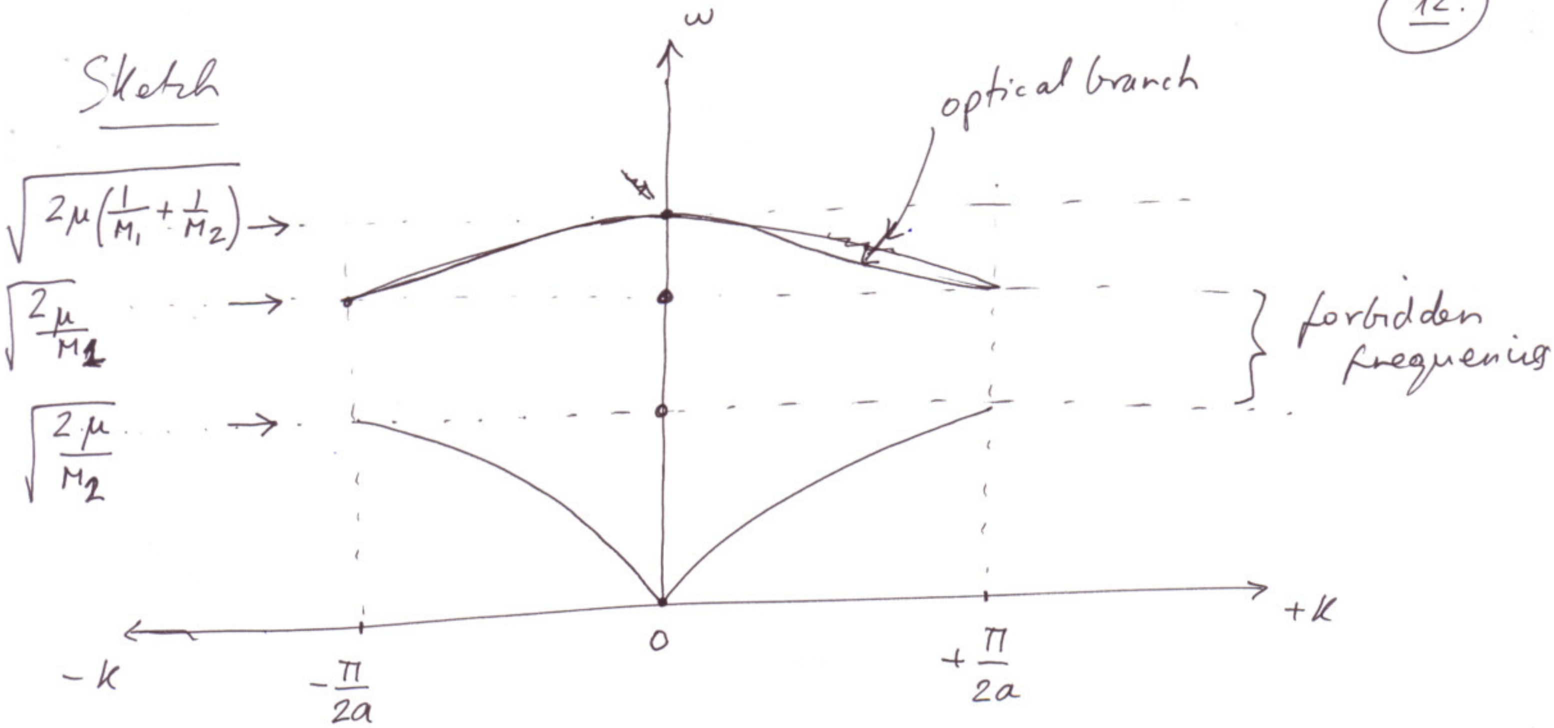
$$\omega_2^2\left(\pm\frac{\pi}{2a}\right) = a - b\left(\pm\frac{\pi}{2a}\right)$$

$$= \mu\left(\frac{1}{M_1}+\frac{1}{M_2}-\frac{1}{M_2}+\frac{1}{M_1}\right)$$

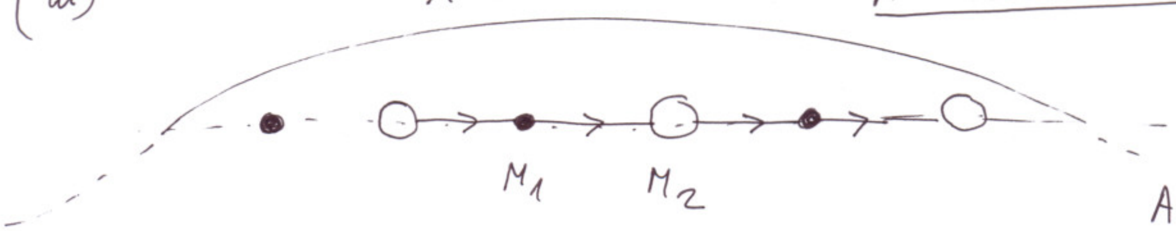
$$= \frac{2\mu}{M_1}$$

$$\therefore \omega_2\left(\pm\frac{\pi}{2a}\right) = \sqrt{\frac{2\mu}{M_1}}$$

Sketch



(iii) $\lambda >> a$ $(k=0)$ <u>Acoustic branch</u>

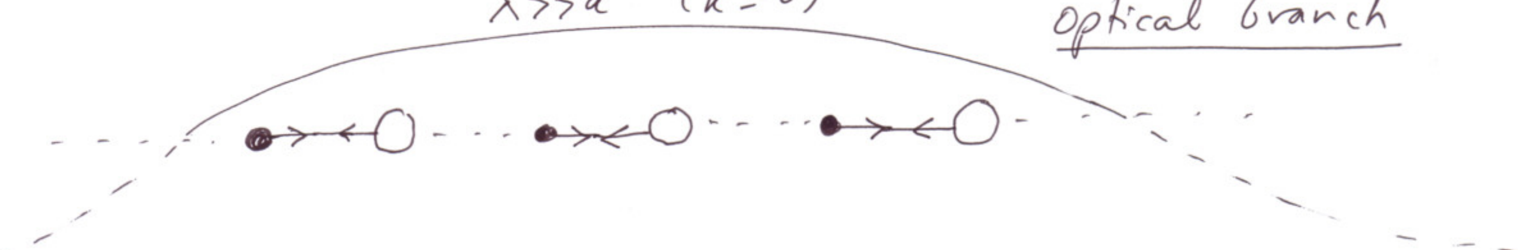


At $k=0$

$A_1 = A_2$

Waves are in phase and have the <u>same amplitude</u>

$\lambda >> a$ $(k=0)$ <u>optical branch</u>



At $k=0$ $(\lambda >> a)$

$$M_1 M_2 + M_2 A_2 = 0$$

$$\Rightarrow \frac{A_1}{A_2} = -\frac{M_1}{M_2}$$

The minus sign means the waves are 180° out of phase but oscillate with common center of mass.

Question 6.

(i) Gold

$\Theta_{D,Au} = ?$

$\rho_{Au} = 19.3 g/cm^3$

$M_{Au} = 197 g/mol$

$V_{Au} = 2100 m/s$

Copper

$\Theta_{D,Cu} = 348K$

$\rho_{Cu} = 8.9 g/cm^3$

$M_{Cu} = 63.5 g/mol$

$V_{Cu} = 3800 m/s$

Soln.

$$\omega_D = V(6\pi^2 n)^{\frac{1}{3}}$$

$$n = \frac{N_A}{V} \quad \text{where} \quad V = \frac{M}{\rho}$$

$$\therefore \quad n = \frac{N_A}{\frac{M}{\rho}} = \frac{\rho N_A}{M}$$

$$n_{Cu} = \frac{\rho_{Cu} N_A}{M_{Cu}} \quad (\text{for copper}) \quad -(1)$$

$$n_{Au} = \frac{\rho_{Au} N_A}{M_{Au}} \quad (\text{for gold}) \quad -(2)$$

$$\Rightarrow \omega_{D,Au} = V_{Au} (6\pi^2)^{\frac{1}{3}} \, n_{Au}^{\frac{1}{3}} \quad -(3)$$

and $\omega_{D,Cu} = V_{Cu} (6\pi^2)^{\frac{1}{3}} \, n_{Cu}^{\frac{1}{3}} \quad -(4)$

(3) ÷ (4)

$$\Rightarrow \frac{\omega_{D,Au}}{\omega_{D,Cu}} = \frac{V_{Au}}{V_{Cu}} \cdot \left(\frac{n_{Au}}{n_{Cu}}\right)^{\frac{1}{3}} = \frac{V_{Au}}{V_{Cu}} \left[\frac{\frac{1}{M_{Au}} \rho_{Au} N_A}{\frac{1}{M_{Cu}} \rho_{Cu} N_A}\right]^{\frac{1}{3}}$$

~~Also,~~

$$\Rightarrow \quad \frac{\omega_{D,Au}}{\omega_{D,Cu}} = \frac{V_{Au}}{V_{Cu}} \left(\frac{\rho_{Au} M_{Cu}}{\rho_{Cu} M_{Au}} \right)^{\frac{1}{3}} \quad ; \quad \frac{\theta_D}{\omega_D} = \frac{\hbar}{k_B}$$

Substituting:

$$\theta_{D,Au} = \left[\frac{2100}{3800} \sqrt[3]{\frac{19.3 \times 63.5}{8.9 \times 197}} \right] 348$$

$$= \underline{\underline{170.67K}}$$

~~since~~ since

$$\frac{\theta_{D,Au}}{\omega_{D,Au}} = \frac{\hbar}{k_B} = \frac{\theta_{D,Cu}}{\omega_{D,Cu}}$$

$$\Rightarrow \quad \frac{\omega_{D,Au}}{\omega_{D,Cu}} = \frac{\theta_{D,Au}}{\theta_{D,Cu}} = \frac{V_{Au}}{V_{Cu}} \left(\frac{\rho_{Au} M_{Cu}}{\rho_{Cu} M_{Au}} \right)^{\frac{1}{3}}$$

$$\underline{\underline{\theta_{D,Au} = 170.67K}}$$

(ii) Well-covered in the study-guide.

Section B

7. (i) $\mathcal{E} = \frac{V}{L}$; $R = \rho \frac{L}{A}$; $J = \frac{I}{A}$

starting from $I = \frac{V}{R}$ (Ohm's Law)

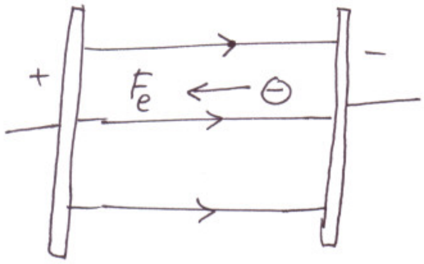
we have

$$J = \frac{V}{R} \cdot \frac{1}{A} = \frac{V}{\rho \frac{L}{A} \cdot A} = \frac{1}{\rho} \cdot \frac{V}{L}$$

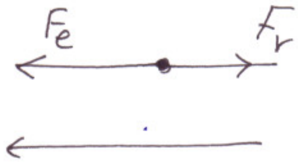
where $\frac{1}{\rho} = \sigma$

$$\therefore \quad \boxed{J = \sigma \mathcal{E}}$$

(ii)



Force diagram



F_n = net force

$$F_n = F_e - F_r$$

where F_r = force due to inter-electron collisions $= m\dfrac{V}{\tau}$

$$F_e = -e\,\mathcal{E}$$

(τ = relaxation time)

V = drift velocity

$$\Rightarrow F_n = F_e - F_r$$

$$\Leftrightarrow m\frac{dv}{dt} = -e\,\mathcal{E} - \frac{mv}{\tau} \quad \text{(per electron)}$$

Under equilibrium $F_n = 0 \Rightarrow v$ = constant.

$$\Rightarrow V = -\frac{e\tau}{m}\mathcal{E}$$

Since $n = \dfrac{\text{number of electrons}}{\text{volume containing the electrons}}$

$J = (-ne)\,V_d$ is the amount of charge flowing in unit time (i.e. current) through a unit area = current density

$$= (-ne)\left(-\frac{e\tau}{m}\mathcal{E}\right)$$

$$\Rightarrow J = \frac{ne^2\tau}{m}\mathcal{E}$$

$$\therefore \boxed{\sigma = \frac{ne^2\tau}{m}}$$

e.g. in 1 sec, each electron travels a distance V_d

(iii) $Z_{Cu} = 2$

$\rho_{Cu} = 8.95 g/cm^3$

$\sigma = 1.55 \times 10^{-8} \Omega m$

$m_e = 9.109 \times 10^{-31} kg$

$M_{Cu} = 63.5g$

$$V_{Cu} = \frac{M_{Cu}}{\rho_{Cu}} = \frac{63.5}{8.95} cm^3 = \frac{63.5}{8.95} \times 10^{-6} m^3$$

$$n = \frac{Z_v \rho_{Cu} N_A}{M_{Cu}} = \frac{2 \times 8.95 \times 10^3 \times 6.022 \times 10^{23}}{63.5 \times 10^{-3}}$$

(electrons /m^3)

$$= 1.69754 \times 10^{29} m^{-3}$$

From $\sigma = \dfrac{ne^2 \tau}{m_e}$

$$\tau = \frac{\sigma m_e}{ne^2} = \frac{1.55 \times 10^{-8} \times 9.109 \times 10^{-31}}{1.69754 \times 10^{29} \times (1.6022 \times 10^{-19})^2}$$

$$\boxed{\tau = 3.24 \times 10^{-30} s}$$

Question 8

(i) Mathiesen's rule – states that electrical resistivity (ρ) has a temperature dependant part and a temperature independent part, i.e.

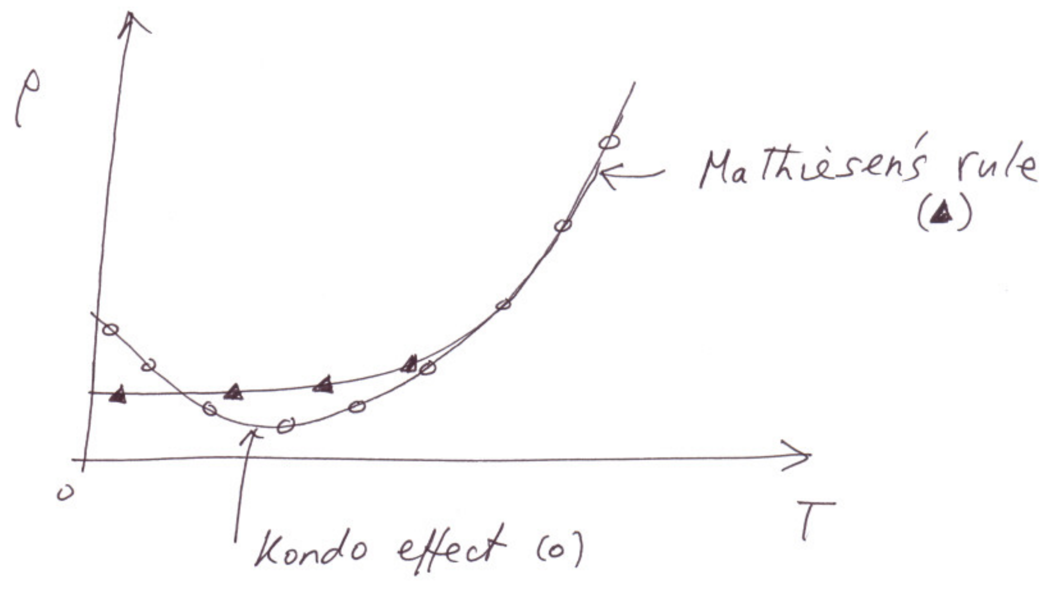
$\rho = \rho_i + \rho_f(T)$ Almost linear with (T).

dominates at high temperature due to phonon scattering.

dominates at low temperature with negligible phonon scattering

(ii) Kondo effect

Describes the deviation from Mathiesen's rule and is seen as an anomaly due to the scattering of electrons by magnetic moments of impurities. For example, Fe impurities in copper (Cu) exhibit the Kondo effect.



(iii) Lorentz number

The Wiedemann-Franz Law states that the ratio of the electronic contribution to the thermal conductivity (κ_e) and the electrical conductivity (σ) of a metal is proportional to the temperature (T).

That is, $\frac{\kappa_e}{\sigma} = LT$ with L being the constant of proportionality and known as the Lorentz number

kappa

$$L = \frac{\kappa_e}{\sigma T} \approx 2.22 \times 10^{-8}\, W\Omega K^{-2}.$$