FSK 324 Test 2 _ Memo (2012)

Sect A

Q1. (i) $$\bar{\varepsilon} = \frac{\sum_{n=0}^{\infty} \varepsilon_n e^{-\frac{\varepsilon_n}{KT}}}{\sum_{n=0}^{\infty} e^{-\frac{\varepsilon_n}{KT}}}, \quad \varepsilon_n = n\hbar\omega, \; n = 0, 1, 2, \ldots$$

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

But $\sum_{n=0}^{\infty} x^n = \dfrac{1}{1-x}$ if and only if ~~...~~ $n < 0$ (i.e. n is negative)

Then

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

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

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

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

Hence $$\bar{\varepsilon} = \hbar\omega \frac{\frac{x}{(1-x)^2}}{\frac{1}{(1-x)}} = \hbar\omega \frac{x}{1-x} = \hbar\omega \frac{e^{-\frac{\hbar\omega}{KT}}}{1 - e^{-\frac{\hbar\omega}{KT}}}$$

$$\therefore \bar{\varepsilon} = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{KT}} - 1}$$ (per atomic oscillator, per degree of freedom).

(ii)

$\Rightarrow$ For 3-degrees of freedom,

$$\bar{\varepsilon} = \frac{3\hbar\omega}{e^{\frac{\hbar\omega}{KT}} - 1}$$

Therefore, per mole

$$E = N_A \bar{\varepsilon}\Big|_{3\,\text{degrees}} = \frac{3 N_A \hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$$

Then

$$C_V = \frac{\partial E}{\partial T}\Big|_V = 3N_A \cdot \hbar\omega \left[\frac{\partial}{\partial \left(e^{\frac{\hbar\omega}{kT}} - 1\right)} \cdot \left(e^{\frac{\hbar\omega}{kT}} - 1\right)^{-1} \cdot \frac{\partial}{\partial T}\left(e^{\frac{\hbar\omega}{kT}} - 1\right) \right]$$

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

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

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

But $R = kN_A$ and $\omega \rightarrow \omega_E$, the Einstein frequency

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

which is the required expression.

Q2. At the low-temperature limit of C_V in the Debye model,

$$C_V \approx \frac{12}{5}\pi^4 k\left(\frac{T}{\theta_D}\right)^3 \Rightarrow C_V = \alpha\left(\frac{T}{\theta_D}\right)^3$$

$$\therefore \quad \alpha = \frac{C_V}{(T/\theta_D)^3} = C_V\left(\frac{\theta_D}{T}\right)^3$$

Using KCl at 5K,

$$\alpha = \left(\frac{230}{5}\right)^3 (3.8\times10^{-2}) = 3.6988 * 10^3 \, JK^{-1}mol^{-1}.$$

$$\Rightarrow C_V = 3.6988\times10^3\left(\frac{T}{\theta_D}\right)^3$$

Hence for NaCl at 5K,

$$C_V = 3.6988 * 10^3\left(\frac{5}{310}\right)^3$$

$$\approx 1.552\times 10^{-2} \, JK^{-1}mol^{-1}.$$

Similarly, for KCl at 2K,

$$C_V = 3.6988 * 10^3\left(\frac{2}{230}\right)^3$$

$$\approx 2.432 * 10^{-3} \, JK^{-1}mol^{-1}$$

Q3. Let the mass of each particle be m. Then

$$m\ddot{u}_r = F_r \quad -(1)$$

But $U_x = Ae^{i(kx-\omega t)} \Rightarrow U_r = Ae^{i(kra-\omega t)}$, where $x = ra$.

$$\Rightarrow \frac{d^2u_r}{dt^2} = -\omega^2 u_r \quad \text{or} \quad \ddot{u}_r = -\omega^2 u_r \quad -(2)$$

(2) into (1) gives

$$-m\omega^2 u_r = F_r \quad -(3)$$

From Hooke's law, the force on the r_th atom is

$$F_r = \mu(u_{r+1}-u_r) - \mu(u_r - u_{r-1})$$

where μ is the atomic force constant (i.e. elasticity at inter-atomic level)

$$\therefore F_r = \mu \left[u_{r+1} + u_{r-1} - 2u_r \right] \quad -(4)$$

But (3) = (4)

$$\Rightarrow \omega^2 = + \frac{\mu}{m u_r}\left[2 - \frac{u_{r+1} + u_{r-1}}{u_r} \right] \quad -(5)$$

But $u_r = A e^{i(kra - \omega t)} = A e^{ikra} e^{-i\omega t}$

$$u_{r+1} = A e^{i[k(r+1)a - \omega t]} = A e^{-i\omega t} e^{ikr} e^{ika}$$

$$u_{r-1} = A e^{i[k(r-1)a - \omega t]} = A e^{-i\omega t} e^{ikr} e^{-ika}$$

Hence (5) becomes

$$\omega^2 = \frac{\mu}{m}\left(2 - e^{ika} - e^{-ika} \right).$$

But $e^{\pm i\phi} = \cos\phi \pm i \sin\phi \Rightarrow \cos\phi = \frac{e^{i\phi} - e^{-i\phi}}{2}$

where if $\phi = ka$ then

$$\omega^2 = \frac{\mu}{m}(2 - 2\cos ka)$$

$$= \frac{2\mu}{m}(1 - \cos ka).$$

Furthermore, $\cos 2\phi = 1 - 2\sin^2\phi$

$$\therefore \frac{1 - \cos 2\phi}{2} = \sin^2\phi$$

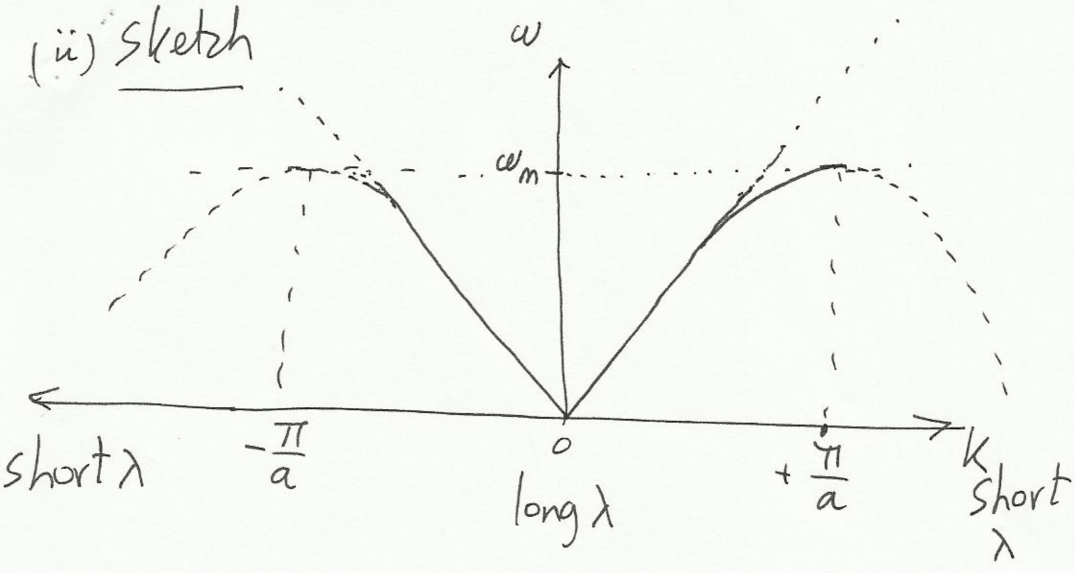
Let $2\phi = ka \Rightarrow \phi = \frac{ka}{2}$

$$\therefore \omega^2 = \frac{4\mu}{m} \cdot \left(\frac{1 - \cos ka}{2} \right) = \frac{4\mu}{m} \sin^2\left(\frac{ka}{2}\right)$$

$$\Rightarrow \omega = \pm 2\sqrt{\frac{\mu}{m}} \sin\left(\frac{ka}{2}\right) \text{ or } \omega = \pm \omega_m \sin\left(\frac{ka}{2}\right)$$

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

(ii) Sketch



$K = \frac{2\pi}{\lambda}$

($\lambda \to 0$ = short λ $\Rightarrow$ k is large)

$1 = \sin\frac{ka}{2} \equiv$ maximum, when $\frac{ka}{2} = \pm\frac{\pi}{2}$ $\therefore$ $K = \frac{\pm\pi}{a}$

$0 = \sin\frac{ka}{2}$, when $\frac{ka}{2} = \pm\pi \Rightarrow K = \pm\frac{2\pi}{a}$

Q4.

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

$$\omega_D \hbar = kT_D \Rightarrow \frac{kT_D}{\hbar} = v(6\pi^2)^{\frac{1}{3}}\left(\frac{N_A}{\frac{M}{\rho}}\right)^{\frac{1}{3}}$$

const.

$$\Rightarrow T_D = \frac{\hbar}{k} v\,(6\pi^2 N_A)^{\frac{1}{3}}\left(\frac{\rho}{M}\right)^{\frac{1}{3}} = \beta\, v\left(\frac{\rho}{M}\right)^{\frac{1}{3}}$$

$$\Rightarrow \frac{T_D^{(Au)}}{T_D^{(Cu)}} = \frac{V^{(Au)}}{V^{(Cu)}}\left[\frac{\rho^{(Au)}}{M^{(Au)}}\right]^{\frac{1}{3}} * \left[\frac{M^{(Cu)}}{\rho^{(Cu)}}\right]^{\frac{1}{3}}$$

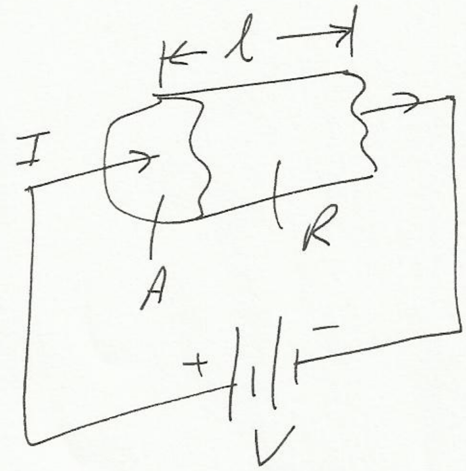
$$\Rightarrow T_D^{(Au)} = \frac{V^{(Au)}}{V^{(Cu)}}\left[\frac{\rho^{(Au)}}{\rho^{(Cu)}} \cdot \frac{M^{(Cu)}}{M^{(Au)}}\right]^{\frac{1}{3}} T_D^{(Cu)}$$

$$= \left(\frac{2.1}{3.8}\right)\left[\frac{19.3}{8.9} * \frac{63.5}{197}\right]^{\frac{1}{3}} 348\,\text{Kelvin}$$

$$\therefore \underline{T_D^{(Au)} = 170.7\,K}$$

Sect B.

5. (i) Ohms Law $\Rightarrow V = I \cdot R.$



$$R = \rho \frac{L}{A}$$

$$\mathcal{E} = \frac{V}{L} \Rightarrow \mathcal{E} \cdot L = V$$

(electric field)

$$J = \frac{I}{A} \Rightarrow I = J \cdot A$$

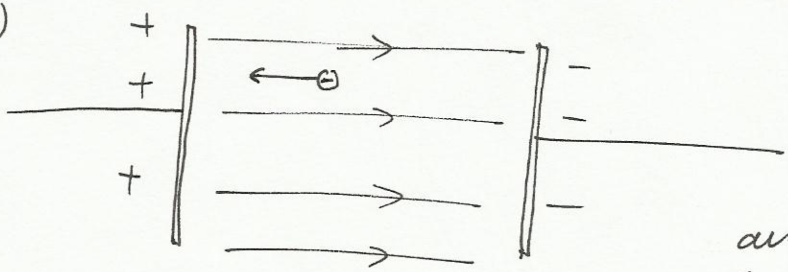
$\therefore$ Since $V = I \cdot R$

$$(\mathcal{E} \cdot L) = (J \cdot A) \cdot \left(\rho \frac{L}{A}\right)$$

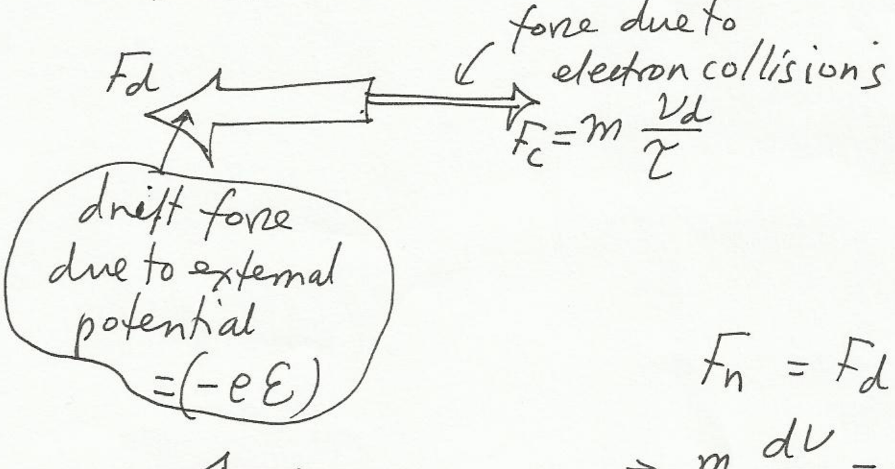
$$\Rightarrow \mathcal{E} = \rho J \quad \text{or} \quad J = \frac{1}{\rho} \mathcal{E}$$

$$\underline{\underline{J = \sigma \mathcal{E}}}$$

(ii)

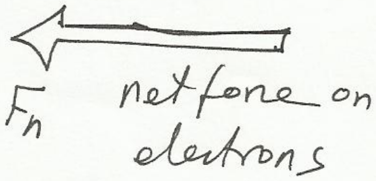


$F = q\mathcal{E}.$



$$F_n = F_d - F_c$$

$$\Rightarrow m \frac{dv}{dt} = -e\mathcal{E} - m\frac{v_d}{\tau}.$$



At equilibrium, $F_n = 0$

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

But $J = -ne v_d$ {where n = number of electrons per unit volume.

To see this, consider a time interval of Δt sec. Hence volume ~~of~~ swept out by cross-section area is $A v_d$, and number of electrons therein is $(nAv_d\Delta t)$.

Hence charge delivered in 1 sec is $(-neAv_d)$ and the current is

$$I = \frac{\Delta\,\text{charge}}{\text{time}} = \frac{-neAv_d\cancel{\Delta t}}{\cancel{\Delta t}} = -neAv_d$$

By definition

$$J = \frac{I}{A} = -nev_d \}$$

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

$\therefore J = \frac{ne^2\tau}{m}\mathcal{E}$ which also equals $(\sigma\mathcal{E})$

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

(iii) $M = 63.5g$

$\rho_{den.} = 8.95 g\,cm^{-3}$

$\rho_{res} = 1.55 \times 10^{-8} (\Omega m)$

$Z_v = 1.$

(a) $n = \dfrac{Z_i\, \rho_{den.} N_A}{M} = \dfrac{1 \times 8.95\, g cm^{-3} \times 6.022 \times 10^{23} mol^{-1}}{63.5 g\, mol^{-1}}$

$= \underline{\underline{8.488 \times 10^{22}}}$ electrons per cm^3

or $\underline{\underline{n = 8.488 \times 10^{28} \text{ per } m^3}}$ $(1cm^3 = 10^{-6} m^3)$

(b) $\sigma = \dfrac{ne^2 \tau}{m} = \dfrac{1}{\rho_{res.}} \quad \therefore \tau = \dfrac{m}{\rho_{res}\, n e^2}$

$= \dfrac{9.11 \times 10^{-31} kg.}{1.55 \times 10^{-8} \Omega m. * 8.488 \times 10^{28} m^{-3} (1.6022 \times 10^{-19} C)^2}$

$= 2.697 * 10^{-14} s$

$= 26.97 fs$ (femtosec)

(c) $\mathcal{E}_F = \dfrac{\hbar^2}{2m} (3\pi^2 n)^{\frac{2}{3}}$

$= \dfrac{(6.626 \times 10^{-34})^2}{(2\pi)^2 2 \times 9.11 \times 10^{-31}} \left(3\pi^2 \times 8.488 \times 10^{28}\right)^{\frac{2}{3}}$ Joules

$= 1.1283 \times 10^{-18} J$ $\left\{ \begin{array}{l} \text{but } 1eV = 1.6022 \times 10^{-19} J \\ \therefore 1J = \dfrac{1}{1.6022 \times 10^{-19}} eV \end{array} \right.$

$\underline{\underline{= 7.04 eV}}$

(see also Table 4.11 for $\mathcal{E}_F^{(Cu)}$).

(d) Fermi-velocity, V_F is $\sqrt{\dfrac{2\mathcal{E}_F}{m}} = \sqrt{\dfrac{2 \times 1.1283 \times 10^{-18}}{9.11 \times 10^{-31}}}\, m/s = 1.574 \times 10^{6} m/s$

$\therefore$ Mean free path $= l_F = V_F \tau = 2.697 \times 10^{-14} \times 1.574 \times 10^{6} m = 4.245 \times 10^{-8} m$
$= 42.45\, nm.$

6. The Drude theory (a.k.a the Classical Theory).

Successes

(i) correctly derives Ohm's law

(ii) correctly predicts the dependence of resistivity on temperature

(iii) explains the direct link between thermal conductivity and electrical resistivity.

Failures

(i) fails to explain the conduction electron contribution to heat capacity (thermal conductivity)

(ii) also fails to explain the contribution of conduction electrons to magnetic susceptability

(iii) cannot explain why the mean free paths are so much longer than the lattice parameter.

The free electron gas theory

Failures

(i) It's greatest failure is considered to be the sign of the Hall coefficient which can be both positive ~~and~~ or negative. The theory expects that R_H will always be negative.

(ii) It expects that the number of conduction electrons in unit volume will increase with valency. This is not always so.

(iii) It always predicts a spherical fermi-surface whereas measurements often indicate it can be non-spherical.

(iii) Na ; $\varepsilon_F = 3.23\,eV$

(a) Fermi-energy – is the energy level of the highest or most energetic of the ground states of a material at zero Kelvin.

(b) $\varepsilon_F = KT_F \Rightarrow T_F = \frac{\varepsilon_F}{K} = \frac{3.23 \times 1.6022 \times 10^{-19}\,J}{1.38 \times 10^{-23}\,J K^{-1}}$

(assume 1 mole)

$= 3.75 \times 10^4\,K$

(see also Table 4.11)

(c) $f(E) = \frac{1}{e^{\frac{E-E_F}{KT}} + 1}$; $\frac{(E-E_F)eV}{\cancel{KT}} * \frac{1.6022 \times 10^{-19}}{1.38 \times 10^{-23} \times 300} = 38.7(E-E_F)$

where E_F, E in eV.

$= \frac{1}{e^{38.7(E-E_F)} + 1}$

Table

E/E_F	0	0.4	0.8	1	1.4	1.8
$f(E)$	1	0.874	0.66	0.5	0.22	0.07

Example: $\frac{E}{E_F} = 0.4 \Rightarrow E = 0.4 \times 3.23\,eV$

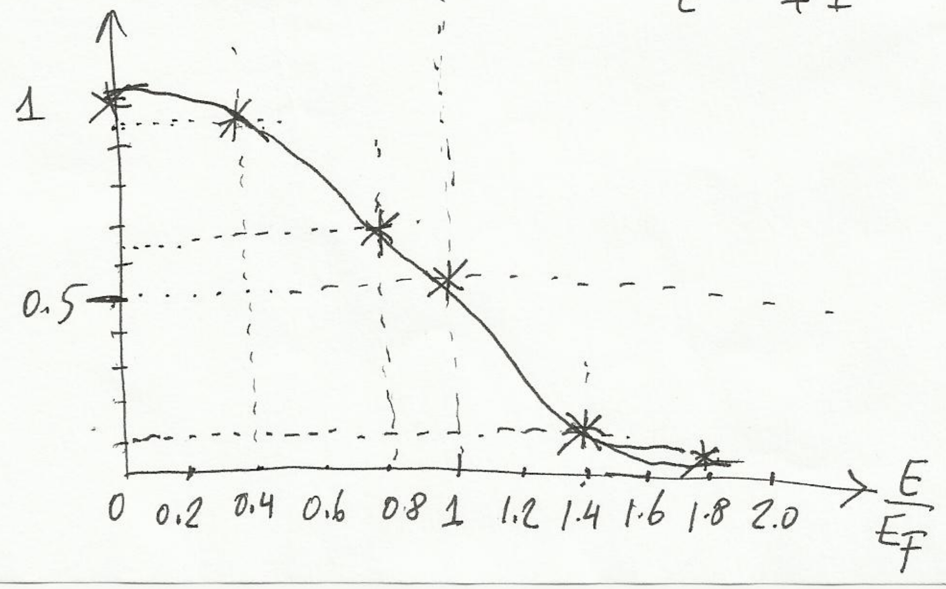
$= \cancel{12}\ 1.292\,eV$

$\therefore E - E_F = (1.292 - 3.23)$

$= -1.938\,eV$

$\therefore \cancel{f(0.4}\ f(1.292) = \frac{1}{e^{-1.938} + 1} = 0.874$

Sketch



(d) $f(E) = \dfrac{1}{e^{38.7(E-E_F)}+1}$ ← eV

$$= \frac{1}{e^{38.7(E-3.23)}+1}$$

$$\Rightarrow \quad e^{38.7(E-3.23)} = f^{-1}(E) - 1$$

$$\Rightarrow \quad 38.7(E-3.23) = \ln\left[f^{-1}(E)-1\right]$$

$$\therefore \quad E = \frac{\ln\left[f^{-1}(E)-1\right]}{38.7} + 3.23$$

$f^{-1}(E)$	0.5	0.8	0.98
E	3.23eV	3.19eV	3.13eV

no need to calculate

Example! $f(E) = 0.8 \Rightarrow E = \dfrac{\ln\left[\dfrac{1}{0.8}-1\right]}{38.7} + 3.23$

$$= \frac{\ln(0.25)}{38.7} + 3.23$$

$$= 3.19\,\text{eV}$$