

Solutions to Problems in Solid State Physics II

Problem 2005-I

ε_h is the maximum energy of band 1 (follows from the specification of the Fermi surface). The number of electronic states in one band, within the 1. Brillouin zone, is twice the number of \vec{k} states, i.e. twice the number of unit cells in the system. If $\varepsilon_h < \varepsilon_c$ all states in band 1, and no states in band 2, would be occupied by electrons at zero temperature, implying that

- 1) the system would be an insulator (or semiconductor).

The reciprocal lattice of an fcc is a bcc lattice. In the bcc reciprocal lattice there are 8 equivalent (111) reciprocal lattice points lying at the corners of the 1. Brillouin zone, each counting one eighth. This implies that there is, effectively, one hole and one electron Fermi surface in one Brillouin zone. With the use of the notation introduced on the figure, we have:

$$\varepsilon_F = \varepsilon_e + \frac{(\hbar k_e)^2}{2m_e} = \varepsilon_h - \Delta + \frac{(\hbar k_e)^2}{2m_e}, \quad \varepsilon_F = \varepsilon_h - \frac{(\hbar k_h)^2}{2m_h}. \quad (1)$$

The number of holes (i.e. the number of missing electrons) in band 1 is equal to the number of electrons occupying band 2, i.e.

$$n = p. \quad (2)$$

and since both bands are parabolic, we may use Marder eq. (6.29) to obtain the lengths of the two Fermi wave vectors:

$$k_e = (3\pi^2 n)^{1/3}, \quad \text{and equivalently} \quad k_h = (3\pi^2 p)^{1/3}. \quad (3)$$

These equations are straightforwardly solved, and we get

$$2) \quad \varepsilon_F = \varepsilon_h - \frac{m_e}{m_e + m_h} \Delta.$$

$$3) \quad n = p = \frac{1}{3\pi^2} \left(\frac{2\Delta}{\hbar^2} \frac{m_e m_h}{m_e + m_h} \right)^{3/2}.$$

According to Marder eqs. (6.77) and (6.23), the specific heat is

$$c_V = \frac{\pi^2}{3} k_B^2 T D(\varepsilon_F), \quad D(\varepsilon_F) = \frac{m}{\hbar^3 \pi^2} \sqrt{2m\varepsilon_F} = \frac{m k_F}{\hbar^2 \pi^2}, \quad (4)$$

in the case of a parabolic band, when $T \ll \varepsilon_F/k_B$. In the present case, we need to require $T \ll \Delta/k_B$, and adding the electron- and hole-like contributions,

$$D(\varepsilon_F) = \frac{m_e k_e}{\hbar^2 \pi^2} + \frac{m_h k_h}{\hbar^2 \pi^2} = \frac{m_e + m_h}{\hbar^2 \pi^2} \left(\frac{2\Delta}{\hbar^2} \frac{m_e m_h}{m_e + m_h} \right)^{1/2} \quad (5)$$

the result is

$$4) \quad \gamma = c_V/T = \frac{k_B^2}{3\hbar^3} \sqrt{2m_e m_h (m_e + m_h)} \Delta.$$

The conductivity tensor for each of the two kinds of band electrons is isotropic and according to Marder eqs. (17.55) and (17.57):

$$\sigma_e = \frac{ne^2\tau}{m_e}, \quad \sigma_h = \frac{pe^2\tau}{m_h}. \quad (6)$$

The electrons in each band add independently of each other to the linear response of the system, and the total conductivity is found to be

$$5) \quad \sigma = \sigma_e + \sigma_h = ne^2\tau \frac{m_e + m_h}{m_e m_h} = \frac{e^2\tau}{3\pi^2\hbar^3} \left(8\Delta^3 \frac{m_e m_h}{m_e + m_h} \right)^{1/2}.$$

The individual Hall coefficients for the two bands are, (17.97):

$$\mathcal{R}_e = -\frac{1}{nec}, \quad \mathcal{R}_h = \frac{1}{pec} = -\mathcal{R}_e \quad (7)$$

In the limit of $|\mathcal{R}B\sigma_0| \gg 1$, we get

$$\begin{aligned} \overline{\overline{\sigma}} &= \frac{\sigma_e}{1 + (\mathcal{R}_e B \sigma_e)^2} \begin{pmatrix} 1 & \mathcal{R}_e B \sigma_e \\ -\mathcal{R}_e B \sigma_e & 1 \end{pmatrix} + \frac{\sigma_h}{1 + (\mathcal{R}_h B \sigma_h)^2} \begin{pmatrix} 1 & \mathcal{R}_h B \sigma_h \\ -\mathcal{R}_h B \sigma_h & 1 \end{pmatrix} \\ &\simeq \begin{pmatrix} 0 & (\mathcal{R}_e B)^{-1} \\ -(\mathcal{R}_e B)^{-1} & 0 \end{pmatrix} + \begin{pmatrix} 0 & (\mathcal{R}_h B)^{-1} \\ -(\mathcal{R}_h B)^{-1} & 0 \end{pmatrix} \end{aligned} \quad (8)$$

Since in this limit $\overline{\overline{\sigma}} \simeq \begin{pmatrix} 0 & (\mathcal{R}B)^{-1} \\ -(\mathcal{R}B)^{-1} & 0 \end{pmatrix}$, the total Hall coefficient \mathcal{R} is

$$6) \quad \mathcal{R} = \left(\frac{1}{\mathcal{R}_e} + \frac{1}{\mathcal{R}_h} \right)^{-1} = -\frac{1}{(n-p)ec} \rightarrow \pm\infty.$$

The two Hall-current components “compensate” each other, so that the total current vanishes in this two-band system.

In the case of $\Delta = 0.1$ meV and $m_e = m_h = 9.109389 \times 10^{-31}$ kg, the electron density is

$$\begin{aligned} n &= \frac{1}{3\pi^2} \left(\frac{2\Delta}{\hbar^2} \frac{m_e m_h}{m_e + m_h} \right)^{3/2} \\ &= \frac{1}{3\pi^2} \left(\frac{2 \times 0.1 \times 1.602177 \cdot 10^{-19} \times 0.5 \times 9.109389 \cdot 10^{-31}}{(1.054572 \cdot 10^{-34})^2} \right)^{3/2} \text{ m}^{-3} \end{aligned}$$

or

$$7) \quad n = 5.078 \times 10^{19} \text{ cm}^{-3}.$$

A small density when compared with the usual electron density in metals, which is of the order of 10^{22} cm^{-3} .

Problem 2005-II

- 1) The Fermi surface determined by $\varepsilon(\vec{k}) = \varepsilon_F$ is ellipsoidal

$$\frac{k_x^2}{a^2} + \frac{k_y^2}{a^2} + \frac{k_z^2}{c^2} = 1$$

with the semi-axes $a = \sqrt{2m_1\varepsilon_F/\hbar}$ and $c = \sqrt{2m_2\varepsilon_F/\hbar}$.

- 2) According to, for instance, eq. (17.48) in Marder:

$$\overline{\overline{\sigma}} = e^2\tau n\overline{\overline{M}}^{-1} = \begin{pmatrix} \frac{ne^2\tau}{m_1} & 0 & 0 \\ 0 & \frac{ne^2\tau}{m_1} & 0 \\ 0 & 0 & \frac{ne^2\tau}{m_2} \end{pmatrix}$$

- 3) The application of the transformation defined by eq. (2) in the problem text implies

$$\varepsilon(\vec{k}') = \frac{(\hbar k')^2}{2m_1}$$

and referring to (6.24) we get

$$\begin{aligned} D(\varepsilon) &= \frac{2}{(2\pi)^3} \int d\vec{k} \delta(\varepsilon - \varepsilon(\vec{k})) = \frac{2}{(2\pi)^3} \sqrt{\frac{m_2}{m_1}} \int d\vec{k}' \delta(\varepsilon - \varepsilon(\vec{k}')) \\ &= \sqrt{\frac{m_2}{m_1}} \frac{m_1}{\hbar^3\pi^2} \sqrt{2m_1\varepsilon} = \frac{1}{\hbar^3\pi^2} \sqrt{2m_1^2m_2\varepsilon} \end{aligned}$$

- 4) By definition

$$\vec{v}' = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}'} = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} \frac{\partial \vec{k}}{\partial \vec{k}'} = \left(v_x, v_y, \sqrt{\frac{m_2}{m_1}} v_z \right) = \overline{\overline{T}}^{-1} \vec{v}$$

Writing the original semiclassical equation of motion, (16.12)

$$\hbar(\dot{k}_x, \dot{k}_y, \dot{k}_z) = -e(E_x, E_y, E_z) - \frac{e}{c} (v_y B_z - v_z B_y, v_z B_x - v_x B_z, v_x B_y - v_y B_x)$$

then we get

$$\begin{aligned} \hbar \dot{\vec{k}}' &= \hbar \left(\dot{k}_x, \dot{k}_y, \sqrt{\frac{m_1}{m_2}} \dot{k}_z \right) = -e \left(E_x, E_y, \sqrt{\frac{m_1}{m_2}} E_z \right) \\ &\quad - \frac{e}{c} \left(v'_y B_z - \sqrt{\frac{m_1}{m_2}} v'_z B_y, \sqrt{\frac{m_1}{m_2}} v'_z B_x - v'_x B_z, \sqrt{\frac{m_1}{m_2}} \{v'_x B_y - v'_y B_x\} \right) \end{aligned}$$

which compares with eq. (3) in the problem text, when:

$$\vec{E}' = \left(E_x, E_y, \sqrt{\frac{m_1}{m_2}} E_z \right) = \overline{\overline{T}} \vec{E}$$

and

$$\vec{B}' = \left(\sqrt{\frac{m_1}{m_2}} B_x, \sqrt{\frac{m_1}{m_2}} B_y, B_z \right) = |\bar{T}| \bar{T}^{-1} \vec{B}, \quad |\bar{T}| = \sqrt{\frac{m_1}{m_2}}$$

5) Since

$$\vec{j}' = -ne \langle \vec{v}' \rangle = -ne \langle \bar{T}^{-1} \vec{v} \rangle = \bar{T}^{-1} \vec{j}$$

then

$$\vec{j}' = \bar{\sigma}' \vec{E}' \quad \Rightarrow \quad \bar{T}^{-1} \vec{j} = \bar{\sigma}' \bar{T} \vec{E}$$

or

$$\bar{\sigma} = \bar{T} \bar{\sigma}' \bar{T}$$

6) The resistivity tensor, eq. (4) in the problem text, is valid for the isotropic system, which means that

$$\bar{\rho}' = \begin{pmatrix} \sigma_1^{-1} & 0 & 0 \\ 0 & \sigma_1^{-1} & -\mathcal{R}B' \\ 0 & \mathcal{R}B' & \sigma_1^{-1} \end{pmatrix}, \quad \sigma_1 = \frac{ne^2\tau}{m_1}, \quad \mathcal{R} = -\frac{1}{nec}$$

For the x component $B' = \sqrt{\frac{m_1}{m_2}} B$, hence the result is

$$\bar{\rho} = \bar{\sigma}^{-1} = \bar{T}^{-1} \bar{\rho}' \bar{T}^{-1} = \begin{pmatrix} \sigma_1^{-1} & 0 & 0 \\ 0 & \sigma_1^{-1} & -\mathcal{R}B \\ 0 & \mathcal{R}B & \frac{m_2}{m_1} \sigma_1^{-1} \end{pmatrix}$$

At zero field, this result agrees with the previous one derived under point 2). The non-diagonal contribution, appearing when a magnetic field is applied along the x axis, is the same as in the isotropic case, hence the Hall coefficient is unchanged, $\mathcal{R} = -\frac{1}{nec}$. We may generalize the result and conclude that the Hall coefficient, within the present approximations, is independent of the mass tensor, if the magnetic field is applied along one of the principal axes of the mass tensor.

Problem 2005-III

- 1) Assuming $\vec{v}_e = v_e e^{-i\omega t}(\hat{x} + i\hat{y})$ then $\vec{E} = (E/v_e)\vec{v}_e$ and $\dot{\vec{v}}_e = -i\omega\vec{v}_e$. Using the relation

$$(\hat{x} + i\hat{y}) \times \hat{z} = i\hat{x} - \hat{y} = i(\hat{x} + i\hat{y}) \quad \Rightarrow \quad \vec{v}_e \times \vec{B} = iB\vec{v}_e$$

the equation-of-motion reads

$$-i\omega m_e \vec{v}_e = -e \left(\frac{E}{v_e} + \frac{iB}{c} \right) \vec{v}_e - \frac{m_e}{\tau} \vec{v}_e,$$

which is fulfilled identically, if

$$-i\omega m_e = -e \left(\frac{E}{v_e} + \frac{iB}{c} \right) - \frac{m_e}{\tau},$$

or if

$$v_e = -i \frac{eE}{m_e \left(\omega - \omega_e + \frac{i}{\tau} \right)}, \quad \omega_e = \frac{eB}{m_e c}.$$

- 2) The equation-of-motion for the holes is the same as (1) after $-e$ has been replaced by e , and m_e and \vec{v}_e by, respectively, m_h and \vec{v}_h . The corresponding solution for the holes is then:

$$v_h = i \frac{eE}{m_h \left(\omega + \omega_h + \frac{i}{\tau} \right)}, \quad \omega_h = \frac{eB}{m_h c}.$$

The conductivity is introduced via the equation

$$\vec{j} = -ne\vec{v}_e + pe\vec{v}_h = -ne(\vec{v}_e - \vec{v}_h) = \sigma \vec{E}$$

and we get

$$\begin{aligned} \vec{j} &= -ne \left(-i \frac{eE}{m_e \left(\omega - \omega_e + \frac{i}{\tau} \right)} - i \frac{eE}{m_h \left(\omega + \omega_h + \frac{i}{\tau} \right)} \right) (\hat{x} + i\hat{y}) e^{-i\omega t} \\ &= ine^2 \left(\frac{1}{m_e \left(\omega - \omega_e + \frac{i}{\tau} \right)} + \frac{1}{m_h \left(\omega + \omega_h + \frac{i}{\tau} \right)} \right) \vec{E} = \sigma(\omega) \vec{E} \end{aligned}$$

or

$$\sigma(\omega) = i \frac{e^2 n (m_e + m_h) \left(\omega + \frac{i}{\tau} \right)}{m_e m_h \left(\omega - \omega_e + \frac{i}{\tau} \right) \left(\omega + \omega_h + \frac{i}{\tau} \right)}$$

(as $m_e \omega_e = m_h \omega_h$).

- 3) In the case of $\omega = 0$ and $B = 0$, or $\omega_e = \omega_h = 0$, the result is

$$\sigma(0) = ne^2 \tau \frac{m_e + m_h}{m_e m_h} = \frac{ne^2 \tau}{m_e} + \frac{ne^2 \tau}{m_h},$$

which is just the obvious generalization of the simple Drude formula to the case where both the electrons and holes contribute to the current.

- 4) In the limit $(\omega_e, \omega_h) \gg \omega \gg 1/\tau$ we may neglect i/τ in the numerator and $\omega + i/\tau$ in the denominator of $\sigma(\omega)$, and the result is

$$\sigma(\omega) = -i \frac{e^2 n (m_e + m_h) \omega}{m_e m_h \omega_e \omega_h} = -i n (m_e + m_h) \left(\frac{c}{B} \right)^2 \omega$$

to leading order in ω .

- 5) According to eq. (20.14) in Marder, the relationship between the conductivity and the dielectric constant is

$$\epsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma(\omega)$$

and hence in the present system

$$\epsilon(\omega) = 1 + 4\pi n (m_e + m_h) \left(\frac{c}{B} \right)^2 \simeq 4\pi n (m_e + m_h) \left(\frac{c}{B} \right)^2,$$

when assuming $\epsilon(\omega) \gg 1$. Introducing this into the equation determining the dispersion relation of the transversely polarized light waves, $\omega^2 \epsilon(\omega) = c^2 q^2$ (20.17 in Marder), the dispersion relation becomes:

$$\omega = \omega(q) = \frac{B}{\sqrt{4\pi n (m_e + m_h)}} q,$$

i.e. because $\epsilon(\omega)$ is independent of ω , to leading order, these Alfvén waves propagate with a constant velocity ω/q (without dispersion).

- 6) When using cgs units (as assumed here), $B = 10 \text{ kG} = 10^4 \text{ G}$ corresponds to $H = 10^4 \text{ Oe}$, and since $B = H$ then $B^2 = BH = 10^8 \text{ G} \times \text{Oe}$, which unit is equivalent to erg/cm^3 , hence

$$\begin{aligned} v = \frac{\omega(q)}{q} &= \frac{B}{\sqrt{4\pi n (m_e + m_h)}} = \left(\frac{10^8}{4\pi \times 10^{19} \times 2 \times 9 \times 10^{-28}} \right)^{1/2} \text{ cm/s} \\ &= 2.1 \times 10^7 \text{ cm/s}. \end{aligned}$$

nearly 1500 times smaller than the velocity of light in vacuum.

Problem 2006: The Ising model in a transverse field

1) From Heisenberg's equation-of-motion we get,

$$\begin{aligned}\frac{d\sigma^z}{dt} &= \frac{i}{\hbar}[\mathcal{H}_1, \sigma^z] = -\frac{i}{\hbar}\Gamma[\sigma^x, \sigma^z] = -\frac{2}{\hbar}\Gamma\sigma^y \quad \Rightarrow \\ \frac{d^2\sigma^z}{dt^2} &= -\frac{2i\Gamma}{\hbar^2}[\mathcal{H}_1, \sigma^y] = -\frac{2i\Gamma}{\hbar^2}[-\Gamma(2i\sigma^z) - \mu_B H(-2i\sigma^x)]\end{aligned}\quad (1)$$

or

$$\frac{d^2\sigma^z}{dt^2} = -\frac{4\Gamma^2}{\hbar^2}\sigma^z + \frac{4\Gamma\mu_B H}{\hbar^2}\sigma^x \quad (2)$$

2) Introducing the $|\pm\rangle$ states by $\sigma^z|\pm\rangle = \pm|\pm\rangle$, the eigenstates at zero field are $|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ and $|1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$, where $\mathcal{H}_1|0\rangle = -\Gamma|0\rangle$ and $\mathcal{H}_1|1\rangle = \Gamma|1\rangle$. Using these eigenstates, the thermal expectation values are $\langle\sigma^z\rangle = 0$ and $\langle\sigma^x\rangle = \tanh(\beta\Gamma)$. Introducing $H = H_0 e^{-i\omega t}$ we may solve the thermal average of (2) by assuming $\langle\sigma^z(t)\rangle = \sigma_0^z e^{-i\omega t}$

$$\frac{d^2\langle\sigma^z(t)\rangle}{dt^2} = (-i\omega)^2\langle\sigma^z(t)\rangle = -\frac{4\Gamma^2}{\hbar^2}\langle\sigma^z(t)\rangle + \frac{4\Gamma\mu_B H}{\hbar^2}\tanh(\beta\Gamma) \quad (3)$$

to linear order in the field, in which case any time dependence of σ^x may be neglected and the time derivation and thermal averaging may be interchanged. When isolating $n\mu_B\langle\sigma^z(t)\rangle$ and dividing it by H we get

$$\chi_0(\omega) = n\mu_B^2 \frac{4\Gamma \tanh(\beta\Gamma)}{4\Gamma^2 - (\hbar\omega)^2} \quad (4)$$

3) In the mean-field approximation $\sigma_i^z\sigma_j^z \simeq \sigma_i^z\langle\sigma_j^z\rangle + \sigma_j^z\langle\sigma_i^z\rangle - \langle\sigma_i^z\rangle\langle\sigma_j^z\rangle$ and

$$\mathcal{H} = \sum_i \mathcal{H}_{\text{MF}}(i) = \sum_i \left[-\Gamma\sigma_i^x - \mu_B H\sigma_i^z - zJ\langle\sigma^z\rangle\sigma_i^z + \frac{1}{2}zJ\langle\sigma^z\rangle^2 \right] \quad (5)$$

If $\langle\sigma^z\rangle = 0$ at zero field, then in the presence of the uniform (time-dependent) field $\langle\sigma_i^z(t)\rangle$ is the same for all sites, and $n\mu_B\langle\sigma^z(t)\rangle = \chi_0(\omega)H_{\text{eff}}(t)$ with $\mu_B H_{\text{eff}}(t) = \mu_B H(t) + zJ\langle\sigma^z(t)\rangle$. Per definition, $n\mu_B\langle\sigma^z(t)\rangle = \chi(\omega)H(t)$ and the combination of these equations leads to

$$n\mu_B\langle\sigma^z(t)\rangle = \chi(\omega)H(t) = \chi_0(\omega) \left(H(t) + zJ \frac{\chi(\omega)H(t)}{n\mu_B^2} \right)$$

or

$$\chi(\omega) = \frac{\chi_0(\omega)}{1 - \chi_0(\omega) \frac{zJ}{n\mu_B^2}} \quad (6)$$

4) The condition for the occurrence of a transition between the paramagnetic and a ferromagnetic phase, where $\langle\sigma^z\rangle \neq 0$, is that $\chi(0) \rightarrow \infty$, or

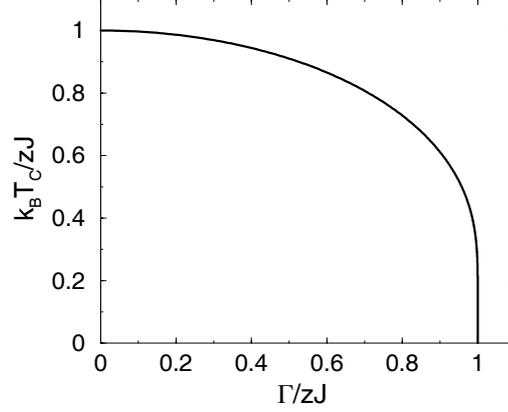
$$\chi_0(0) \frac{zJ}{n\mu_B^2} \rightarrow 1 \quad \Rightarrow \quad \frac{zJ}{\Gamma} \tanh\left(\frac{\Gamma}{k_B T_C}\right) = 1 \quad (7)$$

$|\tanh x| \leq 1$ and the critical condition that this equation has a solution is

$$\Gamma \leq zJ \quad \text{or} \quad T_C \rightarrow 0 \text{ when } \Gamma \rightarrow zJ \quad (8)$$

In the other limit, $T_C \rightarrow zJ/k_B$ when $\Gamma \rightarrow 0$ (the simple Ising model).

The following figure shows $k_B T_C/zJ$ as a function of Γ/zJ :



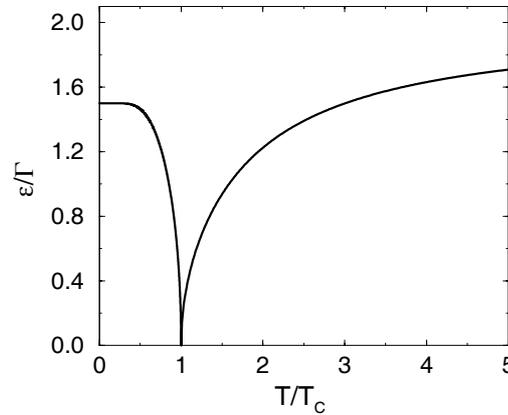
5) From eq. (6) we get,

$$\chi(\omega) = \frac{n\mu_B^2 4\Gamma \tanh(\beta\Gamma)}{4\Gamma^2 - 4zJ\Gamma \tanh(\beta\Gamma) - (\hbar\omega)^2} \quad (9)$$

or that the excitation energies are

$$\hbar\omega = \pm\varepsilon(T) = \pm 2\Gamma \sqrt{1 - (zJ/\Gamma) \tanh(\beta\Gamma)}, \quad T \geq T_C \quad (10)$$

The square root is well-defined as long as $T > T_C$ and vanishes at $T = T_C$. In the high-temperature limit, $\hbar\omega \rightarrow \pm 2\Gamma$, which are the energies of the non-interacting system. In the ordered phase, one has to account for that $\langle \sigma^z \rangle$ is non-zero, implying that the eigenstates $|0\rangle$ and $|1\rangle$ become mixed, and the energy separation of the two levels becomes larger than 2Γ . As a consequence, the excitation energies become non-zero below T_C . The figure below shows ε/Γ as a function of T/T_C , both above and below T_C , in the particular case of $\Gamma/zJ = 0.8$, in which case $k_B T_C/\Gamma = 0.91024$:



Problem 2007: Surface plasmons

1) The relation between $\sigma(\omega)$ and $\epsilon(\omega)$ is, Marder's Eq. (20.14),

$$\epsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma(\omega) = 1 + \frac{4\pi i}{\omega} \frac{ne^2\tau}{m} \frac{1}{1-i\omega\tau} = 1 + \frac{\omega_p^2}{\omega} \frac{i\tau}{1-i\omega\tau} \quad (a1)$$

where we have used that, according to Marder's Eq. (23.7), $\omega_p^2 = \frac{4\pi ne^2}{m}$. In the limit of $\omega\tau \gg 1$, $\epsilon(\omega)$ becomes real and is determined by

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \quad \omega\tau \gg 1 \quad (a2)$$

2) The boundary condition $\vec{E}_1 \times \hat{x} = \vec{E}_2 \times \hat{x}$ is fulfilled at $x = 0$, since the y components are zero and the z components are equal, $E_{1z}(0, y, z) = E_{2z}(0, y, z)$. In the case of the x components at $x = 0$, then $E_{1x} = \epsilon E_{2x}$ or $D_{1x} = E_{1x} = \epsilon E_{2x} = D_{2x}$, showing that the normal component of \vec{D} is continuous at the interface. When $x \neq 0$ we have

$$\nabla \cdot \vec{E} = \begin{cases} A \left(\lambda + 0 + \frac{i\lambda}{k}(ik) \right) e^{\lambda x} e^{i(kz-\omega t)} = 0 & , \quad x < 0 \\ A \left(\frac{\epsilon\lambda}{\epsilon} + 0 + \frac{i\lambda}{k}(ik) \right) e^{\epsilon\lambda x} e^{i(kz-\omega t)} = 0 & , \quad x > 0 \end{cases} \quad (a3)$$

as required. The solution (2) only describes a surface wave, if $|\vec{E}|$ decreases exponentially for increasing values of $|x|$ (the opposite would be an improper solution in any case). For $x < 0$ this is only the situation if $\lambda > 0$, and for $x > 0$ the requirement is that $\epsilon\lambda$ has to be negative. Hence the necessary conditions are $\lambda > 0$ and $\epsilon < 0$.

3) The vector identity $\nabla \times \nabla \times \vec{E} = \nabla(\nabla \cdot \vec{E}) - \nabla^2 \vec{E}$ implies $\nabla \times \nabla \times \vec{E} = -\nabla^2 \vec{E}$, because $\nabla \cdot \vec{E} = 0$ when $x \neq 0$. Inserting (2) in (3), we get

$$\begin{cases} \{\lambda^2 + (ik)^2\} \vec{E}_1 = \frac{(-i\omega)^2}{c^2} \vec{E}_1 & , \quad x < 0 \\ \{(\epsilon\lambda)^2 + (ik)^2\} \vec{E}_2 = \frac{(-i\omega)^2}{c^2} \epsilon \vec{E}_2 & , \quad x > 0 \end{cases} \quad (a4)$$

and the solution of these equations, with respect to λ and k , is

$$\lambda = \left(\frac{-1}{1+\epsilon} \right)^{\frac{1}{2}} \frac{\omega}{c}, \quad k = \left(\frac{\epsilon}{1+\epsilon} \right)^{\frac{1}{2}} \frac{\omega}{c} \quad (a5)$$

which solution is well-defined only if $\epsilon < -1$.

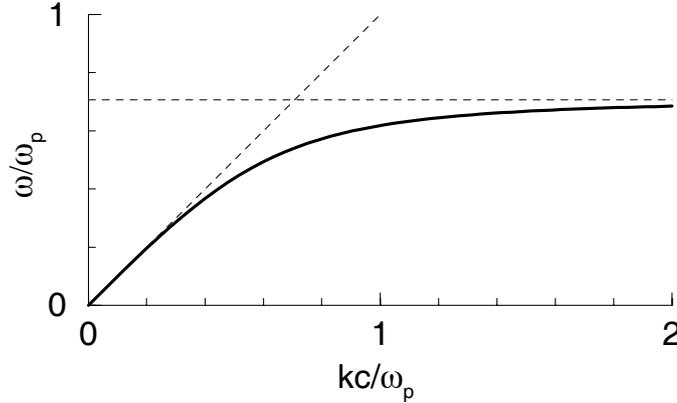
4) Introducing (a2) then the relation between k and ω in (a5) may be written

$$(kc)^2 = \frac{\epsilon}{1+\epsilon} \omega^2 = \frac{\omega^2 - \omega_p^2}{2\omega^2 - \omega_p^2} \omega^2, \quad \omega^2 < \frac{1}{2}\omega_p^2 \quad (a6)$$

In the two limits we get $(kc)^2 \simeq \omega^2$ when $\omega \ll \omega_p$, and $kc \rightarrow \infty$ when $\omega^2 \rightarrow \omega_p^2/2$, or

$$\omega \simeq kc \quad \text{if} \quad kc \ll \omega_p, \quad \omega \simeq \frac{\omega_p}{\sqrt{2}} \quad \text{if} \quad kc \gg \omega_p \quad (a7)$$

The behaviour in the two limits plus a single point, as for instance $kc = 0.907\omega_p$ for $\omega = 0.6\omega_p$, determine the dispersion relation $\omega = \omega(k)$ sketched in the figure:



5) In the limit of $kc \gg \omega_p$ then $\epsilon \simeq -1$, in which case (a5) shows that $\underline{\lambda} = k$. Introducing this condition in the expressions for the electric field vectors, we get: $\vec{E}_1 = A(1, 0, i)e^{-k|x|}e^{i(kz-\omega t)}$ and $\vec{E}_2 = A(-1, 0, i)e^{-k|x|}e^{i(kz-\omega t)}$. Hence, the surface is a mirror plane for the electrical field, $\vec{E}_1 \leftrightarrow \vec{E}_2$ when $x \rightarrow -x$. Both fields are circular polarized, where \vec{E}_1 and \vec{E}_2 are respectively left-handed and right-handed polarized. The total (average) field at $x = 0$ is longitudinal polarized.

Using Marder's Eq. (23.3), the plasma frequency of potassium is found to be $\omega_p = \underline{6.50 \cdot 10^{15} \text{ s}^{-1}}$. The corresponding value of $k = k_p = \omega_p/c = [6.50 \cdot 10^{15}/3 \cdot 10^{18}] \text{ \AA}^{-1} = \underline{2.17 \cdot 10^{-3} \text{ \AA}^{-1}}$. The Fermi wave number is $k_F = (3\pi^2 n)^{1/3} = 0.733 \text{ \AA}^{-1}$, and the ratio $k_p/k_F = \underline{2.96 \cdot 10^{-3}} \ll 1$.

[It is not possible to excite surface plasmons by shining light on the sample. The component of the wave vector along the surface of an incoming light wave is always smaller or equal the length of the total wave vector. Hence the resonance line of the incoming light always have a slope (phase velocity) which is larger than, or equal, the long wavelength behaviour of the surface plasmons, i.e. $\omega_{\text{incoming}} > \omega$ for a certain k component in the $x = 0$ plane. The opposite is neither possible, i.e. the surface plasmons do not emit light waves.]

Problem 2008: Thermodynamics of a superconductor

1) The free energy expression (2) predicts the magnetization along the direction of the applied field to be

$$M = -\frac{1}{V} \frac{\partial G_s}{\partial H_0} = -\frac{1}{4\pi} H_0 \quad \Rightarrow \quad B = H_0 + 4\pi M = 0 \quad (a1)$$

When the sample is a thin needle along the direction of the field, the internal H -field is equal the applied one, and, as should be the case, $B = 0$ in the interior of the superconductor. The field-independent term implies that $G_s \leq G_n$ as long as $|H_0| \leq H_c$, or that the superconducting phase is stable as long as the applied field is smaller than the critical one.

2) The equations (2) and (3) predicts the entropy to be

$$S_s = -\frac{\partial G_s}{\partial T} = V \frac{H_c}{4\pi} \frac{\partial H_c}{\partial T} + S_n = -\frac{V}{2\pi T_c} H_c^2(0) (1 - t^2) t + S_n \quad (a2)$$

S_s is smaller than S_n as long as the superconducting phase is stable. [The entropy changes discontinuously at the transition at $H_c(T)$ when $T < T_c$, i.e. the transition is of first-order with a latent heat of $Q = (S_n - S_s)T$. At zero field the entropy depends continuously on T , i.e. the transition is of second order at T_c .] The heat capacity is

$$C_s = T \frac{\partial S_s}{\partial T} = t \frac{\partial S_s}{\partial t} = \frac{V}{2\pi T_c} H_c^2(0) (3t^2 - 1) t + C_n \quad (a3)$$

This result applies as long as $t \leq 1$, when the applied field is zero.

3) Since the summation in equation (5) does not involve the spin degree of freedom, the \vec{k} -sum is replaced by an energy integral, where the density of states is the half of $D(\varepsilon)$ defined by Marder in equations (6.13)-(6.19) and

$$U = -\sum_{\vec{k}} \frac{(E_{\vec{k}} - |\xi_{\vec{k}}|)^2}{2E_{\vec{k}}} = -V \int_0^\infty \frac{D(\varepsilon)}{2} \frac{(\sqrt{(\varepsilon - \varepsilon_F)^2 + \Delta^2} - |\varepsilon - \varepsilon_F|)^2}{2\sqrt{(\varepsilon - \varepsilon_F)^2 + \Delta^2}} d\varepsilon$$

$\Delta \ll \varepsilon_F$ implies that $D(\varepsilon)$ may be replaced by the constant $D(\varepsilon_F)$, and the introduction of $x = (\varepsilon - \varepsilon_F)/\Delta$ then leads to

$$U = -\frac{1}{4} V D(\varepsilon_F) \Delta^2 \int_{-\varepsilon_F/\Delta}^\infty \frac{(\sqrt{x^2 + 1} - |x|)^2}{\sqrt{x^2 + 1}} dx = -\frac{1}{4} V D(\varepsilon_F) \Delta^2 \quad (a4)$$

The lower limit of the integral may be replaced by $-\infty$, in which case the integral is twice the one given by equation (7).

4) The heat capacity makes a discontinuous jump at $T = T_c$, which according to equation (a3) is

$$C_s - C_n = \frac{V}{\pi T_c} H_c^2(0) \quad (a5)$$

and from equations (2) and (a4) we have

$$H_c^2(0) = -\frac{8\pi}{V}U = 2\pi D(\varepsilon_F)\Delta^2 = 2\pi D(\varepsilon_F)(\alpha k_B T_c)^2 \quad (a6)$$

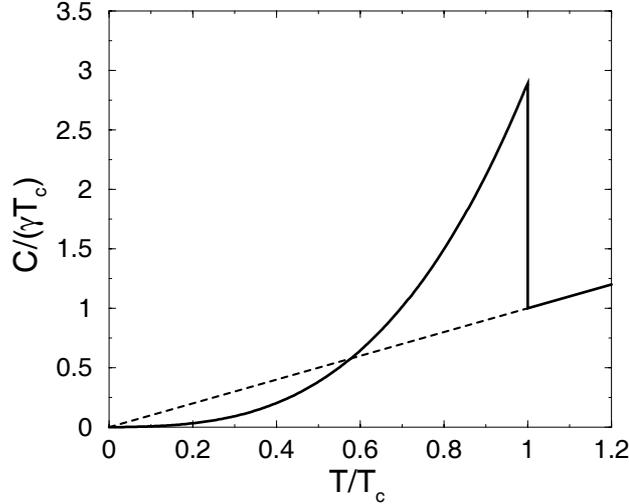
when using the BCS relation $\Delta = \alpha k_B T_c$. Neglecting the phonons, the specific heat of a normal metal is $C_n/V = \frac{\pi^2}{3}D(\varepsilon_F)k_B^2 T$ according to Marder's equation (6.77). From these relations we find at $T = T_c$

$$\frac{C_s - C_n}{C_n} = \frac{V}{\pi T_c} 2\pi D(\varepsilon_F)(\alpha k_B T_c)^2 \left[V \frac{\pi^2}{3} D(\varepsilon_F) k_B^2 T_c \right]^{-1} = \frac{6\alpha^2}{\pi^2} \simeq 1.89 \quad (a7)$$

5) The heat capacity of the normal phase is $C_n = \gamma T$ or $C_n/(\gamma T_c) = t$ when $T > T_c$. It is then straightforwardly found that the relative heat capacity is

$$\frac{C}{\gamma T_c} = t \left[1 + \frac{1.89}{2} (3t^2 - 1) \right] \quad (a8)$$

when $T \leq T_c$, as displayed below.



[In the limit of $t \rightarrow 1$, the BCS theory predicts $H_c(T) = AH_c(0)(1-t)$, where $A \simeq 1.737$. Using this result instead of equation (3), the ratio above is being multiplied by $(A/2)^2$ and becomes equal to $12/[7\zeta(3)] \simeq 1.43$ instead of 1.89. In the other limit $t \rightarrow 0$ the BCS theory predicts the heat capacity to vanish $\propto \exp(-\Delta/k_B T)$ not linearly as found here.]

Using equation (6.31) in Marder and $n = 0.1806 \text{ \AA}^{-3}$ the free-electron like Fermi energy is found to be $\underline{\varepsilon_F = 11.65 \text{ eV}}$. The corresponding density-of-states at the Fermi surface is, (6.33), $D(\varepsilon_F) = 0.02323 \text{ eV}^{-1} \text{ \AA}^{-3}$. The BCS energy gap is $\Delta = \alpha k_B T_c = 1.764 \times 8.617385 \cdot 10^{-5} \times 1.18 \text{ eV}$, or $\underline{\Delta = 0.179 \text{ meV}} \simeq 1.5 \cdot 10^{-5} \varepsilon_F$. Finally, $H_c^2(0) = 2\pi D(\varepsilon_F)\Delta^2 = 2\pi \times 0.02323 (1.79 \cdot 10^{-4})^2 \text{ eV \AA}^{-3} = 0.4677 \cdot 10^{-8} \times 1.60218 \cdot 10^{-12} \cdot 10^{24} \text{ erg cm}^{-3}$ implying $\underline{H_c(0) = 86.6 \text{ Oe}}$. Experimentally, $\gamma = 1.48 \gamma(\text{free}) \Rightarrow H_c(0) = \sqrt{1.48} \cdot 86.6 \text{ Oe} = 105 \text{ Oe}$, which value is in agreement with experiments.

Problem 2009: Transport due to electrons belonging to a single band

1) It is straightforwardly found that

$$\begin{aligned}\varepsilon(\vec{k}) &= \varepsilon_{\min} = 0 & \text{at} & \quad \vec{k} = (0, 0, 0) \\ \varepsilon(\vec{k}) &= \varepsilon_{\max} = 6E_0 & \text{at} & \quad \vec{k} = \frac{\pi}{a}(1, 1, 1)\end{aligned}\quad (a1)$$

The first Brillouin zone is determined by:

$$-\frac{\pi}{a} < k_x < \frac{\pi}{a}, \quad -\frac{\pi}{a} < k_y < \frac{\pi}{a}, \quad -\frac{\pi}{a} < k_z < \frac{\pi}{a} \quad (a2)$$

At the boundaries one or more components of \vec{k} are equal $\pm\pi/a$, and the smallest value of $\varepsilon(\vec{k}) = \varepsilon_F$, where this may occur, is

$$\varepsilon_F(\text{threshold}) = 2E_0 \quad (a3)$$

According to the 1. semiclassical rule the band index i is a constant of motion (page 415 in Marder) allowing the contributions from the different bands to be considered separately. The total current density $\vec{j} = \sigma_{\text{tot}}\vec{E}$ (using that $\vec{\sigma}_{\text{tot}}$ is a scalar in the cubic case) is the sum of the individual contributions from the different electrons and

$$\sigma_{\text{tot}} = \sum_i \sigma_i \quad (a4)$$

2) The inverse mass tensor is defined by Marder in eq. (16.28). In the present case it is diagonal and ($\alpha = x, y, \text{ or } z$)

$$\frac{1}{M_{\alpha\alpha}} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(\vec{k})}{\partial k_\alpha^2} = \frac{E_0 a^2}{\hbar^2} \cos(ak_\alpha) = \frac{1}{m_0} \cos(ak_\alpha) \quad (a5)$$

when introducing m_0 as defined in the text. This result implies that

$$\text{Tr}(\mathbf{M})^{-1} = \frac{1}{m_0} \left[\cos(ak_x) + \cos(ak_y) + \cos(ak_z) \right] = \frac{1}{m_0} \left[3 - \frac{\varepsilon(\vec{k})}{E_0} \right] \quad (a6)$$

Introducing this result in Marder's eq. (17.50) we get

$$\frac{m_0}{m^*} = \frac{m_0}{3n} \int [d\vec{k}] f_{\vec{k}} \text{Tr}(\mathbf{M}^{-1}) = \frac{1}{3n} \int [d\vec{k}] f_{\vec{k}} \left[3 - \frac{\varepsilon(\vec{k})}{E_0} \right] = 1 - \frac{\langle \varepsilon \rangle}{3E_0} \quad (a7)$$

3) In the limit $\varepsilon(\vec{k}) \leq \varepsilon_F \ll E_0$ then $|ak_\alpha| \ll 1$ and $\cos(ak_\alpha) \simeq 1 - \frac{1}{2}(ak_\alpha)^2$ or

$$\varepsilon(\vec{k}) \simeq E_0 \left[\frac{a^2 k_x^2}{2} + \frac{a^2 k_y^2}{2} + \frac{a^2 k_z^2}{2} \right] = \frac{E_0 a^2 k^2}{2} = \frac{\hbar^2 k^2}{2m_0}, \quad k^2 = k_x^2 + k_y^2 + k_z^2 \quad (a9)$$

Hence, in this limit the band electrons behave as free electrons with mass $m_0 = \hbar^2/(E_0 a^2)$. For a three dimensional gas of free electrons, the Fermi wave number is $k_F = (3\pi^2 n)^{1/3}$, eq. (6.29) in Marder, and

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m_0} = \frac{1}{2} E_0 (3\pi^2 a^3 n)^{2/3} \quad (a10)$$

and, when $T \ll T_F$, (see also problem 6.3 in Marder)

$$\begin{aligned} \langle \varepsilon \rangle &= \frac{1}{n} \int [d\vec{k}] \theta(\varepsilon_F - \varepsilon(\vec{k})) \varepsilon(\vec{k}) = \frac{1}{n} \frac{2}{(2\pi)^3} \int_0^{k_F} dk 4\pi k^2 \frac{\hbar^2 k^2}{2m_0} \\ &= \frac{\hbar^2}{n\pi^2 2m_0} \frac{k_F^5}{5} = \frac{1}{5} \frac{k_F^3}{n\pi^2} \varepsilon_F = \frac{3}{5} \varepsilon_F = \frac{3}{10} E_0 (3\pi^2 a^3 n)^{2/3} \end{aligned} \quad (a11)$$

The contribution of this band to the conductivity is then

$$\sigma = \frac{ne^2\tau}{m^*} = \frac{e^2\tau}{\hbar^2} E_0 a^2 n \left[1 - \frac{1}{10} (3\pi^2 a^3 n)^{2/3} \right] \quad (a12)$$

4) Introducing the density of holes in the band $p = \int [d\vec{k}] (1 - f_{\vec{k}})$, then

$$n + p = \int [d\vec{k}] = \frac{2}{(2\pi)^3} \int_{-\pi/a}^{\pi/a} dk_x \int_{-\pi/a}^{\pi/a} dk_y \int_{-\pi/a}^{\pi/a} dk_z = \frac{2}{(2\pi)^3} \left(\frac{2\pi}{a} \right)^3 = \frac{2}{a^3} \quad (a13)$$

(as also obtained by elementary considerations). The case where $n = 2/a^3$ is then the one where the band is completely filled with electrons, $p = 0$ and $\varepsilon_F \geq 6E_0$. Since the conductivity of a completely filled band is zero, then

$$\langle \varepsilon \rangle = 3E_0, \quad \sigma = 0 \quad (a14)$$

The transformation $\vec{k} \mapsto \vec{k}' = \frac{\pi}{a}(1, 1, 1) - \vec{k}$ and $\varepsilon(\vec{k}) \mapsto 6E_0 - \varepsilon(\vec{k}')$ leaves the expression for the band energies unchanged. This symmetry shows that the hole and the electron pictures are completely equivalent in the present case. The holes in the limit of $0 < 6E_0 - \varepsilon_F \ll E_0$, or $n \gg p$, behave in the same way as the electrons in the limit $0 < \varepsilon_F \ll E_0$, or $n \ll p$, and

$$\sigma = \frac{pe^2\tau}{m^*} = \frac{e^2\tau}{\hbar^2} E_0 a^2 p \left[1 - \frac{1}{10} (3\pi^2 a^3 p)^{2/3} \right], \quad p = \frac{2}{a^3} - n \quad (a15)$$

replaces (a12) in this opposite limit.

According to eq. (a4), the Fermi surface does not touch the Brillouin zone boundaries if $0 < \varepsilon_F < 2E_0$. In this energy interval the Fermi surface only supports closed orbits. These closed orbits are lying on the outside of the occupied states, i.e. they are “electron like”, and

$$\mathcal{R} = -\frac{1}{nec}, \quad 0 < \varepsilon_F < 2E_0 \quad (a16)$$

The electron-hole symmetry implies the presence of an equivalent closed Fermi surface if replacing ε_F with $6E_0 - \varepsilon_F$. This surface, centered around $\frac{\pi}{a}(1, 1, 1)$, only contains closed “hole-like” orbits on the outside of unoccupied states, and

$$\mathcal{R} = \frac{1}{pec}, \quad 4E_0 < \varepsilon_F < 6E_0, \quad p = \frac{2}{a^3} - n \quad (a17)$$

[In the interval $2E_0 < \varepsilon_F < 4E_0$, the Fermi surface involves open orbits, except if the field is applied exactly along a cubic axis, but then the orbits are mixed between being electron- and hole-like.]

Problem 2010: Magnetic properties of band electrons

1) The number of states in a single band is 2 spin states times N different \vec{k} states, and introducing $n_0 = N/V$

$$V \int_0^\infty D(\varepsilon) d\varepsilon = V \int_0^W D d\varepsilon = VDW = 2N \quad \Rightarrow \quad D = \frac{2n_0}{W} \quad (a1)$$

The number of electrons in the band is N , which determines the Fermi energy ε_F^0

$$N = V \int_0^{\varepsilon_F^0} D(\varepsilon) d\varepsilon = V \int_0^{\varepsilon_F^0} \frac{2n_0}{W} d\varepsilon \quad \Rightarrow \quad \varepsilon_F^0 = \frac{W}{2} \quad (a2)$$

2) In the mean-field approximation, one or the other of the operators in products of two are being replaced by their thermal mean values. In the present case,

$$\hat{n}_{\vec{k}\uparrow} \hat{n}_{\vec{k}'\downarrow} \cong \hat{n}_{\vec{k}\uparrow} \langle \hat{n}_{\vec{k}'\downarrow} \rangle + \langle \hat{n}_{\vec{k}\uparrow} \rangle \hat{n}_{\vec{k}'\downarrow} - \langle \hat{n}_{\vec{k}\uparrow} \rangle \langle \hat{n}_{\vec{k}'\downarrow} \rangle \quad (a3)$$

and inserting this in (2) we get the results

$$\begin{aligned} E_{\vec{k}\uparrow} &= \varepsilon_{\vec{k}} + \frac{U}{N} \sum_{\vec{k}} \langle \hat{n}_{\vec{k}'\downarrow} \rangle + \mu_B H \quad \Rightarrow \quad \Delta_{\uparrow} = U \frac{n_{\downarrow}}{n_0} + \mu_B H \\ E_{\vec{k}\downarrow} &= \varepsilon_{\vec{k}} + \frac{U}{N} \sum_{\vec{k}} \langle \hat{n}_{\vec{k}'\uparrow} \rangle - \mu_B H \quad \Rightarrow \quad \Delta_{\downarrow} = U \frac{n_{\uparrow}}{n_0} - \mu_B H \\ \mathcal{E}_0 &= -\frac{U}{N} \sum_{\vec{k}, \vec{k}'} \langle \hat{n}_{\vec{k}\uparrow} \rangle \langle \hat{n}_{\vec{k}'\downarrow} \rangle = -N U \frac{n_{\uparrow} n_{\downarrow}}{n_0^2} \end{aligned} \quad (a4)$$

The mean-field Hamiltonian is in the same form as that of a gas of independent Fermions, and

$$\langle \hat{n}_{\vec{k}\sigma} \rangle = f_{\vec{k}\sigma} = \frac{1}{e^{\beta(E_{\vec{k}\sigma} - \mu)} + 1} \quad (a5)$$

$\beta = 1/k_B T$ and μ is determined by the condition that the total number of electrons is N , i.e.

$$N = \sum_{\vec{k}} (f_{\vec{k}\uparrow} + f_{\vec{k}\downarrow}) = V(n_{\uparrow} + n_{\downarrow}) \quad \Rightarrow \quad n_{\uparrow} + n_{\downarrow} = n_0 \quad (a6)$$

3) The electron energies are $E_{\vec{k}\sigma} = \varepsilon_{\vec{k}} + \Delta_{\sigma}$ implying that the spin-dependent density of states is

$$D_{\sigma}(\varepsilon) = \frac{1}{V} \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}} - \Delta_{\sigma}) = \begin{cases} \frac{D}{2} = \frac{n_0}{W} & \Delta_{\sigma} < \varepsilon < W + \Delta_{\sigma} \\ 0 & \varepsilon < \Delta_{\sigma}, W + \Delta_{\sigma} < \varepsilon \end{cases} \quad (a7)$$

At zero temperature

$$n_{\sigma} = \frac{1}{V} \sum_{\vec{k}} f_{\vec{k}\sigma} = \int^{\varepsilon_F} D_{\sigma}(\varepsilon) d\varepsilon = \int_{\Delta_{\sigma}}^{\varepsilon_F} \frac{n_0}{W} d\varepsilon = \frac{\varepsilon_F - \Delta_{\sigma}}{W} n_0 \quad (a8)$$

The Fermi energy is determined by

$$n_0 = n_\uparrow + n_\downarrow = \frac{2\varepsilon_F - \Delta_\uparrow - \Delta_\downarrow}{W} n_0 \quad \Rightarrow \quad \varepsilon_F = \frac{1}{2}(W + U) \quad (a9)$$

since $\Delta_\uparrow + \Delta_\downarrow = U$ according to (a4). Using the two same equations (a8) and (a4), the polarization is found to be

$$n_\downarrow - n_\uparrow = \frac{\Delta_\uparrow - \Delta_\downarrow}{W} n_0 = \frac{U}{W}(n_\downarrow - n_\uparrow) + \frac{2n_0}{W}\mu_B H \quad (a10)$$

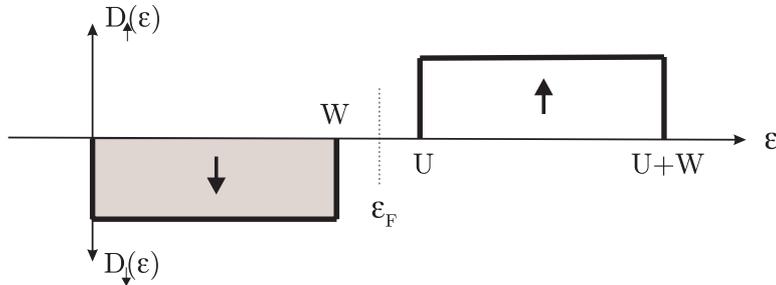
This equation of ‘‘self-consistency’’ is solved straightforwardly and the magnetic susceptibility is found to be

$$\chi = \frac{\mu_B(n_\downarrow - n_\uparrow)}{H} = \frac{2n_0}{W} \frac{1}{1 - \frac{U}{W}} \mu_B^2 \quad (a11)$$

The coulomb interaction U implies an enhancement of the Pauli susceptibility, $D(\varepsilon_F)\mu_B^2$, by the factor $[1 - U/W]^{-1} = [1 - D(\varepsilon_F)U/2n_0]^{-1}$.

4) χ diverges when $U \rightarrow W$, hence the critical value of U is $U_c = W$. When U is smaller than the critical value, $U < W$, the energy density \mathcal{E}/V at zero field, as given by Eq. (7), is at its minimum when $M = 0$, and the minimum energy density is $\mathcal{E}/V = n_0(W + U)/4 = n_0\varepsilon_F/2$. The ground state is paramagnetic and the magnetization is proportional to the field all the way up to its saturation value $M_s = n_0\mu_B$. The saturation of the magnetization is achieved when all electrons are in the same spin state ($n_\downarrow = n_0$ and $n_\uparrow = 0$).

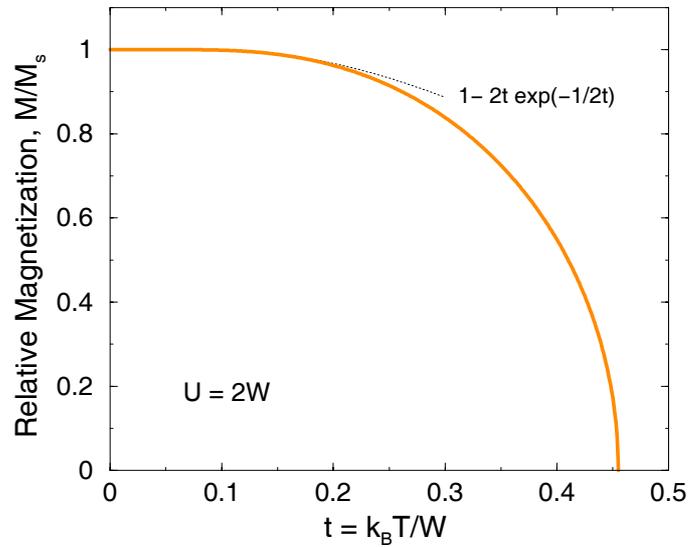
In the opposite case, when $U > W$, the coefficient to M^2 in the energy density (7) becomes negative and the energy is minimized when M^2 is maximized, i.e. $|M| = M_s = n_0\mu_B$ in equilibrium (independent of the value of H). The ground state is ferromagnetic and the energy density is $\mathcal{E}/V = n_0W/2$ at $H = 0$. The magnetization is saturated at all values of H (the magnetization vector is parallel to the field if H is non zero). The figure below shows the density of states for the spin-up and spin-down electrons at $H = 0$, where $\Delta_\downarrow = 0$ and $\Delta_\uparrow = U > W$.



All the electrons are in the spin-down band and the band is completely filled, $W < \varepsilon_F < U$. There are no empty states lying near by in energy and it is not possible to accelerate the electrons by an electric field. Hence, the paramagnetic metal becomes a ferromagnetic insulator when $U > W$. At non-zero temperatures the spin-up states are going to be thermally populated and M is reduced, but because of the gap the magnetization depends exponentially

on temperature, $M_s - M \propto \exp[-\beta(U - W)/2]$, in contrast to the $T^{3/2}$ law predicted by the spin-wave theory for a normal Heisenberg ferromagnet. At sufficiently high temperature, at $T = T_C$, this “Stoner ferromagnet” becomes a paramagnetic metal, though still with an enhanced Pauli susceptibility.

The figure below shows, as an example, the calculated magnetization curve in the case of $U = 2W$.



Condensed Matter Physics 2

Skriftlig eksamen - April 2011

Answer to Problem 1: Ferromagnet

a) When J_1 and J_2 are positive, the ground state is the saturated ferromagnet, where $\langle \vec{s}_i \rangle = s \hat{z} = \frac{1}{2} \hat{z}$ for all i . The ground state energy U is

$$U = -\frac{1}{2}N(z_1 J_1 + z_2 J_2)s^2 = \underline{\underline{-(6J_1 + 3J_2)\frac{V}{a^3}}} \quad (a1)$$

The fcc structure has 4 atoms per cubic unit cell, which implies $N = 4V/a^3$. The number of nearest neighbours is $z_1 = 12$, and the number of next-nearest neighbours is $z_2 = 6$.

b) Applying an infinitesimal field along the z axis, only the z component of the thermal average $\langle \vec{s}_i \rangle$ may be non zero. In this case, the mean-field approximation implies

$$\begin{aligned} \vec{s}_i \cdot \vec{s}_j &\stackrel{\text{MF}}{=} \vec{s}_i \cdot \langle \vec{s}_j \rangle + \langle \vec{s}_i \rangle \cdot \vec{s}_j - \langle \vec{s}_i \rangle \cdot \langle \vec{s}_j \rangle \\ &= (s_i^z + s_j^z - \langle s^z \rangle) \langle s^z \rangle = \frac{1}{4}(\sigma_i^z + \sigma_j^z - \langle \sigma^z \rangle) \langle \sigma^z \rangle \end{aligned} \quad (a2)$$

where $\sigma_i^z = 2s_i^z$ may take on the values $+1$ or -1 . Hence, within the mean-field approximation, $\vec{s}_i \cdot \vec{s}_j$ is replaced by the same expression as derived from the Ising interaction $\frac{1}{4}\sigma_i\sigma_j$ within the same approximation.

c) The mean-field transition temperature for the simple Ising model is derived by Marder in Section 24.4 to be determined by $k_B T = zJ$. For the present system, this temperature is determined by the same expression except that zJ is replaced by $\frac{1}{4}(z_1 J_1 + z_2 J_2)$, i.e.

$$T_C = \underline{\underline{(3J_1 + \frac{3}{2}J_2)/k_B}} \quad (a3)$$

Answer to Problem 2: Non-interacting spin-dimer system

a) The spin-operator sum is defined $\vec{S}(i) = \vec{s}_1(i) + \vec{s}_2(i)$, where the spin quantum number S for the total spin may take on the values 0 or 1.

$$[\vec{S}(i)]^2 = [\vec{s}_1(i)]^2 + [\vec{s}_2(i)]^2 + 2\vec{s}_1(i) \cdot \vec{s}_2(i) = \frac{3}{2} + 2\vec{s}_1(i) \cdot \vec{s}_2(i) = S(S+1) \quad (a4)$$

using $[\vec{s}_1(i)]^2 = [\vec{s}_2(i)]^2 = s(s+1) = \frac{3}{4}$, and the Hamiltonian for the i th dimer may be written

$$\mathcal{H}(i) = -J \left[\frac{1}{2}S(S+1) - \frac{3}{4} \right] - g\mu_B H S_z(i) \quad (a5)$$

when defining the z axis to be parallel with the field. The eigenenergies are:

$$\begin{aligned} \varepsilon_{00} &= \frac{3}{4}J, & S=0, S_z=0 \\ \varepsilon_{1-1} &= -\frac{1}{4}J + g\mu_B H, & S=1, S_z=-1 \\ \varepsilon_{10} &= -\frac{1}{4}J, & S=1, S_z=0 \\ \varepsilon_{11} &= -\frac{1}{4}J - g\mu_B H, & S=1, S_z=1 \end{aligned} \quad (a6)$$

b) When $J = 0$ the system is $2N$ non-interacting $s = \frac{1}{2}$ ions, and the susceptibility is given by Curie's law, eqs. (25.31) and (25.32) in Marder, i.e.

$$\chi = (g\mu_B)^2 \frac{2N}{V} \frac{s(s+1)}{3k_B T} = \frac{n(g\mu_B)^2}{4k_B T} \quad (a6)$$

c) When $k_B T \ll |J|$ and $J > 0$, then only the triplet $S = 1$ is populated and the dimer system is equivalent to N non-interacting $S = 1$ ions. If $J < 0$ only the $S = 0$ singlet is populated and the system becomes non-magnetic:

$$\chi_1 = (g\mu_B)^2 \frac{N}{V} \frac{S(S+1)}{3k_B T} = \frac{n(g\mu_B)^2}{3k_B T} \quad (J > 0) \quad (a7)$$

$$\chi_0 = 0 \quad (J < 0)$$

Notice that $\chi = (3\chi_1 + \chi_0)/4$.

Answer to Problem 3: Anisotropic band electrons

a) The constant energy surface in \vec{k} space at $\varepsilon = \varepsilon_F$, the Fermi surface, is an ellipsoid with semi axes a_i , $i = 1, 2, 3$:

$$\left(\frac{k_x}{a_1}\right)^2 + \left(\frac{k_y}{a_2}\right)^2 + \left(\frac{k_z}{a_3}\right)^2 = 1, \quad a_i = \frac{\sqrt{2m_i\varepsilon_F}}{\hbar} \quad (a8)$$

b) According to, for instance, eq. (17.48) in Marder:

$$\vec{\sigma} = ne^2\tau\vec{M}^{-1} = ne^2\tau \begin{pmatrix} \frac{1}{m_1} & 0 & 0 \\ 0 & \frac{1}{m_2} & 0 \\ 0 & 0 & \frac{1}{m_3} \end{pmatrix} \quad (a9)$$

in the (x, y, z) coordinate system. Applying a field $\vec{E} = E_0(1, 1, 0)$, then the current density is $\vec{j} = \vec{\sigma}\vec{E} = ne^2\tau(E_0/m_1, E_0/m_2, 0)$, which is a vector in the (xy) plane making an angle ϕ with the x axis, where $\tan\phi = m_1/m_2$.

c) Introducing a new vector variable

$$\vec{k}' = \left(\sqrt{\frac{m}{m_1}}k_x, \sqrt{\frac{m}{m_2}}k_y, \sqrt{\frac{m}{m_3}}k_z \right) \Rightarrow \varepsilon(\vec{k}') = \frac{(\hbar k')^2}{2m} \quad (a10)$$

then the density of states is [using eq. (6.23) in Marder]

$$\begin{aligned} D(\varepsilon) &= \frac{2}{(2\pi)^3} \int d\vec{k} \delta(\varepsilon - \varepsilon(\vec{k})) = \left(\frac{m_1 m_2 m_3}{m^3}\right)^{\frac{1}{2}} \frac{2}{(2\pi)^3} \int d\vec{k}' \delta(\varepsilon - \varepsilon(\vec{k}')) \\ &= \left(\frac{m_1 m_2 m_3}{m^3}\right)^{\frac{1}{2}} \frac{\sqrt{2m^3\varepsilon}}{\hbar^3\pi^2} = \frac{\sqrt{2(m^*)^3\varepsilon}}{\hbar^3\pi^2}, \quad \underline{m^* = (m_1 m_2 m_3)^{\frac{1}{3}}} \end{aligned} \quad (a11)$$

The Sommerfeld constant [eq. (6.77) in Marder] is $\gamma = (\pi^2/3)D(\varepsilon_F)k_B$. The Fermi energy is $\varepsilon_F = (\hbar k'_F)^2/2m$, where $k'_F = (3\pi^2 n)^{1/3}$. Introducing this in (a11) the result is $D(\varepsilon_F) = m^* k'_F / (\hbar\pi)^2$ or

$$\gamma = \frac{k_B}{\hbar^2} \left(\frac{\pi^2}{9} m_1 m_2 m_3 n \right)^{\frac{1}{3}} \quad (a12)$$