

Solutions to Problems in Condensed Matter Physics 2

(Textbook: Michael P. Marder, *Condensed Matter Physics*, Wiley, 2000)

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(Niels Bohr Institute, February 2011)

Solutions to the problems in Chapter 6

6.3 Pressure of a Fermi gas at zero temperature

The number of electrons N and the internal energy U , in the volume V , are

$$N = V \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon, \quad U = V \int_0^\infty \varepsilon D(\varepsilon) f(\varepsilon) d\varepsilon, \quad (1)$$

The Fermi distribution function $f(\varepsilon)$ and the density of states (per unit volume) $D(\varepsilon)$ are

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}, \quad D(\varepsilon) = A\sqrt{\varepsilon}, \quad A = \frac{\sqrt{2m^3}}{\pi^2 \hbar^3}. \quad (2)$$

At zero temperature

$$f(\varepsilon) = \theta(\varepsilon_F - \varepsilon), \quad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}, \quad k_F = (3\pi^2 n)^{1/3} \quad (3)$$

Introducing the step function and $D(\varepsilon) = A\sqrt{\varepsilon}$ in (1), we may determine $U(0)$ and an alternative expression for A :

$$N = V \int_0^{\varepsilon_F} A\sqrt{\varepsilon} d\varepsilon = \frac{2}{3} V A \varepsilon_F^{3/2} \Rightarrow A = \frac{3n}{2\varepsilon_F^{3/2}}, \quad U(0) = V \frac{2}{5} A \varepsilon_F^{5/2} = \frac{3}{5} N \varepsilon_F \quad (4)$$

i.e. $U \propto \varepsilon_F \propto k_F^2 \propto V^{-2/3}$ and the pressure at zero temperature is

$$P = -\frac{\partial U(0)}{\partial V} = \frac{2}{3} \frac{U}{V} = \frac{2}{5} n \varepsilon_F = \frac{(3\pi^2)^{2/3} n^{5/3} \hbar^2}{5m} \quad (5)$$

in sharp contrast to a classical gas, where the zero-temperature pressure is zero.

6.4 Density of states in low dimensions

The density of states in \vec{k} -space is $D_{\vec{k}} = 2/(2\pi)^d$ in d dimensions (6.34)

$$D(\varepsilon) = \int [d\vec{k}] \delta(\varepsilon - \varepsilon_{\vec{k}}) \equiv \int D_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}}) d\vec{k} = \frac{2}{(2\pi)^d} \int \delta(\varepsilon - \varepsilon_{\vec{k}}) d\vec{k} \quad (1)$$

Introducing “spherical coordinates” in d dimensions and $k = |\vec{k}|$, then

$$d\vec{k} = \begin{cases} 2 dk & , \quad d = 1 \\ 2\pi k dk & , \quad d = 2 \\ 4\pi k^2 dk & , \quad d = 3 \end{cases} \quad (2)$$

The factor 2 in the one-dimensional case appears because the one-dimensional wave vector may assume both positive and negative values, whereas $k \geq 0$ per definition.

$$\varepsilon_{\vec{k}} = \varepsilon_k = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \frac{\sqrt{2m\varepsilon_k}}{\hbar}, \quad dk = \left(\frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k \Rightarrow \quad (3)$$

$$D(\varepsilon) = \begin{cases} \frac{2}{2\pi} \int_0^\infty 2 \delta(\varepsilon - \varepsilon_k) \left(\frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k = \frac{\sqrt{2m}}{\pi \hbar} \varepsilon^{-1/2}, & d = 1 \\ \frac{2}{(2\pi)^2} \int_0^\infty 2\pi \frac{\sqrt{2m\varepsilon_k}}{\hbar} \delta(\varepsilon - \varepsilon_k) \left(\frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k = \frac{m}{\pi \hbar^2}, & d = 2 \\ \frac{2}{(2\pi)^3} \int_0^\infty 4\pi \frac{2m\varepsilon_k}{\hbar^2} \delta(\varepsilon - \varepsilon_k) \left(\frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k = \frac{\sqrt{2m^3}}{\pi^2 \hbar^3} \varepsilon^{1/2}, & d = 3 \end{cases}$$

6.5 Fermi pancakes

Thin layer of Ag: $L_x = L_y = L = 10^6 \text{ \AA}$ and $L_z = d$.

The density of electrons is the same as the density of atoms (one conduction electron per Ag atom), i.e. $n = 5.86 \cdot 10^{22} \text{ cm}^{-3} = 0.0586 \text{ \AA}^{-3}$, according to the properties given in the periodic table on the front page of Marder. The wave function of the “free” electrons should vanish at the boundaries $z = 0$ and $z = d$. This condition is fulfilled if assuming the one-electron wave function to be

$$\psi(x, y, z) \propto e^{i(k_x x + k_y y)} \sin(pqz), \quad q = \frac{\pi}{d}, \quad p = 1, 2, \dots \quad (1)$$

The electron states are characterized by the two-dimensional wave vector $\vec{k} = (k_x, k_y, 0)$ and the “band index” p . The eigenenergies are ($k^2 = k_x^2 + k_y^2$):

$$\varepsilon_{p\vec{k}} = \frac{\hbar^2}{2m} (k^2 + p^2 q^2) \geq \varepsilon_{1\vec{0}} = \frac{\hbar^2 q^2}{2m} \quad (2)$$

At $T = 0$ ($T \ll T_F$), as assumed implicitly in the exercise, the occupied states are all those with energies smaller than ε_F . The number of electrons in the p th band, N_p , is zero if $\varepsilon_{p\vec{0}} > \varepsilon_F$. In the opposite case:

$$N_p = L^2 \int_0^{k_p} \frac{2}{(2\pi)^2} 2\pi k dk = L^2 \frac{k_p^2}{2\pi} \quad (3)$$

where k_p is the Fermi wave number of the p th band, i.e. the largest value of k of occupied states in the p th band, as determined by

$$\varepsilon_{pk_p} = \frac{\hbar^2}{2m} (k_p^2 + p^2 q^2) = \varepsilon_F \quad \Rightarrow \quad k_p^2 = \frac{2m\varepsilon_F}{\hbar^2} - p^2 q^2 = q^2 \left(\frac{\varepsilon_F}{\varepsilon_{1\vec{0}}} - p^2 \right) \quad (4)$$

(a) In the first case $d = 4.1 \text{ \AA}$ or $q = \pi/d = 0.76624 \text{ \AA}^{-1}$, and

$$\varepsilon_{1\vec{0}} = \frac{\hbar^2 q^2}{2m} = \frac{(1.054572 \cdot 10^{-27} \times 0.76624 \cdot 10^8)^2}{2 \times 9.109389 \cdot 10^{-28} \times 1.602177 \cdot 10^{-12}} \text{ eV} = 2.2369 \text{ eV} \quad (5)$$

Assuming the Fermi energy to be smaller than the lowest energy of the ($p = 2$) band, $\varepsilon_F < \varepsilon_{2\vec{0}} = 4\varepsilon_{1\vec{0}}$, then only the ($p = 1$) states are occupied, in which case N_1 has to be equal the total number N of free electrons:

$$N = L^2 d n = N_1 = L^2 \frac{k_1^2}{2\pi} \quad \Rightarrow \quad k_1 = \sqrt{2\pi d n} = 1.22866 \text{ \AA}^{-1} \quad (6)$$

Introducing this result in (3) we get the Fermi energy and the band width W of the occupied states:

$$\varepsilon_F = \varepsilon_{1k_1} = \varepsilon_{1\vec{0}} \left[(k_1/q)^2 + 1 \right] = 7.99 \text{ eV}, \quad W = \varepsilon_F - \varepsilon_{1\vec{0}} = \underline{5.75 \text{ eV}} \quad (7)$$

which is in accordance with our starting assumption of $\varepsilon_F < \varepsilon_{2\vec{0}} = 8.948 \text{ eV}$. These results may be compared with that obtained for bulk Ag:

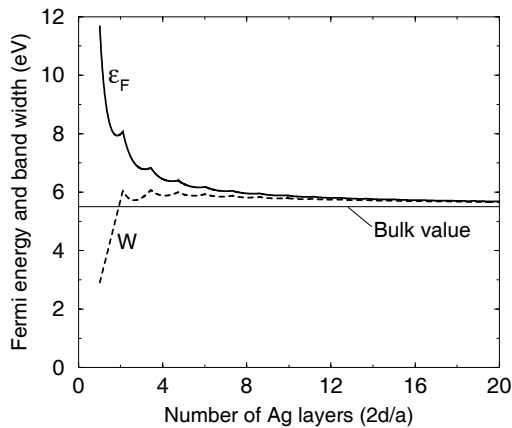
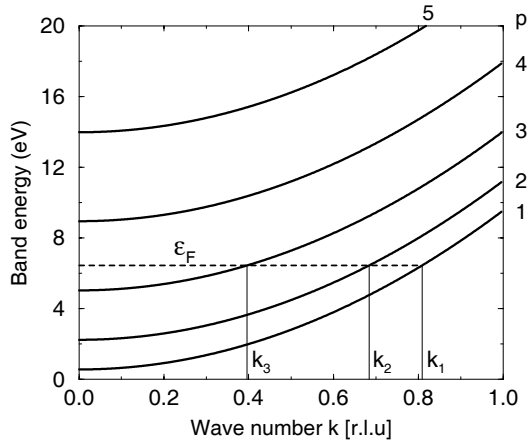
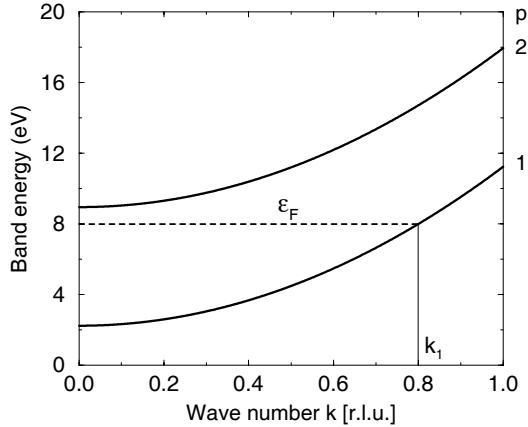
$$\varepsilon_F(\text{bulk}) = W(\text{bulk}) = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} = 5.50 \text{ eV} \quad (8)$$

(b) In the case of $d = 8.2 \text{ \AA}$, $q = \pi/d = 0.38312 \text{ \AA}^{-1}$ and $\varepsilon_{10} = 0.5592 \text{ eV}$. In order to determine ε_F in this case, we need to include more bands than the lowest one. The number of bands turns out to be 3, and

$$N = N_1 + N_2 + N_3 \Rightarrow 2\pi dn = q^2 \left[\left(\frac{\varepsilon_F}{\varepsilon_{10}} - 1^2 \right) + \left(\frac{\varepsilon_F}{\varepsilon_{10}} - 2^2 \right) + \left(\frac{\varepsilon_F}{\varepsilon_{10}} - 3^2 \right) \right] \quad (9)$$

Solving this equation with respect to $\varepsilon_F/\varepsilon_{10}$, we get $\varepsilon_F/\varepsilon_{10} = 11.523$, which is larger than 3^2 but smaller than 4^2 , in accordance with the assumption that all electrons are found in the three lowest bands. Hence the results are:

$$\varepsilon_F = 6.44 \text{ eV}, \quad W = \varepsilon_F - \varepsilon_{10} = \underline{5.89 \text{ eV}} \quad (10)$$



The two first figures show the energy bands as functions of k in the cases (a) and (b), where the unit of k is the length of a reciprocal lattice vector $2\pi/a$ [r.l.u.]. The last figure shows the Fermi energy (and the band width) as a function of the number of atomic layers of Ag. The crystal structure of Ag is fcc with the lattice parameter $a = 4.09 \text{ \AA}$. This is very nearly the thickness d assumed in (a), i.e. this case corresponds to a film with two atomic layers of Ag atoms.

Solutions to the problems in Chapter 7

7.1 Normals to surfaces

$\vec{r} = (x_1, x_2, x_3) = \vec{s}(t)$ is the parametrization of a curve lying within the surface defined by $f(\vec{r}) = \varepsilon$. Since $f(\vec{s}(t))$ is a constant ε , the derivative of this function is 0:

$$\frac{d}{dt}f(\vec{s}(t)) = \sum_{\alpha} \frac{\partial f}{\partial x_{\alpha}} \frac{ds_{\alpha}}{dt} = \nabla f \cdot \frac{d\vec{s}}{dt} = 0 \quad (1)$$

Because $\vec{s}(t)$ may be any arbitrary curve lying within the surface, the same is true for the curve tangent $d\vec{s}(t)/dt$, and (1) is only generally valid if ∇f is normal to the surface.

7.3 Van Hove singularities

(a) The problem becomes the same as the one considered in problem 7.1 if making the replacements $\vec{k} \rightarrow \vec{r}$ and $\varepsilon_{n\vec{k}} \rightarrow f(\vec{r})$, hence $\nabla_{\vec{k}} \varepsilon_{n\vec{k}}$ is perpendicular to the energy surface defined by $\varepsilon_{n\vec{k}} = \varepsilon$.

(b) The energy is assumed to be $\varepsilon_{n\vec{k}} = \varepsilon_{\max} - k^2$, and in the two-dimensional case

$$\begin{aligned} D(\varepsilon) &= \int [d\vec{k}] \delta(\varepsilon - \varepsilon_{n\vec{k}}) = \frac{2}{(2\pi)^2} \int_0^{\infty} 2\pi k \delta(\varepsilon - \varepsilon_{\max} + k^2) dk \\ &= \frac{1}{2\pi} \int_0^{\infty} \delta(\varepsilon - \varepsilon_{\max} + k^2) d(k^2) = \frac{1}{2\pi} \theta(\varepsilon_{\max} - \varepsilon) \end{aligned} \quad (1)$$

The density of states is zero if $\varepsilon > \varepsilon_{\max}$ and $1/(2\pi)$ when $\varepsilon < \varepsilon_{\max}$.

(c) In the three dimensional case, the result is

$$\begin{aligned} D(\varepsilon) &= \int [d\vec{k}] \delta(\varepsilon - \varepsilon_{n\vec{k}}) = \frac{2}{(2\pi)^3} \int_0^{\infty} 4\pi k^2 \delta(\varepsilon - \varepsilon_{\max} + k^2) dk \\ &= \frac{1}{2\pi^2} \int_0^{\infty} k \delta(\varepsilon - \varepsilon_{\max} + k^2) d(k^2) = \frac{1}{2\pi^2} \sqrt{\varepsilon_{\max} - \varepsilon} \theta(\varepsilon_{\max} - \varepsilon) \end{aligned} \quad (2)$$

Solution to HS's problem 1

Heat capacity of a two-dimensional electron gas

GaAs/AlGaAs heterostructure (see Marder Section 19.5):

$$n = 10^{11} \text{ cm}^{-2}, \quad \varepsilon = \frac{\hbar^2 k^2}{2m^*}, \quad m^* = 0.067m_e \quad (1)$$

The present situation corresponds to the case (a) of the previous problem 6.5 in Marder, i.e. the gas is purely two-dimensional in the sense that only the ($p = 1$) band needs to be considered, and \vec{k} is a two-dimensional vector with the length $k = \sqrt{k_x^2 + k_y^2}$. The most important quantity is the Fermi energy, which is determined by evaluating N at zero temperature:

$$n = \frac{N}{A} = \int_{k \leq k_F} D_{\vec{k}} d\vec{k} = \frac{2}{(2\pi)^2} \int_0^{k_F} 2\pi k dk = \frac{k_F^2}{2\pi} \Rightarrow k_F = \sqrt{2\pi n} \quad (2a)$$

The same result is obtained by using that, according to problem 6.4 or equation (6.35), $D(\varepsilon) = m^*/\pi\hbar^2$ in the two-dimensional case:

$$n = \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon = \frac{m^* \varepsilon_F}{\pi\hbar^2} \Rightarrow \varepsilon_F = \frac{n\pi\hbar^2}{m^*} \quad \text{or} \quad k_F = \sqrt{2\pi n} \quad (2b)$$

Introducing the numbers, and using that $k_F = 1 \text{ \AA}^{-1}$ corresponds to a Fermi energy $\varepsilon_F = 3.81 \text{ eV}$ when the mass is m_e , then we get

$$k_F = 0.793 \cdot 10^{-2} \text{ \AA}^{-1}, \quad \varepsilon_F = \frac{(0.793 \cdot 10^{-2})^2}{0.067} 3.81 \text{ eV} = 3.58 \text{ meV} \quad (3)$$

This Fermi energy corresponds to a Fermi temperature $T_F = \varepsilon_F/k_B = 41.5 \text{ K}$.

1) $T = 1 \text{ K}$ is much smaller than the Fermi temperature and the heat capacity may be determined by the leading order expression (6.77)

$$c_V = \frac{\pi^2}{3} D(\varepsilon_F) k_B^2 T = \frac{\pi}{6} \frac{T}{T_F} k_F^2 k_B, \quad \text{as} \quad D(\varepsilon_F) = \frac{m^*}{\pi\hbar^2} = \frac{k_F^2}{2\pi\varepsilon_F} = \frac{k_F^2}{2\pi k_B T_F} \quad (4)$$

In the case of a sample with the area $A = 1 \text{ cm}^2$ the result is

$$C_V(\text{el}) = A c_V = A \frac{\pi}{6} \frac{1}{41.5} (0.793 \cdot 10^6 \text{ cm}^{-1})^2 \times 1.38066 \cdot 10^{-23} \text{ J/K} = \underline{1.1 \cdot 10^{-13} \text{ J/K}} \quad (5)$$

The explicit result is $C_V(\text{el}) = A\pi m^* k_B^2 T / (3\hbar^2)$. Hence, the small value of C_V is not due to the low electron density n but to the two-dimensionality of the system and the small effective mass.

2) In order to estimate the phonon contribution to the heat capacity we shall use the Debye model (Section 13.3.2 in Marder). The Debye temperature of GaAs is $\Theta_D = 344 \text{ K}$ (which value is not changed much when some of the Ga ions are replaced by Al ions). Using (13.70), (13.75) in Marder (2.Ed.) and

$$\int_0^\infty \frac{x^4 e^x}{(e^x - 1)^2} dx = \frac{4\pi^4}{15} \Rightarrow c_V = \frac{12\pi^4}{5} n_A k_B \left(\frac{T}{\Theta_D} \right)^3 \quad (T \ll \Theta_D) \quad (6)$$

According to Table 2.5 (page 27) in Marder, GaAs has the zincblende structure (\sim diamond structure) with the lattice parameter $a = 5.63 \text{ \AA}$. In this structure there are 8 atoms per unit cell, and the density of atoms is $n_A = 8/a^3 = 4.48 \cdot 10^{22} \text{ cm}^{-3}$. [The mean atomic mass (periodic table) is $(69.72 + 74.92)/2 = 72.3 \text{ u}$, implying a mass density $\rho = 5.38 \text{ g cm}^{-3}$]. Assuming $V = 1 \text{ cm}^3$ and $T = 1 \text{ K}$, the phonon contribution becomes

$$C_V(\text{ph}) = \frac{12\pi^4}{5} \times 4.48 \cdot 10^{22} \times 1.38066 \cdot 10^{-23} \left(\frac{1}{344} \right)^3 \text{ J/K} = \underline{3.55 \cdot 10^{-6} \text{ J/K}} \quad (7)$$

which is much larger than the electronic contribution. Utilizing that $C_V(\text{el}) \propto T$ and $C_V(\text{ph}) \propto T^3$, the temperature T_0 at which the two contributions are equal, is determined by (T_0 in K)

$$1.10 \cdot 10^{-13} T_0 = 3.55 \cdot 10^{-6} T_0^3 \Rightarrow T_0 = \underline{1.8 \cdot 10^{-4} \text{ K}} \quad (8)$$

A more fair comparison would be to consider a film of thickness $\sim 100 \mu\text{m}$, i.e. $A = 1 \text{ cm}^2$ and $V = 10^{-2} \text{ cm}^3$, in which case $T_0 = 1.8 \text{ mK}$, a temperature within an accessible range (however, the reduction of the size of the sample makes it more difficult to determine the heat capacity).

Solution to the problem in Chapter 11

11.2 Zinc in copper

Copper is a monovalent fcc and zinc a divalent hcp (not fcc) metal. At a small concentration of Zn^{++} , the crystal structure is fcc until the Fermi surface touches some point on the edge of the Brillouin zone:

(a) In the nearly free electron approximation, the Fermi wave vector is (nearly) determined as in the free electron case,

$$n = \int_{|\vec{k}| \leq k_F} D_{\vec{k}} d\vec{k} = \frac{2}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk = \frac{1}{3\pi^2} k_F^3 \quad \Rightarrow \quad k_F = (3\pi^2 n)^{1/3} \quad (1)$$

Defining c to be the concentration of Zn^{++} ions and a to be the lattice parameter of the fcc lattice, then the electron density is

$$n = \frac{4}{a^3} [(1-c) + 2c] = \frac{4}{a^3} (1+c) \quad \Rightarrow \quad k_F = \left[\frac{12\pi^2}{a^3} (1+c) \right]^{1/3} = \frac{4.9109}{a} (1+c)^{1/3} \quad (2)$$

(b) The primitive unit vectors of the face-centered cubic lattice are, (2.2):

$$\vec{a}_1 = \frac{a}{2}(1, 1, 0), \quad \vec{a}_2 = \frac{a}{2}(1, 0, 1), \quad \vec{a}_3 = \frac{a}{2}(0, 1, 1) \quad (3)$$

and the corresponding primitive vectors of the reciprocal lattice are

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi}{a}(1, 1, -1), \quad \vec{b}_2 = \frac{2\pi}{a}(1, -1, 1), \quad \vec{b}_3 = \frac{2\pi}{a}(-1, 1, 1) \quad (4)$$

The boundaries of the 1. Brillouin zone are established by the planes perpendicular to $\pm \vec{b}_i$ at the distance $k_1 = |\vec{b}_i|/2$ from the origin. Hence the shortest distance from the origin to the zone boundaries is

$$k_1 = \frac{|\vec{b}_i|}{2} = \frac{\pi\sqrt{3}}{a} = \frac{5.4414}{a} \quad (5)$$

$k_F(c=0)$ is smaller than k_1 , and $k_F(c)$ becomes equal to k_1 at the zinc concentration $c = c_1$

$$4.9109(1+c_1)^{1/3} = 5.4414 \quad \Rightarrow \quad c_1 = \underline{0.36} \quad (6)$$

The experimental phase diagram (see Fig. 4 in Chapter 21 of Kittel) shows a transition from fcc to bcc, for increasing c values, at about the Zn concentration determined here.

(c) The primitive unit vectors of the body-centered cubic lattice are, (2.3):

$$\vec{a}_1 = \frac{a}{2}(1, 1, -1), \quad \vec{a}_2 = \frac{a}{2}(1, -1, 1), \quad \vec{a}_3 = \frac{a}{2}(-1, 1, 1) \quad (7)$$

and the corresponding primitive vectors of the reciprocal lattice are

$$\vec{b}_1 = \frac{2\pi}{a}(1, 1, 0), \quad \vec{b}_2 = \frac{2\pi}{a}(1, 0, 1), \quad \vec{b}_3 = \frac{2\pi}{a}(0, 1, 1) \quad (8)$$

Notice, that the reciprocal of the bcc lattice is fcc, and equivalently, that the reciprocal lattice of fcc is the bcc lattice.

In the case of bcc there are 2 atoms per cubic unit cell, hence

$$n = \frac{2}{a^3}(1 + c), \quad k_F = \left[\frac{6\pi^2}{a^3}(1 + c) \right]^{1/3} = \frac{3.8979}{a}(1 + c)^{1/3} \quad (9)$$

The shortest distance from the origin to the boundaries of the 1. Brillouin zone is

$$k_2 = \frac{|\vec{b}_i|}{2} = \frac{\pi\sqrt{2}}{a} = \frac{4.4429}{a} \quad \text{and} \quad k_2 = k_F \quad \text{when} \quad c = c_2 = \underline{0.48} \quad (10)$$

Once again, this is about the right Zn concentration at which the Cu-Zn alloy system shows a change of crystal structure (from bcc to a complex γ structure).

If the atomic density is assumed to stay constant at the transition fcc \rightarrow bcc, the Fermi wave vector is the same on each side of the phase line, but the lattice parameter a is changed, $a_{\text{bcc}} = (1/2)^{1/3} a_{\text{fcc}} = 0.794 a_{\text{fcc}}$. The cubic lattice parameter a also changes (increases) gradually with the Zn concentration, in between the phase lines, since $n_{\text{Cu}} = 1.33 n_{\text{Zn}}$, however, all the possible variations of a have no influence on the arguments above. β -brass is the alloy with $c = 0.5$, and it shows an order-disordered phase transition at about 470 °C, which we are going to discuss later on.

Citation from Kittel: “Why is there a connection between the electron concentrations at which a new phase appears and at which the Fermi surface makes contact with the Brillouin zone? We recall that the energy bands split into two at the region of contact on the zone boundary [Marder, Chapter 8, (8.24)]. If we add more electrons to the alloy at this stage, they will have to be accommodated in the upper band or in states of high energy near the zone corners of the lower band. Both options are possible, and both involve an increase of energy. Therefore it may be energetically favorable for the crystal structure to change to one which can contain a Fermi surface of larger volume (more electrons) before contact is made with the zone boundary. In this way H. Jones made plausible the sequence of structures fcc, bcc, γ , hcp with increasing electron concentration.”

Solutions to the problems in Chapter 12

12.4 Elastic constants

(a) The application of a uniform external gas pressure (no shear stress) implies a uniform dilations of an isotropic solid, where only $e_{xx} = e_{yy} = e_{zz}$ are non-zero, or

$$e_{\alpha\beta} = \delta_{\alpha\beta} \frac{V - V_0}{3V_0} = \frac{\Delta V}{3V_0} \quad (1)$$

where V_0 is the zero-pressure equilibrium volume. Introducing this in the free energy expression for an isotropic solid (12.23)

$$\mathcal{F} = \frac{1}{2} \int \left[\lambda \left(\sum_{\alpha} e_{\alpha\alpha} \right)^2 + 2\mu \sum_{\alpha\beta} e_{\alpha\beta}^2 \right] d\vec{r} = \frac{1}{2} (V_0 + \Delta V) \left[\lambda \left(\frac{\Delta V}{V_0} \right)^2 + 2\mu \frac{3}{9} \left(\frac{\Delta V}{V_0} \right)^2 \right] \quad (2)$$

the bulk modulus is found to be

$$B = V \frac{\partial^2 \mathcal{F}}{\partial V^2} = \underline{\lambda + \frac{2}{3}\mu} \quad (3)$$

(when $V \rightarrow V_0$). This result is also obtained from the bulk modulus in the cubic case (12.19), $B = [c_{11} + 2c_{12}]/3$, by replacing the elastic constants with the Lamé constants of the isotropic solid, $c_{12} = \lambda$, $c_{44} = \mu$, and $c_{11} = c_{12} + 2c_{44} = \lambda + 2\mu$.

(b) According to (12.31), or Fig. 12.2, Young's modulus Y is defined to be $Y = \sigma_{zz}/e_{zz}$, when applying a uniform stress σ_{zz} in the z direction. In the cubic case, the diagonal elements of stress and strain tensors are related by, (12.14)-(12.17),

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \end{pmatrix} = \bar{c} \begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \end{pmatrix}, \quad \bar{c} = \begin{pmatrix} c_{11} & c_{12} & c_{12} \\ c_{12} & c_{11} & c_{12} \\ c_{12} & c_{12} & c_{11} \end{pmatrix} \quad (4)$$

[the “off-diagonal elements relations” are $\sigma_{\alpha} = c_{44}e_{\alpha}$, where $\alpha = 4, 5, 6$. In the case of $\alpha = 4$ this equation reads $\sigma_{yz} = 2c_{44}e_{yz}$]. In order to determine e_{zz} when σ_{zz} is non-zero, we need to determine the inverse matrix. The determinant of \bar{c} is $D = c_{11}^3 + 2c_{12}^3 - 3c_{11}c_{12}^2 = (c_{11} + 2c_{12})(c_{11} - c_{12})^2$, and the inverse matrix is found to be

$$\bar{c}^{-1} = \begin{pmatrix} A & B & B \\ B & A & B \\ B & B & A \end{pmatrix}, \quad A = \frac{c_{11} + c_{12}}{(c_{11} + 2c_{12})(c_{11} - c_{12})}, \quad B = -\frac{c_{12}}{c_{11} + c_{12}} A \quad (5)$$

showing that $e_{zz} = A\sigma_{zz}$, hence

$$Y = A^{-1} = \frac{(c_{11} + 2c_{12})(c_{11} - c_{12})}{c_{11} + c_{12}} \quad (6)$$

[In order to complete the cubic case, then Poisson's ratio (12.34) is $-B/A$ or $\nu = \frac{c_{12}}{c_{11} + c_{12}}$, and the shear modulus is $G = c_{44}$].

12.5 Waves in cubic crystals

(a) Combining (12.14) and (12.16) we may write the free energy of a cubic solid as

$$\mathcal{F} = \frac{1}{2} \int d\vec{r} \left[c_{11} (e_{xx}^2 + e_{yy}^2 + e_{zz}^2) + 2c_{12} (e_{xx}e_{yy} + e_{xx}e_{zz} + e_{yy}e_{zz}) + 2c_{44} (e_{xy}^2 + e_{yx}^2 + e_{xz}^2 + e_{zx}^2 + e_{yz}^2 + e_{zy}^2) \right] = \frac{1}{2} \int d\vec{r} \sum_{\alpha\beta} \sigma_{\alpha\beta} e_{\alpha\beta} \quad (1)$$

which shows that the stress-strain relations are

$$\sigma_{\alpha\alpha} = c_{11}e_{\alpha\alpha} + c_{12} \sum_{\beta \neq \alpha} e_{\beta\beta}, \quad \sigma_{\alpha\beta} = 2c_{44}e_{\alpha\beta} \quad (\alpha \neq \beta), \quad e_{\alpha\beta} \equiv \frac{1}{2} \left(\frac{\partial u_\alpha}{\partial r_\beta} + \frac{\partial u_\beta}{\partial r_\alpha} \right) \quad (2)$$

Introducing these relations in the equations of motion, (12.25), we get

$$\rho \ddot{u}_\alpha = \sum_\beta \frac{\partial \sigma_{\alpha\beta}}{\partial r_\beta} = c_{11} \frac{\partial^2 u_\alpha}{\partial r_\alpha^2} + \sum_{\beta \neq \alpha} \left[c_{12} \frac{\partial^2 u_\beta}{\partial r_\alpha \partial r_\beta} + c_{44} \frac{\partial}{\partial r_\beta} \left(\frac{\partial u_\alpha}{\partial r_\beta} + \frac{\partial u_\beta}{\partial r_\alpha} \right) \right] \quad (3)$$

(b) Introducing a plane-wave solution

$$\vec{u}(\vec{r}, t) = \vec{u}^0 e^{i(\vec{k} \cdot \vec{r} - \omega t)} \quad (4)$$

into these equations (3), we get

$$-\rho \omega^2 u_\alpha^0 = -c_{11} k_\alpha^2 u_\alpha^0 - c_{12} \sum_{\beta \neq \alpha} k_\alpha k_\beta u_\beta^0 - c_{44} \sum_{\beta \neq \alpha} (k_\beta^2 u_\alpha^0 + k_\alpha k_\beta u_\beta^0) \quad (5)$$

leading to the following matrix equation for determining \vec{u}^0 and ω

$$\left(c_{11} k_\alpha^2 + c_{44} \sum_{\beta \neq \alpha} k_\beta^2 - \rho \omega^2 \right) u_\alpha^0 + (c_{12} + c_{44}) \sum_{\beta \neq \alpha} k_\alpha k_\beta u_\beta^0 = 0 \quad (6)$$

(c) In the case of waves propagation along [100], the k -vector is $\vec{k} = (k, 0, 0)$ and the matrix equation is diagonal:

$$\left(c_{11} k^2 - \rho \omega^2 \right) u_1^0 = 0, \quad \left(c_{44} k^2 - \rho \omega^2 \right) u_2^0 = 0, \quad \left(c_{44} k^2 - \rho \omega^2 \right) u_3^0 = 0 \quad (7)$$

The sound velocities are

$$\begin{aligned} c_l &= \frac{\omega}{k} = \sqrt{\frac{c_{11}}{\rho}}, & \vec{u}_0 &\parallel \vec{k} \quad (\text{longitudinal}) \\ c_t &= \frac{\omega}{k} = \sqrt{\frac{c_{44}}{\rho}}, & \vec{u}_0 &\perp \vec{k} \quad (\text{transverse}) \end{aligned} \quad (8)$$

i.e. one longitudinal and two degenerate transverse sound waves. Table 12.1 shows that $c_{11} = 165$ GPa, $c_{44} = 79.24$ GPa, and $c_{12} = 64$ GPa in the case of silicon. From the periodic table: the atomic density is $n = 4.99 \cdot 10^{22} \text{ cm}^{-3}$ and the atomic mass is 28.09 u implying $\rho = 28.09 \times 1.66054 \cdot 10^{-27} [\text{kg}] \times 4.99 \cdot 10^{28} [\text{m}^{-3}] = 2328 \text{ kg/m}^3$. Introducing these numbers in (8), we get

$$c_l = \underline{8420 \text{ m/s}}, \quad c_t = \underline{5830 \text{ m/s}} \quad (9)$$

(d) Waves propagating along [111], in which case we assume $\vec{k} = (k/\sqrt{3})(1, 1, 1)$, and the eigenvalue equation for determining $\lambda = \rho\omega^2$ is found to be

$$\begin{pmatrix} A - \lambda & B & B \\ B & A - \lambda & B \\ B & B & A - \lambda \end{pmatrix} \begin{pmatrix} u_1^0 \\ u_2^0 \\ u_3^0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (10a)$$

where

$$\lambda = \rho\omega^2, \quad A = \frac{1}{3}(c_{11} + 2c_{44})k^2, \quad B = \frac{1}{3}(c_{12} + c_{44})k^2 \quad (10b)$$

The characteristic determinant is

$$(A - \lambda) \left((A - \lambda)^2 - B^2 \right) - 2B \left((A - \lambda) - B^2 \right) = (A + 2B - \lambda)(A - B - \lambda)^2 = 0 \quad (11)$$

Introducing the solution $\lambda = A + 2B$ in (10a), we get $u_1^0 = u_2^0 = u_3^0$ or $\vec{u}^0 \parallel \vec{k}$, whereas the two other degenerate solutions $\lambda = A - B$ imply $u_1^0 + u_2^0 + u_3^0 = 0$ or $\vec{u}^0 \cdot \vec{k} = 0$. Hence the sound velocities are

$$\begin{aligned} c_l &= \frac{\omega}{k} = \sqrt{\frac{c_{11} + 2c_{12} + 4c_{44}}{3\rho}} = \underline{9340 \text{ m/s}}, & \vec{u}_0 \parallel \vec{k} & \text{ (longitudinal)} \\ c_t &= \frac{\omega}{k} = \sqrt{\frac{c_{11} - c_{12} + c_{44}}{3\rho}} = \underline{5080 \text{ m/s}}, & \vec{u}_0 \perp \vec{k} & \text{ (transverse)} \end{aligned} \quad (12)$$

Solutions to the problems in Chapter 17

17.4 AC conductivity

In the presence of a time-dependent (uniform) electrical field

$$\vec{E} = \vec{E}_0 e^{-i\omega t} \quad (1)$$

we may use the general solution of the Boltzmann equation given by (17.24), before the integration with respect to t' is performed:

$$g = f - \int_{-\infty}^t dt' e^{(t'-t)/\tau_\varepsilon} e^{-i\omega t'} \vec{v}_{\vec{k}} \cdot \vec{E}_0 e \frac{\partial f(t')}{\partial \mu} \quad (2)$$

Considering only effects which are linear in the applied field (the linearized solution of the Boltzmann equation), then $\vec{v}_{\vec{k}} = \vec{v}_{\vec{k}}(t')$ and $f(t')$ within the integral may be replaced by their time-independent equilibrium values at zero field, and the time integration may be performed straightforwardly

$$g = f - \frac{\tau_\varepsilon}{1 - i\omega\tau_\varepsilon} \vec{v}_{\vec{k}} \cdot \vec{E}_0 e \frac{\partial f}{\partial \mu} e^{-i\omega t} = f - \frac{\tau_\varepsilon}{1 - i\omega\tau_\varepsilon} \vec{v}_{\vec{k}} \cdot \vec{E} e \frac{\partial f}{\partial \mu} \quad (3)$$

Introducing this expression into (17.43)-(17.44) we get the frequency-dependent conductivity (valid in the limit of $\vec{E}_0 \rightarrow \vec{0}$)

$$\sigma_{\alpha\beta}(\omega) = e^2 \int [d\vec{k}] \frac{\tau_\varepsilon}{1 - i\omega\tau_\varepsilon} v_\alpha v_\beta \frac{\partial f}{\partial \mu} \quad (4)$$

or in the case of a cubic or an isotropic (free electron) system:

$$\sigma(\omega) = \frac{ne^2}{m^*} \frac{\tau}{1 - i\omega\tau} = \frac{ne^2\tau}{m^*} \frac{1 + i\omega\tau}{1 + (\omega\tau)^2} \quad (5)$$

17.5 Current driven by thermal gradient

We shall consider a metal subject to a constant temperature gradient

$$\nabla T = \left(\frac{\partial T}{\partial x}, 0, 0 \right) \quad \text{and} \quad \varepsilon_{\vec{k}} = \varepsilon_k = \frac{1}{2} m^* \bar{v}_k^2 \quad (1)$$

According to (17.60), (17.62), and (17.68) the electrical current, in the case of $G = 0$, is

$$\vec{j} = \mathbf{L}^{12} \left(-\frac{\nabla T}{T} \right), \quad \mathbf{L}^{12} = -\frac{1}{e} \mathcal{L}^{(1)} = -\frac{1}{e} \frac{\pi^2}{3} (k_B T)^2 \bar{\sigma}'(\varepsilon_F) \quad (2)$$

The assumption of an isotropic mass, (1), implies $\bar{\sigma}(\varepsilon)$ to be diagonal, and according to (17.64) the diagonal element is

$$\sigma_{\alpha\alpha}(\varepsilon) = e^2 \tau \int d\vec{k} D_{\vec{k}} v_{\vec{k}\alpha}^2 \delta(\varepsilon - \varepsilon_{\vec{k}}) = e^2 \tau \int d\varepsilon_k D(\varepsilon_k) \frac{1}{3} \bar{v}_k^2 \delta(\varepsilon - \varepsilon_k) \quad (3)$$

The integration of $v_{\vec{k}\alpha}^2$ over all solid angles, at a constant $|\vec{k}|$, is 1/3 of the result deriving from $\text{Tr} v_{\vec{k}\alpha}^2 = \bar{v}_k^2$ and using $\bar{v}_k^2 = 2\varepsilon_k/m^*$, we get

$$\sigma_{\alpha\alpha}(\varepsilon) = e^2 \tau D(\varepsilon) \frac{2\varepsilon}{3m^*} \quad \Rightarrow \quad \sigma'_{\alpha\alpha}(\varepsilon) = \frac{2e^2 \tau}{3m^*} [D(\varepsilon) + \varepsilon D'(\varepsilon)] \quad (4)$$

This result is introduced in (2)

$$\vec{j} = \frac{1}{e} \frac{\pi^2}{3} (k_B T)^2 \frac{2e^2 \tau}{3m^*} D(\varepsilon_F) \left(1 + \varepsilon_F \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} \right) \frac{\nabla T}{T} \quad (5)$$

In terms of the heat capacity $c_V = (\pi^2/3) k_B^2 T D(\varepsilon_F)$, (6.77), we finally get

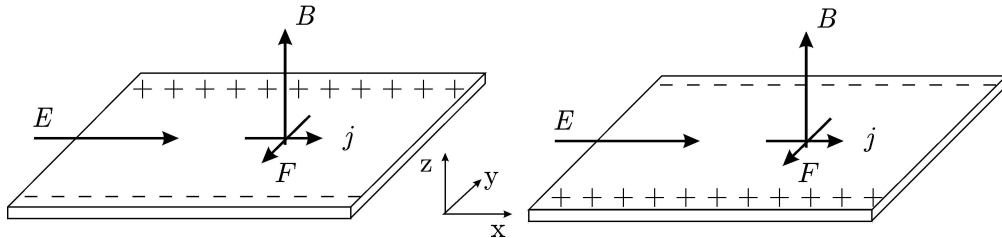
$$j_x = \frac{2e\tau c_V}{3m^*} \frac{\partial T}{\partial x} \left(1 + \varepsilon_F \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} \right) = \frac{e\tau c_V}{m^*} \frac{\partial T}{\partial x} \quad (6)$$

where the last equality sign is valid only if $D(\varepsilon) \propto \sqrt{\varepsilon}$.

17.8 Hall effect – elementary argument

a) Electrons

b) Holes



The Hall effect geometry: The applied field \vec{E} is along the x axis leading to a current \vec{j} in this direction, i.e. an electron (hole) current in the minus (plus) x direction. The magnetic part of the Lorentz force $\vec{F} \propto \vec{j} \times \vec{B}$ is in the minus y direction, when \vec{B} is along z , leading to opposite signs of the resulting charge distributions in the electron and hole cases.

(a) The equation of motion, when assuming the Drude model, is

$$m\dot{\vec{v}} = -e \left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B} \right) - \frac{m\vec{v}}{\tau} \quad (1)$$

in the case of electrons with charge $-e$. Using $\vec{B} = (0, 0, B)$, then we get $\vec{v} \times \vec{B} = (v_y B, -v_x B, 0)$ and since the current, by geometry, is constrained to be along x , the steady state is characterized by v_x being constant and $v_y = 0$. These conditions imply

$$m\dot{v}_y = -e \left(E_y - \frac{v_x B}{c} \right) - 0 = 0 \quad \Rightarrow \quad E_y = \frac{v_x B}{c} \quad (2)$$

(b) The current is $\vec{j} = (j_x, 0, 0)$ with $j_x = -nev_x$, and the Hall coefficient is

$$\mathcal{R} = \frac{E_y}{B j_x} = \frac{v_x B}{c} \frac{1}{B(-nev_x)} = -\frac{1}{nec}, \quad E_y = \mathcal{R} B j_x \quad (3)$$

The electric field in the x direction may be determined from $\dot{v}_x = 0$, or

$$m\dot{v}_x = -eE_x - \frac{mv_x}{\tau} = 0 \quad \Rightarrow \quad E_x = -\frac{me}{\tau} v_x = -\frac{me}{\tau} \frac{j_x}{(-ne)} = \frac{m j_x}{ne^2 \tau} = \frac{j_x}{\sigma} \quad (4)$$

i.e. E_x is determined by the Drude resistivity σ^{-1} as in the case of $B = 0$.

17.9 Hall effect – Boltzmann equation

The Boltzmann equation in the relaxation-time approximation is given by (17.17) and (17.18)

$$\frac{dg}{dt} = \frac{\partial g}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial g}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial g}{\partial \vec{k}} = -\frac{g-f}{\tau} \quad (1)$$

When the state is uniform in space and steady in time, this equation reduces to

$$\dot{\vec{k}} \cdot \frac{\partial g}{\partial \vec{k}} = -\frac{g-f}{\tau} \quad (2)$$

The semiclassical equation of motion is

$$\dot{\hbar\vec{k}} = -e \left(\vec{E} + \frac{1}{c} \vec{v}_{\vec{k}} \times \vec{B} \right), \quad \vec{v}_{\vec{k}} = \dot{\vec{r}} = \frac{1}{\hbar} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} = \frac{\hbar\vec{k}}{m^*} \quad (3)$$

where the second equation expresses that the mass tensor is assumed to be isotropic for simplicity. Like in Problem 17.4 we are only interested in the response (current) which is linear in the electric field. This means that g may be replaced by f in products on the left hand side of (2) which already involve \vec{E} . The linearized version of the Boltzmann equation (2) is therefore

$$-\frac{e}{\hbar} \vec{E} \cdot \frac{\partial f}{\partial \vec{k}} - \frac{e}{\hbar c} \vec{v}_{\vec{k}} \times \vec{B} \cdot \frac{\partial (g-f)}{\partial \vec{k}} = -\frac{g-f}{\tau} \quad (4)$$

when using that $\vec{v}_{\vec{k}} \times \vec{B} \cdot \frac{\partial f}{\partial \vec{k}} = 0$ because $\frac{\partial f}{\partial \vec{k}}$ is parallel with $\vec{v}_{\vec{k}}$, as

$$\frac{\partial f}{\partial \vec{k}} = \frac{\partial f}{\partial \varepsilon_{\vec{k}}} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} = -\frac{\partial f}{\partial \mu} \hbar \vec{v}_{\vec{k}} \quad (5)$$

(a) The geometry is the same as applied in problem 17.8, hence we define $\vec{B} = (0, 0, B)$ and assume the resulting $\vec{E} = (E_x, E_y, 0)$ to be perpendicular to \vec{B} . In this geometry, we guess that the solution has the form

$$g = f + a k_x + b k_y \quad (6)$$

Introducing this in eq. (4) and utilizing (5), we get

$$\frac{e\hbar}{m^*} \frac{\partial f}{\partial \mu} (E_x k_x + E_y k_y) - \frac{eB}{m^*c} (a k_y - b k_x) = -\frac{a k_x + b k_y}{\tau} \quad (7)$$

Since k_x and k_y are independent variables, this equation leads to two independent conditions, which determine a and b to be

$$a = \frac{E_x - \omega_c \tau E_y}{1 + (\omega_c \tau)^2} \left(-\frac{e\hbar\tau}{m^*} \right) \frac{\partial f}{\partial \mu}, \quad b = \frac{E_y + \omega_c \tau E_x}{1 + (\omega_c \tau)^2} \left(-\frac{e\hbar\tau}{m^*} \right) \frac{\partial f}{\partial \mu} \quad (8)$$

where we have introduced the cyclotron frequency $\omega_c = \frac{eB}{m^*c}$.

The α component of the current density \vec{j} is, according to Marder's eq. (17.43),

$$\begin{aligned} j_\alpha &= -e \int [d\vec{k}] v_{k\alpha}^- (g_{\vec{k}} - f_{\vec{k}}) = -e \int [d\vec{k}] v_{k\alpha}^- (a k_x + b k_y) \\ &= -\frac{em^*}{\hbar} \int [d\vec{k}] (a v_{kx}^2 \delta_{\alpha x} + b v_{ky}^2 \delta_{\alpha y}) \end{aligned} \quad (9)$$

where the last equality sign follows because the off-diagonal terms vanish, when the mass tensor is assumed to be diagonal (isotropic). Using the same procedure as in Marder's eqs. (17.44)-(17.50), we have

$$-\frac{em^*}{\hbar} \int [d\vec{k}] v_{k\alpha}^2 \left(-\frac{e\hbar\tau}{m^*} \right) \frac{\partial f}{\partial \mu} = e^2 \tau \int [d\vec{k}] v_{k\alpha}^2 \frac{\partial f}{\partial \mu} = \frac{ne^2\tau}{m^*} \equiv \sigma_0 \quad (10)$$

and combining the three equations (8)-(10), we finally get

$$j_x = \frac{E_x - \omega_c \tau E_y}{1 + (\omega_c \tau)^2} \sigma_0, \quad j_y = \frac{E_y + \omega_c \tau E_x}{1 + (\omega_c \tau)^2} \sigma_0 \quad (11)$$

In the case where \vec{E} is assumed to be along the z axis parallel to the field, we have to add a term $c_z k_z$ to the trial function g in (6). In this situation, the magnetic field does not contribute to the Boltzmann equation, and we get $j_z = \sigma_0 E_z$. Hence, for a system with an isotropic mass m^* , the total conductivity tensor is found to be

$$\vec{\sigma} = \frac{\sigma_0}{1 + (\omega_c \tau)^2} \begin{pmatrix} 1 & -\omega_c \tau & 0 \\ \omega_c \tau & 1 & 0 \\ 0 & 0 & 1 + (\omega_c \tau)^2 \end{pmatrix}, \quad \omega_c = \frac{eB}{m^*c} \quad (12)$$

when the magnetic field B is applied along the z axis.

This result may also be expressed in terms of the Hall coefficient \mathcal{R} , where

$$\omega_c \tau = -\mathcal{R} B \sigma_0, \quad \text{or} \quad \mathcal{R} = -\frac{1}{nec} \quad (13)$$

The resistivity tensor $\bar{\rho}$, defined by the relation $\vec{E} = \bar{\rho}\vec{j}$, is the inverse of the conductivity tensor and is particularly simple

$$\bar{\rho} = \bar{\sigma}^{-1} = \frac{1}{\sigma_0} \begin{pmatrix} 1 & \omega_c\tau & 0 \\ -\omega_c\tau & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{\sigma_0} \begin{pmatrix} 1 & -\sigma_0\mathcal{R}B & 0 \\ \sigma_0\mathcal{R}B & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (14)$$

which is in perfect agreement with the results derived from the Drude model (problem 17.8). The calculations in section 17.4.8 assume $\omega_c\tau \gg 1$, in which case the diagonal elements of $\bar{\sigma}$ may be neglected in comparison with the off-diagonal ones, $\sigma_{xx} = \sigma_{yy} \simeq 0$ and $\sigma_{xy} = -\sigma_{yx} \simeq -(\omega_c\tau)^{-1}$.

Solution to HS's problem 3

Hall effect of a two-dimensional electron gas

A two-dimensional electron gas with an anisotropic dispersion

$$\varepsilon = a(k_x^2 + k_y^2) + b(k_x^4 + k_y^4), \quad a > 0, \quad b > 0 \quad (1)$$

Introducing the polar angle θ in the (k_x, k_y) -coordinate system of the reciprocal lattice, the dispersion relation may be written

$$\varepsilon = a k^2 + \frac{1}{4}b(3 + \cos 4\theta)k^4, \quad k_x = k \cos \theta, \quad k_y = k \sin \theta \quad (2)$$

reflecting directly the four-fold, cubic symmetry of the dispersion.

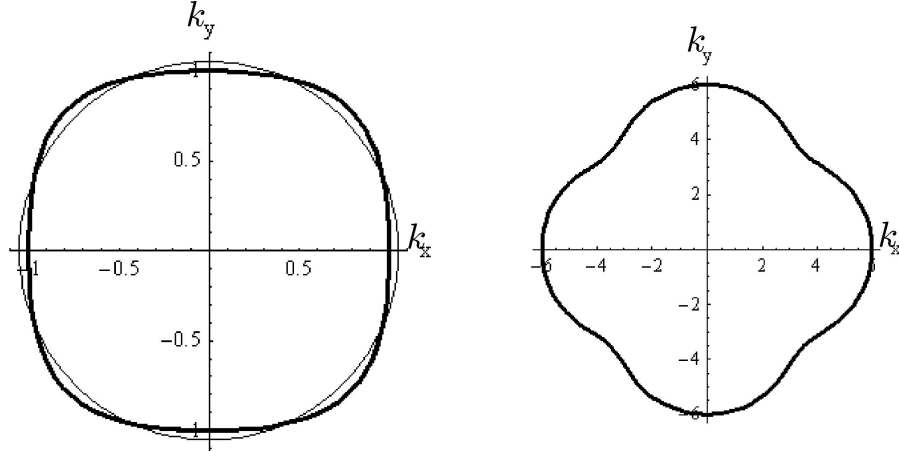
- 1) The equation determining the constant energy contour is obtained by solving (2) with respect to k^2

$$k^2 = k^2(\varepsilon) = \frac{2a}{b(3 + \cos 4\theta)} \left[\left(1 + \frac{b\varepsilon}{a^2}(3 + \cos 4\theta) \right)^{1/2} - 1 \right] \quad (3)$$

In the case of $b\varepsilon \ll a^2$, the square root may be expanded, and to second order ($\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2$) the result is

$$k^2(\varepsilon) \simeq \frac{\varepsilon}{a} \left(1 - \frac{3b\varepsilon}{4a^2} \right) - \frac{b\varepsilon^2}{4a^3} \cos 4\theta \quad (4)$$

In the figure below (to the left) I show a constant energy contour, which differs visible from a circle. It is obtained by a numerical evaluation of (3) (Mathematica program) in the case of $a = b = 1$ and $\varepsilon = 2$ (assuming dimensionless quantities). The thin line shows the average length of $\vec{k}(\varepsilon)$. The figure to the right show the corresponding $|\nabla_{\vec{k}}\varepsilon_{\vec{k}}|$ as a function of the angle θ . The gradient, and hence the velocity $\vec{v}_{\vec{k}} = \nabla_{\vec{k}}\varepsilon_{\vec{k}}/\hbar$, is perpendicular to the constant energy contour. Notice that $|\vec{v}_{\vec{k}}|$ is smallest along the $\langle 11 \rangle$ directions, where $|\vec{k}(\varepsilon)|$ has its maxima.



2) The Boltzmann equation in the relaxation-time approximation, (17.17)-(17.18),

$$\frac{dg}{dt} = \frac{\partial g}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial g}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial g}{\partial \vec{k}} = -\frac{g-f}{\tau} \quad \Rightarrow \quad \dot{\vec{k}} \cdot \frac{\partial g}{\partial \vec{k}} = -\frac{g-f}{\tau} \quad (5)$$

when considering the steady state of a uniform system. The fields are assumed to be $\vec{E} = (E, 0, 0)$ and $\vec{B} = (0, 0, B)$, and the semiclassical equation of motion is

$$\hbar \dot{\vec{k}} = -e \left(\vec{E} + \frac{1}{c} \vec{v}_{\vec{k}} \times \vec{B} \right), \quad \vec{v}_{\vec{k}} = \dot{\vec{r}} = \frac{1}{\hbar} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} \quad (6)$$

Introducing this in the right-hand part of (5) we get

$$-\frac{e}{\hbar} \left(\vec{E} + \frac{1}{c} \vec{v}_{\vec{k}} \times \vec{B} \right) \cdot \left(\frac{\partial(g-f)}{\partial \vec{k}} + \frac{\partial f}{\partial \vec{k}} \right) = -\frac{g-f}{\tau} \quad (7)$$

where

$$\frac{\partial f}{\partial \vec{k}} = \frac{\partial f}{\partial \varepsilon_{\vec{k}}} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} = \hbar \vec{v}_{\vec{k}} \frac{\partial f}{\partial \varepsilon_{\vec{k}}} \quad (8)$$

This gradient is perpendicular to $\vec{v}_{\vec{k}} \times \vec{B}$, and the linearized version of (7) is

$$-e \vec{E} \cdot \vec{v}_{\vec{k}} \frac{\partial f}{\partial \varepsilon_{\vec{k}}} - \frac{e}{\hbar c} \vec{v}_{\vec{k}} \times \vec{B} \cdot \frac{\partial(g-f)}{\partial \vec{k}} = -\frac{g-f}{\tau} \quad (9)$$

Since $(g-f)$ is going to scale with E , the term neglected, $-\frac{e}{\hbar} \vec{E} \cdot \frac{\partial(g-f)}{\partial \vec{k}}$, is of second order in E . Inserting $\vec{E} = (E, 0, 0)$ and $\vec{B} = (0, 0, B)$ in (9), we finally get

$$-e v_x E \frac{\partial f}{\partial \varepsilon_{\vec{k}}} = \left[\frac{eB}{\hbar c} \left(v_y \frac{\partial}{\partial k_x} - v_x \frac{\partial}{\partial k_y} \right) - \frac{1}{\tau} \right] (g-f) \quad (10)$$

3) With the assumption of $g-f = k_y F(\varepsilon)$, we find

$$\begin{aligned} v_y \frac{\partial(g-f)}{\partial k_x} - v_x \frac{\partial(g-f)}{\partial k_y} &= v_y k_y \frac{dF}{d\varepsilon} \frac{\partial \varepsilon}{\partial k_x} - v_x F - v_x k_y \frac{dF}{d\varepsilon} \frac{\partial \varepsilon}{\partial k_y} \\ &= v_y k_y \frac{dF}{d\varepsilon} \hbar v_x - v_x F - v_x k_y \frac{dF}{d\varepsilon} \hbar v_y = -v_x F \end{aligned} \quad (11)$$

When introducing this result in (10) and neglecting $1/\tau$, we get

$$-ev_x E \frac{\partial f}{\partial \varepsilon_{\vec{k}}} = \frac{eB}{\hbar c} [-v_x F(\varepsilon)] \Rightarrow F(\varepsilon) = \frac{\hbar c E}{B} \frac{\partial f}{\partial \varepsilon_{\vec{k}}} \quad (12)$$

The current in the y direction is then

$$\begin{aligned} j_y &= -e \int [d\vec{k}] v_y (g - f) = -\frac{e\hbar c E}{B} \int [d\vec{k}] v_y k_y \frac{\partial f}{\partial \varepsilon_{\vec{k}}} \\ &= -\frac{e\hbar c E}{B} \int dk_x \int dk_y D_{\vec{k}} \frac{\partial \varepsilon_{\vec{k}}}{\partial (\hbar k_y)} k_y \frac{\partial f}{\partial \varepsilon_{\vec{k}}} = -\frac{ecE}{B} \int dk_x \int dk_y D_{\vec{k}} k_y \frac{\partial f}{\partial k_y} \\ &= \frac{ecE}{B} \int dk_x \int dk_y D_{\vec{k}} f = \frac{ecE}{B} \int [d\vec{k}] f = \frac{necE}{B} = -\frac{1}{\mathcal{R}B} E, \quad \mathcal{R} = -\frac{1}{nec} \end{aligned} \quad (13)$$

when performing the y integration by parts, where $D_{\vec{k}} = 2/(2\pi)^2$ is a constant and the boundaries of the integral is the boundaries of the first Brillouin zone. (13) is the usual high-field result for the off-diagonal conductivity $\sigma_{yx} = -1/(\mathcal{R}B)$.

Solutions to the problems in Chapter 22 and 23

22.2 Faraday rotation

The combination of the semiclassical equation of motion and the Drude relaxation-time model leads to the following equation of motion for the electrons (when $\hbar \dot{\vec{k}} = m^* \ddot{\vec{v}} = m^* \ddot{\vec{r}}$)

$$\ddot{\vec{r}} = -\frac{e}{m^* c} \dot{\vec{r}} \times \vec{B} - \frac{e}{m^*} \vec{E} - \frac{\dot{\vec{r}}}{\tau} \quad \text{or} \quad \ddot{\vec{r}} + \frac{\dot{\vec{r}}}{\tau} + \frac{e}{m^* c} \dot{\vec{r}} \times \vec{B} = -\frac{e}{m^*} \vec{E} \quad (1)$$

The (applied) magnetic field is assumed along \hat{z} . The electrical field vector, due to an incident light wave, is assumed to be circular polarized in the plane perpendicular to z

$$\vec{B} = (0, 0, B), \quad \vec{E} = \vec{E}^{\pm} = E_0 (\hat{x} \pm i\hat{y}) e^{-i\omega t} \quad (2)$$

If the light wave propagates in the positive z direction, i.e. $E \propto e^{i(qz - \omega t)}$, then the plus (minus) sign in (2) corresponds to the left (right) circular polarization. In the case of the right circular polarization, the end point of the E -vector is making a right-handed screw line in the direction of propagation at a certain time t (see for instance Griffiths, "Introduction to electrodynamics", p. 374).

(a) Introducing the expressions for the fields in (1), the equation may be solved, with respect to $\dot{\vec{r}}$, by assuming

$$\dot{\vec{r}} = A^{\pm} (\hat{x} \pm i\hat{y}) e^{-i\omega t} \quad (3)$$

Because $(\hat{x} \pm i\hat{y}) \times \hat{z} = -\hat{y} \pm i\hat{x} = \pm i(\hat{x} \pm i\hat{y})$, we get from (1)

$$\left[(-i\omega) + \frac{1}{\tau} \pm i \frac{eB}{m^* c} \right] A^{\pm} (\hat{x} \pm i\hat{y}) e^{-i\omega t} = -\frac{e}{m^*} E_0 (\hat{x} \pm i\hat{y}) e^{-i\omega t} \quad (4)$$

or

$$A^{\pm} = -\frac{eE_0}{m^*} \left[(-i\omega) + \frac{1}{\tau} \pm i \frac{eB}{m^* c} \right]^{-1} = -\frac{eE_0}{m^*} \frac{\tau}{1 - i\omega\tau \pm i\omega_c\tau}, \quad \omega_c = \frac{eB}{m^* c} \quad (5)$$

where ω_c is the cyclotron frequency (section 21.2). The current density and the conductivity tensor are determined from

$$\vec{j} = -ne\dot{\vec{r}}, \quad \vec{j} = \vec{\sigma} \vec{E} \quad (6)$$

The calculations show that $\dot{\vec{r}} = (A^\pm/E_0)\vec{E}$ and defining $\vec{j}^\pm = j_0(\hat{x} \pm i\hat{y})$, then $\vec{j}^+ = \sigma_{++}\vec{E}^+ + \sigma_{+-}\vec{E}^- = \sigma^+\vec{E}^+$ and $\vec{j}^- = \sigma_{-+}\vec{E}^+ + \sigma_{--}\vec{E}^- = \sigma^-\vec{E}^-$. The current has the same circular polarization as the electric field, i.e. the conductivity tensor is diagonal with respect to the choice of sign, $\sigma_{+-} = \sigma_{-+} = 0$. The diagonal components are ($\sigma_{++} \equiv \sigma^+$ and $\sigma_{--} \equiv \sigma^-$)

$$\sigma^\pm = -ne \frac{A^\pm}{E_0} = \frac{\sigma_0}{1 - i\omega\tau \pm i\omega_c\tau}, \quad \sigma_0 = \frac{ne^2\tau}{m^*} \quad (7)$$

(b) In the case of $\omega\tau \gg 1$ and $\omega \gg \omega_c$, we get

$$\sigma^\pm = \frac{\sigma_0}{1 - i\omega\tau \pm i\omega_c\tau} = \frac{\sigma_0}{(-i\omega\tau)} \left[1 + \frac{i}{\omega\tau} \mp \frac{\omega_c}{\omega} \right]^{-1} \simeq \frac{i\sigma_0}{\omega\tau} \left(1 - \frac{i}{\omega\tau} \pm \frac{\omega_c}{\omega} \right) \quad (8)$$

(c) The dielectric constant, (20.14), is

$$\epsilon^\pm = 1 + \frac{4\pi i}{\omega} \sigma^\pm \simeq 1 - \frac{\omega_p^2}{\omega^2} \left(1 - \frac{i}{\omega\tau} \pm \frac{\omega_c}{\omega} \right) \quad (9)$$

where ω_p is the plasma frequency introduced by (20.32) or (23.7)

$$\omega_p^2 = \frac{4\pi ne^2}{m^*} = \frac{4\pi\sigma_0}{\tau} \quad (10)$$

The index of refraction, (20.18), is

$$\tilde{n}_\pm = \bar{n}_\pm + i\kappa_\pm = \sqrt{\epsilon^\pm} \simeq 1 - \frac{\omega_p^2}{2\omega^2} \left(1 - \frac{i}{\omega\tau} \pm \frac{\omega_c}{\omega} \right), \quad \omega \gg \omega_p \quad (11)$$

The Faraday rotation θ of the polarization vector per unit length along the sample is then found to be

$$\theta = \frac{\omega}{2c} (\bar{n}_- - \bar{n}_+) = \frac{\omega}{2c} \cdot 2 \frac{\omega_p^2}{2\omega^2} \frac{\omega_c}{\omega} = \frac{\omega_p^2 \omega_c}{2c\omega^2} \quad (12)$$

Notice, that the sign of θ is determined by the sign of ω_c , or B , i.e. if \vec{B} is along the negative z direction then θ is negative. If the active carriers are holes rather than electrons, we may perform exactly the same calculation except that e is replaced by $-e$ in all expressions (m^* is then the positive hole mass), hence the sign of θ , like the Hall voltage, depends on the kind of carriers.

Derivation of the expression for the Faraday rotation angle: Assuming the incident light wave to be linearly polarized along the x axis at $z = 0$, then we want to find the angle of rotation of the polarization vector in the xy plane as a function of z .

$$\vec{E}(z)/E_0 = \frac{1}{2}(\hat{x} + i\hat{y})e^{i(q_+z - \omega t)} + \frac{1}{2}(\hat{x} - i\hat{y})e^{i(q_-z - \omega t)} \quad (13)$$

At $z = 0$, the polarization vector is parallel to \hat{x} , $\vec{E}(0)/E_0 = \hat{x}e^{-i\omega t}$. Introducing $\psi = \frac{1}{2}(q_+ + q_-)z$ and $\Delta\psi = \frac{1}{2}(q_+ - q_-)z$, or $q_+z = \psi + \Delta\psi$ and $q_-z = \psi - \Delta\psi$, then we get

$$\vec{E}(z)/E_0 = \left[\frac{1}{2}(\hat{x} + i\hat{y})e^{i\Delta\psi} + \frac{1}{2}(\hat{x} - i\hat{y})e^{-i\Delta\psi} \right] e^{i(\psi - \omega t)} \quad (14)$$

The polarization vector at z is determined by the factor in the square bracket, which is found to be

$$\frac{1}{2}(\hat{x} + i\hat{y})(\cos \Delta\psi + i \sin \Delta\psi) + \frac{1}{2}(\hat{x} - i\hat{y})(\cos \Delta\psi - i \sin \Delta\psi) = \hat{x} \cos \Delta\psi - \hat{y} \sin \Delta\psi$$

This expression shows that the polarization vector at z is making the angle $\theta z = -\Delta\psi = -\frac{1}{2}(q_+ - q_-)z$ with the x axis. According to (20.18) $q_{\pm} = \omega\bar{n}_{\pm}/c$, and the rotation angle per unit length, along the direction of light propagation, is

$$\theta = -\frac{1}{2}(q_+ - q_-) = \frac{\omega}{2c}(\bar{n}_- - \bar{n}_+) \quad (15)$$

In the case where the carriers are electrons, then $\theta > 0$, which sign corresponds to a counter-clockwise or left-handed rotation of the polarization vector along z .

23.3 Helicon waves

(a) From the Maxwell equations (23.71) and (23.72) we find

$$-c \nabla \times (\nabla \times \vec{E}) = \nabla \times \frac{\partial B}{\partial t} = \frac{1}{c} \frac{\partial^2 \vec{E}}{\partial t^2} + \frac{4\pi}{c} \frac{\partial \vec{j}}{\partial t} = \frac{1}{c} \frac{\partial^2 \vec{E}}{\partial t^2} + \frac{4\pi\bar{\sigma}}{c} \frac{\partial \vec{E}}{\partial t} \quad (1)$$

when utilizing the linear relation $\vec{j}(\omega) = \bar{\sigma}(\omega)\vec{E}(\omega)$. Assuming

$$\vec{E} = \vec{E}_0 e^{i(\vec{k}\cdot\vec{r} - \omega t)}, \quad \vec{k} = (0, 0, k), \quad k_0 \equiv \frac{\omega}{c} \quad (2)$$

we get from the left- and right-hand sides of (1)

$$-c(i\vec{k}) \times ((i\vec{k}) \times \vec{E}) = \frac{1}{c}(-i\omega)^2 \vec{E} + \frac{4\pi\bar{\sigma}}{c}(-i\omega)\vec{E} = -\frac{\omega^2}{c} \left(\bar{1} + i\frac{4\pi\bar{\sigma}}{\omega} \right) \vec{E} = -\frac{\omega^2}{c} \bar{\epsilon} \vec{E} \quad (3)$$

when introducing the dielectric tensor $\bar{\epsilon}$, (20.14). Leaving out the common phase factor, we finally get

$$\vec{k} \times (\vec{k} \times \vec{E}_0) + k_0^2 \bar{\epsilon} \vec{E}_0 = \vec{0} \quad (4)$$

(b) Symmetry analysis of the relation $\vec{j} = \bar{\sigma} \vec{E}$: The conducting sample is assumed to be isotropic (in the shape of a sphere, if surface effects are of importance). In the presence of a magnetic field $\vec{B} = B\hat{z}$, the sample, or alternatively the coordinate axes, may be rotated any angle around the z axis without changing the coordinate representation (the matrix equation) for the tensor relation between \vec{j} and \vec{E} . If the coordinate axes are rotated by an angle of 90 degrees around the z axis, then (j_x, j_y, j_z) is renamed $(-j_y, j_x, j_z)$ and (E_x, E_y, E_z) is replaced by $(-E_y, E_x, E_z)$, whereas the components $\sigma_{\alpha\beta}$ determined by the sample are kept unchanged:

$$\begin{cases} j_x = \sigma_{xx}E_x + \sigma_{xy}E_y + \sigma_{xz}E_z \\ j_y = \sigma_{yx}E_x + \sigma_{yy}E_y + \sigma_{yz}E_z \\ j_z = \sigma_{zx}E_x + \sigma_{zy}E_y + \sigma_{zz}E_z \end{cases} \rightarrow \begin{cases} -j_y = -\sigma_{xx}E_y + \sigma_{xy}E_x + \sigma_{xz}E_z \\ j_x = -\sigma_{yx}E_y + \sigma_{yy}E_x + \sigma_{yz}E_z \\ j_z = -\sigma_{zx}E_y + \sigma_{zy}E_x + \sigma_{zz}E_z \end{cases} \quad (5)$$

A comparison of the two sets of relations then shows that $\sigma_{xx} = \sigma_{yy}$, $\sigma_{xy} = -\sigma_{yx}$, and $\sigma_{zx} = \sigma_{zy} = \sigma_{xz} = \sigma_{yz} = 0$.

[Extension of the symmetry arguments: At zero field, the isotropic sample is insensitive to a rotation around any arbitrary direction and $\sigma_{\alpha\beta} = \sigma_{xx}\delta_{\alpha\beta}$, which result shows that $\sigma_{xy} \rightarrow 0$ when $B \rightarrow 0$. A reflection of the system with respect to, for instance, the yz plane implies that the axial vector \vec{B} along \hat{z} is reversed, whereas it is the x components of the polar vectors \vec{j} and \vec{E} which change sign. Because of this different behaviour of the polar and axial vectors it is straightforwardly shown that σ_{xy} changes sign if \vec{B} is reversed, whereas nothing happens with the diagonal elements. This symmetry element is in accordance with the general *Onsager relation* $\sigma_{\alpha\beta}(-B) = \sigma_{\beta\alpha}(B)$. Hence, in the case of an isotropic sample the diagonal components may only involve terms quadratic (even powers) in B , whereas the off-diagonal ones are linear (of odd powers) in B .]

These symmetry relations are consistent with the results obtained in the previous problems 17.9 and 22.2, and they apply as well for the dielectric tensor $\bar{\epsilon}$, or

$$\bar{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & 0 \\ -\epsilon_{xy} & \epsilon_{xx} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix} \quad (6)$$

Introducing this in (4) in combination with $\vec{k} \times (\vec{k} \times \vec{E}_0) = -k^2\vec{E}_0 + \vec{k}(\vec{k} \cdot \vec{E}_0)$, the result is

$$\begin{pmatrix} -k^2 + \epsilon_{xx}k_0^2 & \epsilon_{xy}k_0^2 & 0 \\ -\epsilon_{xy}k_0^2 & -k^2 + \epsilon_{xx}k_0^2 & 0 \\ 0 & 0 & \epsilon_{zz}k_0^2 \end{pmatrix} \begin{pmatrix} E_x^0 \\ E_y^0 \\ E_z^0 \end{pmatrix} = \vec{0} \quad (7)$$

which only has a non-zero solution for \vec{E}_0 , if the characteristic determinant vanishes, or if

$$\epsilon_{zz} \left[\left((k/k_0)^2 - \epsilon_{xx} \right)^2 + \epsilon_{xy}^2 \right] = 0 \quad (8)$$

We are going to utilize the solution of problem 22.2 in the following. Here σ^\pm is defined by the vector relation $\vec{j}^\pm = \sigma^\pm \vec{E}^\pm$ in the xy plane, or

$$j_x + ij_y = \begin{cases} \sigma^+(E_x + iE_y) \\ \sigma_{xx}E_x + \sigma_{xy}E_y + i(-\sigma_{xy}E_x + \sigma_{xx}E_y) = (\sigma_{xx} - i\sigma_{xy})(E_x + iE_y) \end{cases} \quad (9)$$

showing that $\sigma^+ = \sigma_{xx} - i\sigma_{xy}$ and correspondingly, (9) in the solution of 22.2,

$$\epsilon^\pm = \epsilon_{xx} \mp i\epsilon_{xy} \Rightarrow \epsilon_{xx} = \frac{1}{2}(\epsilon^+ + \epsilon^-), \quad \epsilon_{xy} = \frac{1}{2}(\epsilon^+ - \epsilon^-)i \quad (10)$$

The latter relations reduce (8) to the diagonal form

$$\epsilon_{zz} \left[(k/k_0)^2 - \epsilon^+ \right] \left[(k/k_0)^2 - \epsilon^- \right] = 0 \quad (11)$$

(c) The situation is exactly the one considered in problem 22.2, and the result found there is [combining (8) and (9) in the solution of 22.2]

$$\begin{aligned} \epsilon^\pm &= 1 + \frac{4\pi i}{\omega} \frac{\sigma_0}{1 - i\omega\tau \pm i\omega_c\tau} = 1 + i \frac{\omega_p^2}{\omega} \frac{\tau}{1 - i\omega\tau \pm i\omega_c\tau} \\ &= 1 + \frac{\omega_p^2}{\omega} \frac{1}{\frac{1}{i\tau} - \omega \pm \omega_c} = 1 - \frac{\omega_p^2}{\omega} \frac{1}{\tilde{\omega} \mp \omega_c}, \quad \tilde{\omega} = \omega + \frac{i}{\tau} \end{aligned} \quad (12)$$

or finally

$$\epsilon^{\pm} = 1 - \frac{\omega_p^2}{\omega\tilde{\omega}} \frac{1 \pm (\omega_c/\tilde{\omega})}{1 - (\omega_c/\tilde{\omega})^2}, \quad \omega_c = \frac{eB}{m^*c}, \quad \omega_p^2 = \frac{4\pi\sigma_0}{\tau} = \frac{4\pi ne^2}{m^*} \quad (13)$$

which result agrees with the expression for $\epsilon_{xx} = (\epsilon^+ + \epsilon^-)/2$ given by (23.82).

(d) The atomic density (front page) of aluminium metal is $6.02 \cdot 10^{22} \text{ cm}^{-3}$. According to Table 6.1, the number of conduction electrons per atom is 3, i.e. the electron density in Al^{3+} -metal is $n = 18.06 \cdot 10^{22} \text{ cm}^{-3}$. The cyclic plasma frequency is $\omega_p = 5.64(15) \cdot 10^{15} \text{ rad/s}$, when $n = 10^{22} \text{ cm}^{-3}$ and $m^* = m$, see (23.3). [Incidentally, the unit of a cyclic frequency is **not** Hz but rad/s or just s^{-1} . The unit Hz (hertz) is reserved for the case of cycles per second, $\nu = \omega/(2\pi)$.] In the case of Al-metal,

$$\omega_p = 24 \cdot 10^{15} \text{ s}^{-1}, \quad \nu_p = 3.8 \cdot 10^{15} \text{ Hz}, \quad \hbar\omega_p = 16 \text{ eV} \quad (14)$$

The cyclotron frequency may be expressed in terms of the fundamental magnetic quantity, the Bohr magneton:

$$\mu_B = \frac{e\hbar}{2mc} = 5.788383 \cdot 10^{-9} \text{ eV/G} \quad \Rightarrow \quad \hbar\omega_c = \hbar \frac{eB}{m^*c} = 2 \frac{m}{m^*} \mu_B B \quad (15)$$

Assuming $m^* = m$ and $B = 1 \text{ T} = 10 \text{ kG} = 10^4 \text{ G}$, we get

$$\hbar\omega_c = 0.12 \text{ meV}, \quad \nu_c = 2.8 \cdot 10^{10} \text{ Hz}, \quad \omega_c = 18 \cdot 10^{10} \text{ s}^{-1} \quad (16)$$

The numbers show that $\omega_c \simeq 10^{-5}\omega_p \ll \omega_p$. In the case of $\omega \approx \omega_c$, the fraction in the expression for ϵ^{\pm} is of the order of 10^{10} , and the adding of one to this fraction has no effect at all.

(e) Assuming $\omega \ll \omega_p$ we get from equation (12)

$$\epsilon^{\pm} = -\frac{\omega_p^2}{\omega(\omega \mp \omega_c + \frac{i}{\tau})} \simeq -\frac{\omega_p^2}{\omega(\omega \mp \omega_c)}, \quad \omega_c\tau \gg 1 \quad (17)$$

In most cases $\epsilon^{\pm} < 0$, which implies a purely imaginary refraction index $\tilde{n} = \sqrt{\epsilon}$ and therefore no light propagation. However, there is one situation, where electromagnetic waves with $\omega \ll \omega_p$ are capable to propagate through the sample, which one is determined by the solution ϵ^+ , when $\omega < \omega_c$ (or ϵ^- if the carriers are holes). Hence, when placing a metal like aluminium in a strong magnetic field, it is possible for low-frequency light to propagate through the metal, but low temperature and high purity is demanded in order to secure that the damping is small, $\omega_c\tau \gg 1$.

The dispersion relation for these ‘‘helicon’’ waves is determined by (11) and (17):

$$k^2 = k_0^2 \epsilon^+ = \left(\frac{\omega}{c}\right)^2 \frac{\omega_p^2}{\omega(\omega_c - \omega)} \quad \Rightarrow \quad \omega = \frac{\omega_c (ck)^2}{\omega_p^2 + (ck)^2} \simeq \frac{\omega_c}{\omega_p^2} (ck)^2, \quad k \ll \frac{\omega_p}{c} \quad (18)$$

showing that the dispersion is not linear but quadratic in k in the long wavelength limit. The name of the waves is a derivative of ‘‘helix’’ and refers to the circular polarization of the waves (ϵ^+ corresponds to left circular polarization) – the polarization vector of the helicon wave is forming a helix along the z direction.

The helicon resonance is related to the Hall effect, and the result may be written in a simple form in terms of the Hall coefficient $\mathcal{R} = -(nec)^{-1}$:

$$\omega = \frac{B|\mathcal{R}|}{4\pi}(ck)^2 \quad (\text{cgs-Gaussian units}) \quad (19)$$

In the experiments of, for instance, R. Bowers, C. Legendy and F. Rose, Phys. Rev. Lett. **7**, 339 (1961), wavelengths of the order of 1 cm are considered. In the case of Al-metal, $\lambda = 1$ cm corresponds to a helicon frequency of $\nu = 1.77$ Hz at $B = 10$ kG. In sodium ($n = 2.54 \cdot 10^{22} \text{ cm}^{-3}$) this frequency is 12.3 Hz. Bowers *et al.* observed a standing wave resonance in a Na sample of length $l = 4$ mm at 32 Hz and 10 kG. The resonance condition is $l = \lambda/2$, and our simple model predicts $\lambda/2$ to be about 3.1 mm at the same frequency and field.

Solutions to the problems in Chapter 24

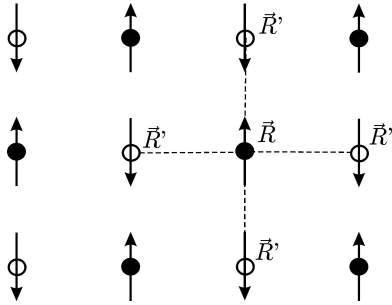
24.4 Mean field theory

The antiferromagnetic two-dimensional Ising model on a square lattice. In this lattice, the number of nearest neighbours is $z = 4$. The Hamiltonian is supposed to be

$$\mathcal{H} = - \sum_{\langle \vec{R}\vec{R}' \rangle} J \sigma_{\vec{R}} \sigma_{\vec{R}'} - \sum_{\vec{R}} H \mu_B \sigma_{\vec{R}} = -\frac{1}{2} \sum_{\vec{R}\vec{R}'} J \sigma_{\vec{R}} \sigma_{\vec{R}'} - \sum_{\vec{R}} H \mu_B \sigma_{\vec{R}}, \quad J < 0 \quad (1)$$

where $\mathcal{H} = \mathcal{E}$ in the usual representation of $\sigma_{\vec{R}} = \pm 1$. Because J is negative, the ground state is not the ferro- but the antiferromagnet. In the sums, \vec{R} and \vec{R}' are nearest neighbours, and the antiferromagnetic ground state is assumed to be determined by the mean field values

$$\langle \sigma_{\vec{R}}, \langle \sigma_{\vec{R}'} \rangle = \begin{cases} (\sigma_{\uparrow}, \sigma_{\downarrow}), & \vec{R} \in \text{sublattice A} \\ (\sigma_{\downarrow}, \sigma_{\uparrow}), & \vec{R} \in \text{sublattice B} \end{cases} \quad (2)$$



The two sublattices of the square lattice: A shown by filled and B by open circles. The figure shows the case, where the site at \vec{R} belongs to the A -sublattice, in which case $\langle \sigma_{\vec{R}} \rangle = \sigma_{\uparrow}$. Its four nearest neighbours at positions \vec{R}' , then all belong to the B sublattice and $\langle \sigma_{\vec{R}'} \rangle = \sigma_{\downarrow}$.

(a) In the mean-field (MF) approximation we get, when inserting (2) in (1),

$$\begin{aligned} \mathcal{E}^{\text{MF}} &= -\frac{1}{2} \sum_{\vec{R}\vec{R}'} J (\sigma_{\vec{R}} \langle \sigma_{\vec{R}'} \rangle + \sigma_{\vec{R}'} \langle \sigma_{\vec{R}} \rangle - \langle \sigma_{\vec{R}} \rangle \langle \sigma_{\vec{R}'} \rangle) - H \mu_B \sum_{\vec{R}} \sigma_{\vec{R}} \\ &= - \sum_{\vec{R}\vec{R}'} J \langle \sigma_{\vec{R}'} \rangle \sigma_{\vec{R}} - H \mu_B \sum_{\vec{R}} \sigma_{\vec{R}} + \frac{1}{2} N z J \sigma_{\uparrow} \sigma_{\downarrow} \\ &= - \sum_{\vec{R} \in A}^{N/2} (z J \sigma_{\downarrow} + \mu_B H) \sigma_{\vec{R}} - \sum_{\vec{R} \in B}^{N/2} (z J \sigma_{\uparrow} + \mu_B H) \sigma_{\vec{R}} + \frac{1}{2} N z J \sigma_{\uparrow} \sigma_{\downarrow} \end{aligned} \quad (3)$$

Because of the MF-approximation, the total energy $\mathcal{E} = \sum_{\vec{R}} \mathcal{E}_{\vec{R}}$ is the sum of the individual contributions of each site, and the partition function of the total system

$$Z = \sum_{\text{all } \mathcal{E}} e^{-\beta \mathcal{E}} = \prod_{\vec{R}} \left(\sum_{\text{all } \mathcal{E}_{\vec{R}}} e^{-\beta \mathcal{E}_{\vec{R}}} \right) = \prod_{\vec{R}} Z_{\vec{R}} \quad (4)$$

is reduced so to become the product of the partition functions $Z_{\vec{R}}$ for the individual sites, see for instance (6.40). For the sites, where \vec{R} belongs to the sublattice A (\uparrow), we get, when omitting the constant energy term $\frac{1}{2}zJ\sigma_{\uparrow}\sigma_{\downarrow}$,

$$Z_{\uparrow} = \sum_{\sigma=\pm 1} e^{-\beta[-(zJ\sigma_{\downarrow} + \mu_B H)\sigma]} = \sum_{\sigma=\pm 1} e^{\beta(zJ\sigma_{\downarrow} + \mu_B H)\sigma} = 2 \cosh [zJ\sigma_{\downarrow} + \mu_B H] \quad (5)$$

which implies that

$$\langle \sigma_{\vec{R}} \rangle = \sigma_{\uparrow} = \frac{1}{Z_{\uparrow}} \sum_{\sigma=\pm 1} \sigma e^{\beta(zJ\sigma_{\downarrow} + \mu_B H)\sigma} = \tanh [\beta(zJ\sigma_{\downarrow} + \mu_B H)] \quad (6)$$

Notice that the omission of a constant energy term does not affect the calculation of a thermal expectation value. Z_{\downarrow} and σ_{\downarrow} are determined equivalently

$$Z_{\downarrow} = 2 \cosh [zJ\sigma_{\uparrow} + \mu_B H], \quad \sigma_{\downarrow} = \tanh [\beta(zJ\sigma_{\uparrow} + \mu_B H)] \quad (7)$$

and the (total) free energy is

$$\begin{aligned} \mathcal{F} &= -\frac{N}{2}k_B T (\ln Z_{\uparrow} + \ln Z_{\downarrow}) + N\frac{1}{2}zJ\sigma_{\uparrow}\sigma_{\downarrow} = \\ &= -\frac{N}{2}k_B T \left\{ \ln [2 \cosh (zJ\sigma_{\downarrow} + \mu_B H)] + \ln [2 \cosh (zJ\sigma_{\uparrow} + \mu_B H)] \right\} + \frac{N}{2}zJ\sigma_{\uparrow}\sigma_{\downarrow} \end{aligned} \quad (8)$$

The constant energy term neglecting in the partition functions adds to \mathcal{F} .

(b) The self-consistent equations determining σ_{\uparrow} and σ_{\downarrow} are derived above.

(c) In the paramagnetic phase, $T > T_N$, σ_{\uparrow} and σ_{\downarrow} vanish in the limit $H \rightarrow 0$. Expanding \tanh to leading order, $\tanh x \simeq x$, we get from (6) and (7)

$$\left. \begin{aligned} \sigma_{\uparrow} &= \tanh [\beta(zJ\sigma_{\downarrow} + \mu_B H)] \simeq \beta(zJ\sigma_{\downarrow} + \mu_B H) \\ \sigma_{\downarrow} &= \tanh [\beta(zJ\sigma_{\uparrow} + \mu_B H)] \simeq \beta(zJ\sigma_{\uparrow} + \mu_B H) \end{aligned} \right\} \sigma_{\uparrow} = \sigma_{\downarrow} = \frac{\mu_B H \beta}{1 - zJ\beta} \quad (9)$$

The expectation values σ_{\uparrow} and σ_{\downarrow} are equal and are proportional to the field. The magnetization is $M = (N/V)\mu_B(\sigma_{\uparrow} + \sigma_{\downarrow})/2$ and the susceptibility is defined as $\chi = M/H$ in the limit of zero field, and we find

$$\chi = \frac{N}{V} \frac{\mu_B^2}{k_B T - zJ} \equiv \frac{N}{V} \frac{\mu_B^2}{k_B (T - \Theta)}, \quad \Theta = -\frac{z|J|}{k_B} = -T_N \quad (10)$$

The paramagnetic Curie, or Curie–Weiss, temperature Θ is defined by (24.41), $\chi \propto (T - \Theta)^{-1}$. In the present system Θ is negative (J is negative), and $|\Theta|$ is, as we shall see, the same as the “Néel temperature”, T_N , below which the system is antiferromagnetically ordered at zero field.

(d) The Néel temperature is the temperature below which the self-consistent equations for σ_\uparrow and σ_\downarrow have a non-zero solution at zero field. The solution is obtained by assuming $\sigma_\uparrow = -\sigma_\downarrow$, and $H = 0$, in which case we get

$$\sigma_\uparrow = \tanh \left[\beta(-z|J|)(-\sigma_\uparrow) \right] = \tanh(\beta z|J|\sigma_\uparrow) = \tanh(\alpha\sigma_\uparrow) \quad (11)$$

This equation is the same as considered in the case of the ferromagnet, (24.56), and it has a non-zero solution, when the coefficient $\alpha \geq 1$. The Néel temperature T_N is the temperature at which $\alpha = z|J|\beta = 1$, or $T_N = z|J|/k_B$. The paramagnetic susceptibility, which diverges at the transition, is obtained by applying a field with the same symmetry as the ordered phase. The application of a “staggered” field, where $H_{\vec{R}} = +H$ at the A sites and $-H$ at the B sites determines straightforwardly (using $\sigma_\uparrow = -\sigma_\downarrow$) the staggered susceptibility to be

$$\chi_{\text{stag}} = \frac{N \mu_B (\sigma_\uparrow - \sigma_\downarrow)}{2H} = \frac{N}{V} \frac{\mu_B^2}{k_B (T - T_N)} \quad (12)$$

which diverges at T_N .

(e) Spin-flip transition: In the ordered phase, the application of a small field along z , in the “up” direction, does not change $\sigma_\uparrow = 1$ or $\sigma_\downarrow = -1$. However, if the field becomes sufficiently large, the spins antiparallel to the field are going to flip so to become parallel to the field. This first-order spin-flip transition happens, when the Zeeman-energy gain is able to compensate for the loss of exchange energy.

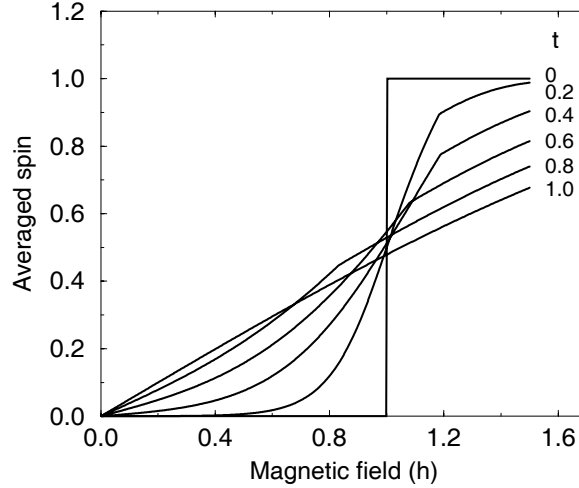
Introducing dimensionless quantities, then

$$\sigma_\uparrow = \tanh \left(\frac{-\sigma_\downarrow + h}{t} \right), \quad \sigma_\downarrow = \tanh \left(\frac{-\sigma_\uparrow + h}{t} \right), \quad h = \frac{\mu_B H}{z|J|}, \quad t = \frac{T}{T_N} \quad (13)$$

In the limit of $t \rightarrow 0$, then the introduction of $\sigma_\uparrow = 1$ in the second equation implies $\sigma_\downarrow = -1$ if $1 > h > 0$ and $\sigma_\downarrow = 1$ if $h > 1$. The first equation then predicts $\sigma_\uparrow = 1$ in both cases, hence assuring that this is the self-consistent solution. Using $\ln[2 \cosh x] = \ln[e^x + e^{-x}] \rightarrow \ln e^{|x|} = |x|$ for $x \rightarrow \pm\infty$, the free energy is found to be determined by

$$\begin{aligned} f &= \frac{\mathcal{F}}{Nz|J|} = -\frac{t}{2} \left\{ \ln \left[2 \cosh \left(\frac{-\sigma_\downarrow + h}{t} \right) \right] + \ln \left[2 \cosh \left(\frac{-\sigma_\uparrow + h}{t} \right) \right] \right\} - \frac{1}{2} \sigma_\uparrow \sigma_\downarrow \\ &\rightarrow -\frac{t}{2} \left\{ \frac{-\sigma_\downarrow + h}{t} + \left| \frac{-\sigma_\uparrow + h}{t} \right| \right\} - \frac{1}{2} \sigma_\uparrow \sigma_\downarrow = \begin{cases} -\frac{1}{2}, & 0 < h < 1 \\ -h + \frac{1}{2}, & h > 1 \end{cases} \end{aligned} \quad (14)$$

Hence, the free energies of the antiferromagnetic phase $f = -1/2$ and of the spin-flipped phase $f = -h + 1/2$ are equal at the transition at $h = 1$. At a finite temperature the spin-flip transition is smeared out due to thermal effects. The figure below shows the numerical calculated “magnetization”, $(\sigma_\uparrow + \sigma_\downarrow)/2$, as a function of the field h at various values of temperature t .

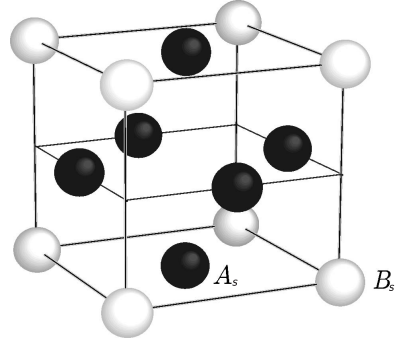


24.6 Superlattices

Model of Cu_3Au – In the fcc lattice, the sites in the centers of the six faces are named A_s and the 8 corners are named B_s as indicated on the figure by, respectively, black and white spheres. There is $8/8 = 1$ B_s site and $6/2 = 3$ A_s sites per unit cell. The distance between nearest neighbours is $a/\sqrt{2}$, and the coordination number is $z = 12$. The kind of nearest neighbours of the two kind of sites are

A_s -site: 8 A_s sites and 4 B_s sites.

B_s -site: 12 A_s sites.



The correct solution to the equations (24.62) and (24.63) is not (24.64), but

$$f(\sigma_{\vec{R}}, \sigma_{\vec{R}'}) = \frac{\epsilon_{BB} - \epsilon_{AA}}{4} (\sigma_{\vec{R}} + \sigma_{\vec{R}'}) - \frac{2\epsilon_{AB} - \epsilon_{AA} - \epsilon_{BB}}{4} \sigma_{\vec{R}} \sigma_{\vec{R}'} \quad (24.64')$$

when leaving out the constant term $C_1 = (2\epsilon_{AB} + \epsilon_{AA} + \epsilon_{BB})/4$. This modification affects the definition of the effective parameters in (24.67), which should read

$$\mu_B H = \mu - \frac{\epsilon_{BB} - \epsilon_{AA}}{2} z, \quad J = \frac{2\epsilon_{AB} - \epsilon_{AA} - \epsilon_{BB}}{4} \quad (24.67')$$

(a) In the present system we have a 3:1 mixture of A and B atoms. The effective Hamiltonian equals the energy minus the chemical potential times the difference between the numbers of B and A atoms, is (leaving out the constant contribution)

$$\mathcal{H} = \mathcal{E} - \mu \sum_{\vec{R}} \sigma_{\vec{R}} = -J \sum_{\langle \vec{R}\vec{R}' \rangle} \sigma_{\vec{R}} \sigma_{\vec{R}'} - \mu_B H \sum_{\vec{R}} \sigma_{\vec{R}} \quad (1)$$

We are going to use the same choice as Marder, that $\sigma_{\vec{R}} = 1$ or -1 signifies a site occupied by, respectively, a B or an A atom. With this choice, the effective energy parameters are those given by (24.67') above. In the mean-field approximation

$$\mathcal{H}^{\text{MF}} = -J \sum_{\langle \vec{R}\vec{R}' \rangle} (\sigma_{\vec{R}} \langle \sigma_{\vec{R}'} \rangle + \sigma_{\vec{R}'} \langle \sigma_{\vec{R}} \rangle - \langle \sigma_{\vec{R}} \rangle \langle \sigma_{\vec{R}'} \rangle) - \mu_B H \sum_{\vec{R}} \sigma_{\vec{R}} = \sum_{\vec{R}} \mathcal{H}_{\vec{R}} \quad (2)$$

where

$$\begin{aligned} \sum_{\langle \vec{R}\vec{R}' \rangle} \left(\sigma_{\vec{R}} \langle \sigma_{\vec{R}'} \rangle + \sigma_{\vec{R}'} \langle \sigma_{\vec{R}} \rangle \right) &= \frac{1}{2} \sum_{\vec{R}\vec{R}'} \left(\sigma_{\vec{R}} \langle \sigma_{\vec{R}'} \rangle + \sigma_{\vec{R}'} \langle \sigma_{\vec{R}} \rangle \right) = \sum_{\vec{R}} \sigma_{\vec{R}} \left(\sum_{\vec{R}'(\text{nn})} \langle \sigma_{\vec{R}'} \rangle \right) \\ &= \sum_{\vec{B}_s}^N \sigma_{\vec{B}_s} \left(12 \langle \sigma_{\vec{A}_s} \rangle \right) + \sum_{\vec{A}_s}^{3N} \sigma_{\vec{A}_s} \left(8 \langle \sigma_{\vec{A}_s} \rangle + 4 \langle \sigma_{\vec{B}_s} \rangle \right) \end{aligned} \quad (3)$$

Here N is the number of unit cells (or B_s sites), and $\sigma_{\vec{R}} = \sigma_{\vec{A}_s}$ ($\sigma_{\vec{B}_s}$), if $\vec{R} = \vec{A}_s$ (\vec{B}_s) is the position of an A_s (B_s) site. The (grand) partition function of the total system is the product of the individual partition functions for each site, because $\mathcal{H} = \sum_{\vec{R}} \mathcal{H}_{\vec{R}}$, and in the case of an A_s site (omitting the constant energy term)

$$Z_{A_s} = \sum_{\sigma=\pm 1} e^{\beta[J(8\langle\sigma_{\vec{A}_s}\rangle+4\langle\sigma_{\vec{B}_s}\rangle)+\mu_B H]\sigma} \quad (4)$$

implying that

$$\begin{aligned} \langle \sigma_{\vec{A}_s} \rangle &= \frac{1}{Z_{A_s}} \sum_{\sigma=\pm 1} \sigma e^{\beta[J(8\langle\sigma_{\vec{A}_s}\rangle+4\langle\sigma_{\vec{B}_s}\rangle)+\mu_B H]\sigma} \\ &= \tanh \left\{ \beta \left[8J \langle \sigma_{\vec{A}_s} \rangle + 4J \langle \sigma_{\vec{B}_s} \rangle + \mu_B H \right] \right\} \end{aligned} \quad (5)$$

and equivalently

$$\langle \sigma_{\vec{B}_s} \rangle = \tanh \left\{ \beta \left[12J \langle \sigma_{\vec{A}_s} \rangle + \mu_B H \right] \right\} \quad (6)$$

(b) $\sigma_{\vec{R}} = +1$ for the B atoms and the number of these atoms is equal the number of unit cells N , whereas the number of A atoms is $3N$. These conditions imply

$$\sum_{\vec{R}} \sigma_{\vec{R}} = \begin{cases} N - 3N = -2N \\ \sum_{\vec{B}_s}^N \sigma_{\vec{B}_s} + \sum_{\vec{A}_s}^{3N} \sigma_{\vec{A}_s} = N \langle \sigma_{\vec{B}_s} \rangle + 3N \langle \sigma_{\vec{A}_s} \rangle \end{cases} \Rightarrow \langle \sigma_{\vec{B}_s} \rangle = -2 - 3 \langle \sigma_{\vec{A}_s} \rangle \quad (7)$$

(c) The chemical potential, or effectively $\mu_B H$, has to be adjusted so that the two equations (5) and (6) are in accordance with the relation $\langle \sigma_{\vec{B}_s} \rangle = -2 - 3 \langle \sigma_{\vec{A}_s} \rangle$. The effective Zeeman term may be eliminated:

$$\begin{aligned} \tanh^{-1} \langle \sigma_{\vec{A}_s} \rangle - \tanh^{-1} \langle \sigma_{\vec{B}_s} \rangle &= \beta \left[8J \langle \sigma_{\vec{A}_s} \rangle + 4J \langle \sigma_{\vec{B}_s} \rangle + \mu_B H \right] \\ -\beta \left[12J \langle \sigma_{\vec{A}_s} \rangle + \mu_B H \right] &= 4\beta J \left(\langle \sigma_{\vec{B}_s} \rangle - \langle \sigma_{\vec{A}_s} \rangle \right) = -8\beta J \left(1 + 2 \langle \sigma_{\vec{A}_s} \rangle \right) \end{aligned} \quad (8)$$

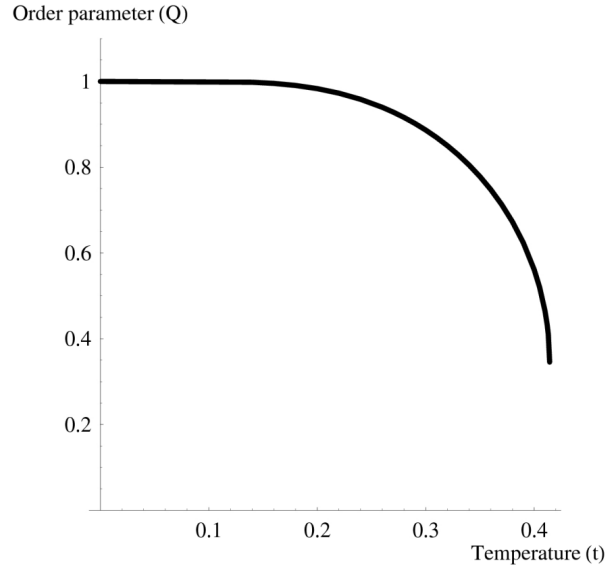
Introducing an effective order parameter Q and $J = -|J|$, we finally get

$$f(Q) \equiv \tanh^{-1} \left(\frac{Q+1}{2} \right) + \tanh^{-1} \left(\frac{3Q-1}{2} \right) = 8\beta|J|Q, \quad Q = -1 - 2 \langle \sigma_{\vec{A}_s} \rangle \quad (9)$$

In the disordered phase both the A_s and the B_s sites are occupied by an A atom with the probability $\frac{3}{4}$ or $\langle \sigma_{\vec{A}_s} \rangle = \langle \sigma_{\vec{B}_s} \rangle = (-1)\frac{3}{4} + (+1)\frac{1}{4} = -\frac{1}{2}$. This result is in accordance with (7) and $Q = -1 - 2 \langle \sigma_{\vec{A}_s} \rangle = 0$. In the completely ordered phase at

zero temperature, all A (B) atoms are placed on the A_s (B_s) sites implying that $\langle \sigma_{\vec{A}_s} \rangle = -1$ and $\langle \sigma_{\vec{B}_s} \rangle = 1$ and hence $Q = 1$.

The numerical solution of (9) is discussed in a Mathematica program. The system orders at a first-order transition, when $f(Q) = Q f'(Q)$ [the line $y = \alpha Q$ with $\alpha = f'(Q_c)$ is parallel to the tangent of $f(Q)$ at $Q = Q_c$, and this line just touches $f(Q)$ at $Q = Q_c$, when $f(Q_c) = \alpha Q_c$. This then becomes a solution to (9) if choosing $\alpha = 8\beta|J|$]. The solution is $Q = Q_c = 0.3455$ and defining the effective temperature scale $t = (8\beta|J|)^{-1}$ then Q jumps from zero to Q_c at the temperature $t = t_c = 1/f'(Q_c) = 0.4143$. The calculated variation of Q as a function of t is shown in the figure.



Solutions to the problems in Chapter 25 and 26

25.2 Classical electrons in a magnetic field

The spin degree-of-freedom does not occur in classical physics. The elementary particles do neither exist, but accepting their existence, they only interact with the electromagnetic fields because of their charges, and with the gravitational field because of their masses. The classical Hamiltonian \mathcal{H} of a many-body system (see for instance Goldstein) is a function of the independent canonical variables (\vec{r}_i, \vec{p}_i) of all the particles. The canonical impulse \vec{p}_i , independent of \vec{r}_i , is defined in terms of the Lagrangian $\mathcal{L} = \mathcal{L}(\vec{r}_i, \dot{\vec{r}}_i, \dots)$ as $\vec{p}_i = \partial\mathcal{L}/\partial\dot{\vec{r}}_i$ (or, in terms of the Hamiltonian theory, as the generator of an infinitesimal translation $\vec{r}_i \rightarrow \vec{r}_i + \delta\vec{r}_i$).

(a) If the external constraints (fields) are independent of time, the Hamiltonian is equal the total (kinetic plus potential) energy of the system. In this case the classical partition function is

$$Z = e^{-\beta\mathcal{F}} = \frac{1}{h^n} \int d\vec{r}_1 d\vec{p}_1 \dots d\vec{r}_n d\vec{p}_n e^{-\beta\mathcal{H}(\vec{r}_1, \vec{p}_1, \dots, \vec{r}_n, \vec{p}_n)} \quad (1)$$

(b) In the presence of a time-independent electromagnetic field, \vec{E} only contributes to the potential energy as determined by the scalar potential. The magnetic field \vec{B} only affects the velocities of the particles via the vector potential $\vec{A} = \vec{A}(\vec{r})$, where $\vec{B} = \nabla \times \vec{A}$. For the i th particle with mass m_i and charge q_i , the canonical impulse is

$$\vec{p}_i = m_i \dot{\vec{r}}_i + \frac{q_i}{c} \vec{A} \quad \Rightarrow \quad T_i = \frac{1}{2} m_i (\dot{\vec{r}}_i)^2 = \frac{1}{2m_i} \left(\vec{p}_i - \frac{q_i}{c} \vec{A} \right)^2 \quad (2)$$

[The magnetic field needs not to be uniform in space, but only to be constant in time – the case of a spatial uniform field is discussed in the next problem 25.4].

(c) The canonical impulse \vec{p}_i appears in the Hamiltonian only via the kinetic energy T_i . Assuming \mathcal{H} in (1) to be the Hamiltonian function of the system, when the magnetic field is zero (but including the potential energy contributions of the electric field), then the introduction of the magnetic field implies that

$$\mathcal{H}(\vec{r}_1, \vec{p}_1, \dots, \vec{r}_n, \vec{p}_n) \rightarrow \mathcal{H}\left(\vec{r}_1, \vec{p}_1 - \frac{q_1}{c}\vec{A}(\vec{r}_1), \dots, \vec{r}_n, \vec{p}_n - \frac{q_n}{c}\vec{A}(\vec{r}_n)\right) \quad (3)$$

The partition function Z in the presence of the magnetic field is then

$$\begin{aligned} Z(\vec{B}) &= \frac{1}{h^n} \int d\vec{r}_1 d\vec{p}_1 \dots d\vec{r}_n d\vec{p}_n e^{-\beta \mathcal{H}(\vec{r}_1, \vec{p}_1 - \frac{q_1}{c}\vec{A}(\vec{r}_1), \dots, \vec{r}_n, \vec{p}_n - \frac{q_n}{c}\vec{A}(\vec{r}_n))} \\ &= \frac{1}{h^n} \int d\vec{r}_1 d\vec{p}_1' \dots d\vec{r}_n d\vec{p}_n' e^{-\beta \mathcal{H}(\vec{r}_1, \vec{p}_1', \dots, \vec{r}_n, \vec{p}_n')} = Z(\vec{0}) \end{aligned} \quad (4)$$

The integration with respect to the canonical impulse \vec{p}_i may be performed before the \vec{r}_i -integrations. Introducing the following change of variables $\vec{p}_i' = \vec{p}_i - \frac{q_i}{c}\vec{A}(\vec{r}_i)$, then $d\vec{p}_i' = d\vec{p}_i$, since $\vec{A}(\vec{r}_i)$ is independent of \vec{p}_i . This transformation of variables therefore leads to the same integral as in (1). The elimination of \vec{B} in the partition function means, for instance, that the magnetic susceptibility of a classical equilibrium system is zero. This result is called the *Bohr–van Leeuwen theorem*. Notice, that it is important for the argumentation that the system is in equilibrium (the basis for the use of the partition function).

25.4 Quantum electrons in a magnetic field

The Hamiltonian of an electron with charge $-e$ in a magnetic field \vec{B} is

$$\mathcal{H} = \frac{1}{2m} \left(\vec{p} + \frac{e}{c}\vec{A} \right)^2 \quad (1)$$

The choice of the “Landau gauge”

$$\vec{A} = (0, Bx, 0) \quad \Rightarrow \quad \vec{B} = \nabla \times \vec{A} = (0, 0, B), \quad \nabla \cdot \vec{A} = 0 \quad (2)$$

i.e. this vector potential corresponds to a spatial uniform field \vec{B} in the z direction. Since the divergence of \vec{A} is zero, the two quantum mechanical operators \vec{A} and \vec{p} commute, $\vec{p} = (\hbar/i)\nabla$ in the \vec{r} -representation. Introducing this choice of gauge in (1), we get

$$\mathcal{H} = \frac{1}{2m} \left[p_x^2 + \left(p_y + \frac{eB}{c}x \right)^2 + p_z^2 \right] \quad (3)$$

The wave function of the electron is assumed to be

$$\psi(\vec{r}) = u(x) e^{i(yk_y + zk_z)} \quad (4)$$

and the eigenvalue equation is

$$\mathcal{H}\psi = e^{i(yk_y + zk_z)} \frac{1}{2m} \left[p_x^2 + \left(\hbar k_y + \frac{eB}{c}x \right)^2 + (\hbar k_z)^2 \right] u(x) \quad (5)$$

When the common phase factor is deleted, this eigenvalue equation is reduced to one, which only involves a determination of $u(x)$, and the equation may be written:

$$\mathcal{H}u(x) = \left[\frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2(x - x_0)^2 + \varepsilon_z \right] u(x) \quad (6)$$

where

$$\omega_c = \frac{eB}{mc}, \quad x_0 = -\frac{\hbar k_y}{m\omega_c}, \quad \varepsilon_z = \frac{\hbar^2 k_z^2}{2m} \quad (7)$$

Equation (6) is the eigenvalue equation for the one-dimensional harmonic oscillator, displaced to be centered around $x = x_0$ and shifted in energy by the constant (with respect to x) energy ε_z . Hence, the final eigenstates are classified by (k_y, k_z) and the occupation number ν , and the energy eigenvalues are

$$\varepsilon_{\nu, k_y, k_z} = \left(\nu + \frac{1}{2}\right) \hbar\omega_c + \frac{\hbar^2 k_z^2}{2m}, \quad \nu = 0, 1, 2, \dots \quad (8)$$

This is the result (25.48) utilized in the analysis of the Landau diamagnetism.

26.2 Ferromagnetic ground state

We are going to discuss the ferromagnetic ground state of the Heisenberg model for an arbitrary integer/half-integer value of S . The Heisenberg Hamiltonian is

$$\mathcal{H} = - \sum_{\langle ll' \rangle} J_{ll'} \vec{S}_l \cdot \vec{S}_{l'} = -\frac{1}{2} \sum_{l \neq l'} J_{ll'} \vec{S}_l \cdot \vec{S}_{l'} \quad (1)$$

according to (26.21) in Marder. The possibility of $J_{ll} \neq 0$ may be excluded, since such a term would contribute only by a constant term $J_{ll}S(S+1)$ to the energy. The components of \vec{S}_l fulfill the usual spin-commutator relations

$$[S_{lx}, S_{ly}] = i \delta_{ll'} S_{lz}, \quad [S_{ly}, S_{l'z}] = i \delta_{ll'} S_{lx}, \quad [S_{lz}, S_{l'x}] = i \delta_{ll'} S_{ly} \quad (2)$$

(a) Defining the following operator:
$$\mathcal{S}_z = \sum_l S_{lz} \quad (3)$$

then the commutator of this operator with a single term $\vec{S}_l \cdot \vec{S}_{l'}$ in (1) is

$$\begin{aligned} [\mathcal{S}_z, \vec{S}_l \cdot \vec{S}_{l'}] &= [\mathcal{S}_z, \vec{S}_l] \cdot \vec{S}_{l'} + \vec{S}_l \cdot [\mathcal{S}_z, \vec{S}_{l'}] \\ &= [S_{lz}, S_{lx}] S_{l'x} + [S_{lz}, S_{ly}] S_{l'y} + S_{lx} [S_{l'z}, S_{l'x}] + S_{ly} [S_{l'z}, S_{l'y}] \\ &= i S_{ly} S_{l'x} - i S_{lx} S_{l'y} + i S_{lx} S_{l'y} - i S_{ly} S_{l'x} = 0 \end{aligned} \quad (4)$$

showing that $[\mathcal{S}_z, \mathcal{H}] = 0$. The S_z -representation for each site is defined by $S_{lz}|m_l\rangle = m_l|m_l\rangle$, where $m_l = -S, -S+1, \dots, S$, and $\mathcal{S}_z \prod_l |m_l\rangle = (\sum_l m_l) \prod_l |m_l\rangle$. Most of these eigenstates are highly degenerated except for the two ‘‘singlets’’, $\prod_l |m_l = \pm S\rangle = \prod_l | + S \rangle$ or $\prod_l | - S \rangle$. Because \mathcal{S}_z and \mathcal{H} commute the two non-degenerate eigenstates of \mathcal{S}_z are also eigenstates to \mathcal{H} , and

$$\mathcal{H} \prod_l |m_l = \pm S\rangle = -\frac{1}{2} N J(\vec{0}) S^2 \prod_l |m_l = \pm S\rangle, \quad J(\vec{k}) = \sum_{l'} J_{ll'} e^{-i\vec{k} \cdot (\vec{r}_l - \vec{r}_{l'})} \quad (5)$$

(b) Defining $\vec{\mathbb{S}} = \vec{S}_{\vec{R}} + \vec{S}_{\vec{R}'}$ and using $\vec{\mathbb{S}}^2 = (\vec{S}_{\vec{R}} + \vec{S}_{\vec{R}'})^2 = \vec{S}_{\vec{R}}^2 + \vec{S}_{\vec{R}'}^2 + 2\vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'}$

$$\langle \Psi | \vec{\mathbb{S}}^2 | \Psi \rangle = \begin{cases} S(S+1) + S(S+1) + 2\langle \Psi | \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'} | \Psi \rangle \\ \mathbb{S}(\mathbb{S}+1), & \mathbb{S} = 0, 1, \dots, 2S \end{cases} \quad (6)$$

which shows that $\langle \Psi | \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'} | \Psi \rangle$ attains its maximum value, when $\mathbb{S} = 2S$, and

$$\text{Max}\{\langle \Psi | \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'} | \Psi \rangle\} = \frac{1}{2}[2S(2S+1) - 2S(S+1)] = S^2 \quad (7)$$

(c) The eigenvalue of \mathcal{H} in (5) for the fully polarized states requires that each pair of operators in (1) contributes by their maximum. Hence, if all exchange constants $J_{ll'} \geq 0$, then the eigenvalue in (5) is the lowest possible value, i.e. the two fully polarized states are the two degenerate ground states.

The lowest excited states are linear combination of the states, where all $m_l = S$ except that $m_l = S - 1$ for one particular site. Naming the product of these states for $|l\rangle$, where l is the site at which $m_l = S - 1$, then it is straightforward to show that the eigenstates of \mathcal{H} constructed from these states are the Fourier transforms of $|l\rangle$. These excited states are characterized by the wave vector \vec{k} of the Fourier transformation, and the energy difference between one excited \vec{k} -state and the ground state is the spin wave energy, $S[J(\vec{0}) - J(\vec{k})]$. Hence, these lowest excited states, the one-magnon states, are exact solutions to the Heisenberg Hamiltonian – but this is no longer the case if proceeding to the two-magnon states, where the eigenvalue of S_z is $NS - 2$.

26.4 Diagonalizing spin waves

The result derived in (26.62) may be written in a reduced form:

$$\begin{aligned} \hat{h} &= \frac{1}{2z|J|S} \left(\mathcal{H} + Nz|J|S^2 \right) = \frac{1}{2z} \sum_{\vec{\delta}} \left[2a_{\vec{k}}^{\dagger} a_{\vec{k}} + \left(a_{\vec{k}}^{\dagger} a_{-\vec{k}}^{\dagger} + a_{\vec{k}} a_{-\vec{k}} \right) \cos(\vec{k} \cdot \vec{\delta}) \right] \\ &= \sum_{\vec{k}} \left[a_{\vec{k}}^{\dagger} a_{\vec{k}} + \frac{1}{2} \left(a_{\vec{k}}^{\dagger} a_{-\vec{k}}^{\dagger} + a_{\vec{k}} a_{-\vec{k}} \right) B_{\vec{k}} \right], \quad B_{\vec{k}} = \frac{1}{z} \sum_{\vec{\delta}} \cos(\vec{k} \cdot \vec{\delta}) \end{aligned} \quad (1)$$

The operators are defined by (26.51) in terms of a_l and its hermitean conjugate a_l^{\dagger} , which are the annihilation and creation operators, also named Bose operators, of a harmonic oscillator at the site l . These operators obey the Bose commutator relations $[a_l, a_{l'}^{\dagger}] = \delta_{ll'}$ and $[a_l^{\dagger}, a_{l'}^{\dagger}] = [a_l, a_{l'}] = 0$, which imply

$$[a_{\vec{k}}, a_{\vec{k}'}^{\dagger}] = \frac{1}{N} \sum_{l'} \left[a_l e^{i\vec{k} \cdot \vec{r}_l}, a_{l'}^{\dagger} e^{-i\vec{k}' \cdot \vec{r}_{l'}} \right] = \frac{1}{N} \sum_{l'} \delta_{ll'} e^{i\vec{k} \cdot \vec{r}_l - i\vec{k}' \cdot \vec{r}_{l'}} = \frac{1}{N} \sum_l e^{i(\vec{k} - \vec{k}') \cdot \vec{r}_l} \quad (2)$$

or that the Fourier transforms of the Bose operators, diagonal with respect to the site index, are Bose operators in reciprocal space

$$[a_{\vec{k}}, a_{\vec{k}'}^{\dagger}] = \delta_{\vec{k}\vec{k}'}, \quad [a_{\vec{k}}, a_{\vec{k}'}] = 0, \quad [a_{\vec{k}}^{\dagger}, a_{\vec{k}'}^{\dagger}] = 0 \quad (3)$$

which are diagonal with respect to the wave vector index (notice that the wave vector \vec{k} is assumed to be a discrete variable). The Hamiltonian (1) is not diagonal in the number representations of the harmonic oscillators, since it involves $a_{\vec{k}}^{\dagger} a_{-\vec{k}}^{\dagger} + a_{\vec{k}} a_{-\vec{k}}$. One way to solve an eigenvalue problem is to make a canonical transformation of the Hamiltonian to one for which the eigenvalue equations have been solved. In the present case, we want to find a new Bose operator $\gamma_{\vec{k}}$, in terms of which \hat{h} only depends on the number operators $\gamma_{\vec{k}}^{\dagger} \gamma_{\vec{k}}$, in which case \hat{h} is “diagonal”. This procedure is called *the Bogoliubov transformation*:

$$a_{\vec{k}} = u_{\vec{k}} \gamma_{\vec{k}} + v_{\vec{k}} \gamma_{-\vec{k}}^{\dagger}, \quad a_{\vec{k}}^{\dagger} = u_{\vec{k}}^* \gamma_{\vec{k}}^{\dagger} + v_{\vec{k}}^* \gamma_{-\vec{k}} = u_{\vec{k}} \gamma_{\vec{k}}^{\dagger} + v_{\vec{k}} \gamma_{-\vec{k}} \quad (4)$$

The last equation indicates that $u_{\vec{k}}$ and $v_{\vec{k}}$ are assumed to be real functions. This is a valid simplification in the present case, but it is not a general requirement. The demand that the new operators should also be Bose operators implies

$$[a_{\vec{k}}, a_{\vec{k}'}^+] = [u_{\vec{k}}\gamma_{\vec{k}} + v_{\vec{k}}\gamma_{-\vec{k}}^+, u_{\vec{k}'}\gamma_{\vec{k}'}^+ + v_{\vec{k}'}\gamma_{-\vec{k}'}^+] = u_{\vec{k}}u_{\vec{k}'}\delta_{\vec{k}\vec{k}'} - v_{\vec{k}}v_{\vec{k}'}\delta_{-\vec{k}-\vec{k}'} = \delta_{\vec{k}\vec{k}'} \quad (5)$$

and, similarly, $[a_{\vec{k}}, a_{\vec{k}'}] = u_{\vec{k}}v_{\vec{k}'}\delta_{\vec{k}-\vec{k}'} - v_{\vec{k}}u_{\vec{k}'}\delta_{-\vec{k}\vec{k}'} = 0$. Hence, the fulfillment of the Bose commutator relations for $\gamma_{\vec{k}}$ requires

$$u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1, \quad u_{\vec{k}}v_{-\vec{k}} - v_{\vec{k}}u_{-\vec{k}} = 0 \quad (6)$$

Inserting (4) in (1) we get

$$\begin{aligned} \hat{h} = \sum_{\vec{k}} \left[\left(u_{\vec{k}}\gamma_{\vec{k}}^+ + v_{\vec{k}}\gamma_{-\vec{k}} \right) \left(u_{\vec{k}}\gamma_{\vec{k}} + v_{\vec{k}}\gamma_{-\vec{k}}^+ \right) + \frac{1}{2}B_{\vec{k}} \left\{ \left(u_{\vec{k}}\gamma_{\vec{k}}^+ + v_{\vec{k}}\gamma_{-\vec{k}} \right) \right. \right. \\ \left. \left. \times \left(u_{-\vec{k}}\gamma_{-\vec{k}}^+ + v_{-\vec{k}}\gamma_{\vec{k}} \right) + \left(u_{\vec{k}}\gamma_{\vec{k}} + v_{\vec{k}}\gamma_{-\vec{k}}^+ \right) \left(u_{-\vec{k}}\gamma_{-\vec{k}} + v_{-\vec{k}}\gamma_{\vec{k}}^+ \right) \right\} \right] \quad (7) \end{aligned}$$

Collecting corresponding terms and replacing $-\vec{k}$ with \vec{k} in some of the terms (utilizing $B_{\vec{k}} = B_{-\vec{k}}$ and $\gamma_{\vec{k}}\gamma_{-\vec{k}} = \gamma_{-\vec{k}}\gamma_{\vec{k}}$), then (7) is reduced to

$$\begin{aligned} \hat{h} = \sum_{\vec{k}} \left[\left(u_{\vec{k}}^2 + B_{\vec{k}}u_{\vec{k}}v_{-\vec{k}} \right) \gamma_{\vec{k}}^+\gamma_{\vec{k}} + \left(v_{-\vec{k}}^2 + B_{\vec{k}}u_{\vec{k}}v_{-\vec{k}} \right) \gamma_{\vec{k}}\gamma_{\vec{k}}^+ \right. \\ \left. + \left\{ 2u_{\vec{k}}v_{\vec{k}} + B_{\vec{k}} \left(u_{\vec{k}}u_{-\vec{k}} + v_{\vec{k}}v_{-\vec{k}} \right) \right\} \frac{1}{2} \left(\gamma_{\vec{k}}^+\gamma_{-\vec{k}}^+ + \gamma_{\vec{k}}\gamma_{-\vec{k}} \right) \right] \quad (8) \end{aligned}$$

In order to diagonalize this Hamiltonian we have to search for values of $u_{\vec{k}}$ and $v_{\vec{k}}$, where the last term in (8) vanishes and the requirements of (6) are fulfilled. In order to simplify the search, we make the *ansatz* $u_{-\vec{k}} = u_{\vec{k}}$, which is consistent with the different conditions only if $v_{-\vec{k}} = v_{\vec{k}}$. In this case the equations are

$$2u_{\vec{k}}v_{\vec{k}} = -B_{\vec{k}} \left(u_{\vec{k}}^2 + v_{\vec{k}}^2 \right), \quad u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1 \quad (9)$$

Introducing $v_{\vec{k}}^2 = u_{\vec{k}}^2 - 1$ in the squared version of the first equation, we get an equation of second degree in $u_{\vec{k}}^2$. Determining the solution of this equation subject to the condition $v_{\vec{k}}^2 > 0$ or $u_{\vec{k}}^2 > 1$, we get

$$u_{\vec{k}}^2 = \frac{1 + \varepsilon_{\vec{k}}}{2\varepsilon_{\vec{k}}}, \quad v_{\vec{k}}^2 = \frac{1 - \varepsilon_{\vec{k}}}{2\varepsilon_{\vec{k}}}, \quad 2u_{\vec{k}}v_{\vec{k}} = -\frac{B_{\vec{k}}}{\varepsilon_{\vec{k}}}, \quad \varepsilon_{\vec{k}} = \sqrt{1 - B_{\vec{k}}^2} \quad (10)$$

According to the definition in (1), $|B_{\vec{k}}| \leq 1$ implying $0 \leq \varepsilon_{\vec{k}} \leq 1$. This is the same solution as given by equations (26.63) and (26.64) in Marder, since $u_{\vec{k}} = \cosh(\alpha_{\vec{k}})$ and $v_{\vec{k}} = \sinh(\alpha_{\vec{k}})$ imply $u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1$ and $\tanh(2\alpha_{\vec{k}}) = 2u_{\vec{k}}v_{\vec{k}}/(u_{\vec{k}}^2 + v_{\vec{k}}^2) = -B_{\vec{k}}$. Introducing the solution (10) in (8) we finally get

$$\begin{aligned} \hat{h} = \sum_{\vec{k}} \left[\frac{1}{2} \left(\varepsilon_{\vec{k}} + 1 \right) \gamma_{\vec{k}}^+\gamma_{\vec{k}} + \frac{1}{2} \left(\varepsilon_{\vec{k}} - 1 \right) \gamma_{\vec{k}}\gamma_{\vec{k}}^+ \right] = \sum_{\vec{k}} \left[\frac{1}{2} \left(\varepsilon_{\vec{k}} - 1 \right) + \varepsilon_{\vec{k}}\gamma_{\vec{k}}^+\gamma_{\vec{k}} \right] \\ \mathcal{H} = -Nz|J|S^2 - z|J|S \sum_{\vec{k}} \left(1 - \varepsilon_{\vec{k}} \right) + \sum_{\vec{k}} \mathcal{E}_{\vec{k}} \gamma_{\vec{k}}^+\gamma_{\vec{k}} \quad (11) \\ \mathcal{E}_{\vec{k}} = 2z|J|S \varepsilon_{\vec{k}}, \quad \langle \gamma_{\vec{k}}^+\gamma_{\vec{k}} \rangle = n_{\vec{k}} = [e^{\beta\mathcal{E}_{\vec{k}}} - 1]^{-1} \end{aligned}$$

The antiferromagnetic Néel state, where the spins of the two sublattices are either $+S$ or $-S$ is not an eigenstate of the Hamiltonian. The second term of \mathcal{H} , discussed by Marder, shows that the ground state energy is smaller than that derived from the Néel state. Additionally, the magnitude $|\langle S_z(l) \rangle|$ is smaller than S at zero temperature. This “zero-point” reduction of the antiferromagnetic moment is determined by the site average of $|\langle 0|S_z(l)|0 \rangle| = S - \langle 0|a_l^\dagger a_l|0 \rangle$, where $|0 \rangle$ is the product ground state of the N independent harmonic oscillators, $\gamma_{\vec{k}}|0 \rangle = 0$,

$$\begin{aligned} \Delta S &= \frac{1}{N} \sum_l \langle 0|a_l^\dagger a_l|0 \rangle = \frac{1}{N} \sum_{\vec{k}} \langle 0|a_{\vec{k}}^\dagger a_{\vec{k}}|0 \rangle = \\ &= \frac{1}{N} \sum_{\vec{k}} \langle 0| \left(u_{\vec{k}} \gamma_{\vec{k}}^\dagger + v_{\vec{k}} \gamma_{-\vec{k}} \right) \left(u_{\vec{k}} \gamma_{\vec{k}} + v_{\vec{k}} \gamma_{-\vec{k}}^\dagger \right) |0 \rangle = \frac{1}{N} \sum_{\vec{k}} v_{\vec{k}}^2 = \frac{1}{N} \sum_{\vec{k}} \frac{1 - \varepsilon_{\vec{k}}}{2\varepsilon_{\vec{k}}} \end{aligned} \quad (13)$$

which number is calculated [P.W. Anderson, Phys. Rev. **86**, 694 (1952)] to be 0.078 in the case of a simple cubic lattice ($z = 6$).

Solution to HS’s problem 4

Localized atoms: heat capacity and magnetic susceptibility

1) In the case of non-interacting atoms, the total energy is the sum of the contributions from each site $\mathcal{E} = \sum_l \mathcal{E}_l$. This implies that the partition function is the product of the partition functions determined for each site (see also the note “Magnetic energy and domains”), and when the atoms are identical:

$$\mathcal{Z} = \prod_{l=1}^N Z_l = Z^N, \quad Z_l = Z = \sum_i e^{-\beta \epsilon_i} = e^{\beta \Delta} + 1 + e^{-\beta \Delta} \quad (1)$$

The free energy is

$$F = -k_B T \ln \mathcal{Z} = -N k_B T \ln Z = -N k_B T \ln \left(e^{\beta \Delta} + 1 + e^{-\beta \Delta} \right) \quad (2)$$

The internal energy is $U = F + TS$, where the entropy is

$$\begin{aligned} \mathcal{S} &= -\frac{\partial F}{\partial T} = N k_B \ln Z + N k_B T \frac{1}{Z} \frac{\partial Z}{\partial T} \Rightarrow \\ U &= F + TS = N k_B T^2 \frac{1}{Z} \frac{\partial Z}{\partial T} = -N \frac{1}{Z} \frac{\partial Z}{\partial \beta} = N \frac{1}{Z} \sum_i \epsilon_i e^{-\beta \epsilon_i} \end{aligned} \quad (3)$$

Introducing the population factor for the i th level (the probability that this level is occupied):

$$p_i \equiv \frac{e^{-\beta \epsilon_i}}{Z} \Rightarrow U = N \sum_i \epsilon_i p_i = -N \Delta \frac{e^{\beta \Delta} - e^{-\beta \Delta}}{e^{\beta \Delta} + 1 + e^{-\beta \Delta}} \quad (4)$$

Notice, that $\sum_i p_i = 1$. In terms of the population factors, the thermal expectation value of any single site operator \hat{A} is $\langle \hat{A} \rangle = \sum_i \langle i | \hat{A} | i \rangle p_i$, and the entropy is $\mathcal{S} = -N k_B \sum_i p_i \ln p_i$.

2) In the limit $k_B T \gg \Delta$ or $\beta\Delta \ll 1$, we have from (1)

$$\begin{aligned} Z &\simeq 1 + \beta\Delta + \frac{1}{2}(\beta\Delta)^2 + 1 + 1 - \beta\Delta + \frac{1}{2}(\beta\Delta)^2 = 3 + (\beta\Delta)^2 \Rightarrow \\ F &\simeq -Nk_B T \ln \left[3 + (\beta\Delta)^2 \right] = -Nk_B T \ln 3 \left[1 + \frac{1}{3}(\beta\Delta)^2 \right] = -Nk_B T \ln 3 - \frac{N\Delta^2}{3k_B T} \\ S &= -\frac{\partial F}{\partial T} = Nk_B \ln 3 - \frac{N\Delta^2}{3k_B T^2}, \quad U = F + TS = -\frac{2N\Delta^2}{3k_B T} \end{aligned} \quad (5)$$

The heat capacity may be determined either as

$$C = \frac{\partial U}{\partial T} = \frac{2N\Delta^2}{3k_B T^2} \quad \text{or} \quad C = T \frac{\partial S}{\partial T} = T(-2) \left(-\frac{N\Delta^2}{3k_B T^3} \right) = \frac{2N\Delta^2}{3k_B T^2} \quad (6)$$

3) The derivative of F with respect to Δ is

$$\frac{\partial F}{\partial \Delta} = -Nk_B T \frac{1}{Z} \frac{\partial Z}{\partial \Delta} = -Nk_B T (\beta p_1 + 0 \cdot p_2 - \beta p_3) = N(p_3 - p_1) \simeq -\frac{2N\Delta}{3k_B T} \quad (7)$$

The last equality is most simply obtained from F derived in (5). In the presence of a magnetic field H , applied along the z axis, the Hamiltonian is specified in terms of the Zeeman interaction

$$\mathcal{H} = \sum_l \mathcal{H}_l = -g\mu_B H \sum_l S_{lz}, \quad S = 1 \quad (8)$$

The Hamiltonian of one of the sites is diagonal in the S_z -representation and the eigenenergies are

$$\begin{cases} |S_z = -1\rangle &\Rightarrow \epsilon_i = g\mu_B H = \Delta & (i = 3) \\ |S_z = 0\rangle &\Rightarrow \epsilon_i = 0 & (i = 2) \\ |S_z = 1\rangle &\Rightarrow \epsilon_i = -g\mu_B H = -\Delta & (i = 1) \end{cases} \quad (9)$$

Hence the Hamiltonian (8) leads to the case considered when $g\mu_B H = \Delta$, and the derivative of F with respect to Δ is proportional to the magnetization, or

$$M = -\frac{1}{V} \frac{\partial F}{\partial H} = -\frac{(g\mu_B)}{V} \frac{\partial F}{\partial \Delta} \simeq \frac{N}{V} \frac{2(g\mu_B)^2}{3k_B T} H, \quad \chi = \left. \frac{M}{H} \right|_{H \rightarrow 0} = \frac{N}{V} \frac{2(g\mu_B)^2}{3k_B T} \quad (10)$$

The susceptibility is calculated in the limit of H or $\Delta \rightarrow 0$, hence the expression derived is valid at all T . Notice, that M may also be obtained from

$$MV = g\mu_B \sum_l \langle S_{lz} \rangle = Ng\mu_B \sum_i \langle i | S_z | i \rangle p_i = Ng\mu_B (p_1 - p_3) \quad (11)$$

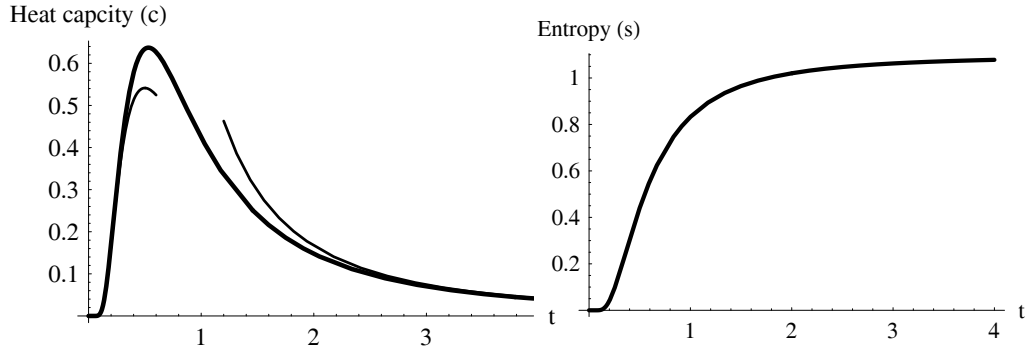
The result for χ in (10) is Curie's law in the case of $S = 1$, see (25.31)-(25.32).

4) Defining $x = \beta\Delta$ the heat capacity derived from U in (4) is

$$\begin{aligned} C &= \frac{\partial U}{\partial T} = -\frac{\Delta}{k_B T^2} \frac{\partial U}{\partial x} = N \frac{\Delta^2}{k_B T^2} \frac{\partial}{\partial x} \left(\frac{e^x - e^{-x}}{e^x + 1 + e^{-x}} \right) = N \frac{\Delta^2}{k_B T^2} \frac{e^x + e^{-x} + 4}{(e^x + 1 + e^{-x})^2} \\ &= N \frac{\Delta^2}{k_B T^2} \frac{e^{\beta\Delta} + e^{-\beta\Delta} + 4}{(e^{\beta\Delta} + 1 + e^{-\beta\Delta})^2} \rightarrow N \frac{\Delta^2}{k_B T^2} e^{-\Delta/(k_B T)} \quad \text{for } T \rightarrow 0 \end{aligned} \quad (12)$$

The figure to the left shows the reduced heat capacity $c = C/(Nk_B)$ as a function of the reduced temperature $t = k_B T/\Delta$ – the thin lines are the results for $c(t)$ in the high- and low-temperature limits, (6) and (12). This characteristic behaviour of the heat capacity is called a *Schottky anomaly*. The number of levels involved in the anomaly for an arbitrary value of S is $(2S + 1)$, i.e. 3 levels in the present case of $S = 1$. This number may be determined from a heat capacity experiment by evaluating the entropy in the high temperature limit, since $\mathcal{S}_\infty = Nk_B \ln(2S + 1)$ for a general value of S . A measurement of $C = T(\partial\mathcal{S}/\partial T)$ determines \mathcal{S} , and

$$\mathcal{S} = \int_0^T \frac{C}{T} dT \quad \Rightarrow \quad s_\infty = \frac{\mathcal{S}_\infty}{Nk_B} = \int_0^\infty \frac{c}{t} dt = \ln(2S + 1) \quad (13)$$



Solutions to the problems in Chapter 27

27.1 Superconducting sphere

The free-energy density of a type-I superconductor is determined by the critical field H_c . Since $\vec{B} = \vec{0}$ throughout the volume of the type-I superconductor, when surface effects are neglected ($\lambda_L \approx 0$ compared to the dimensions of the sample)

$$\vec{B}_i = \vec{H}_i + 4\pi\vec{M} = \vec{0} \quad \Rightarrow \quad \vec{M} = -\frac{1}{4\pi}\vec{H}_i \quad (1)$$

Assuming the sample to be a thin needle along the direction of the applied magnetic field \vec{H}_0 (along z), the demagnetization field $\vec{H}_d = -\mathcal{N}_z\vec{M} \approx \vec{0}$. In this case, the magnetic field within the sample is $\vec{H}_i = \vec{H}_0$ and the magnetization is $\vec{M} = -\vec{H}_0/(4\pi)$. According to eq. (2.6) in the note “Magnetic energy and domains”, the magnetic energy density is then,

$$\frac{1}{V} F_M = \mathcal{G}_M = - \int_{\text{sample}} \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta\vec{H}_0 \right] = \frac{1}{4\pi} \int_0^{H_0} \vec{H}'_0 \cdot d\vec{H}'_0 = \frac{H_0^2}{8\pi} \quad (2)$$

[This energy density corresponds to \mathcal{G} in Marder because \vec{H}_0 is the independent variable, see problem 27.2]. The total energy density is the sum of \mathcal{G}_M and the field-independent condensation-energy density, \mathcal{G}_S . Since the two contributions just outbalance each other at the critical field $H_0 = H_c$, we have a measure for \mathcal{G}_S ,

$$\mathcal{G} = \mathcal{G}_S + \mathcal{G}_M, \quad \mathcal{G}_S = -\frac{H_c^2}{8\pi} \quad (3)$$

If the sample has instead the shape of a sphere, then (1) and (3) still apply, but

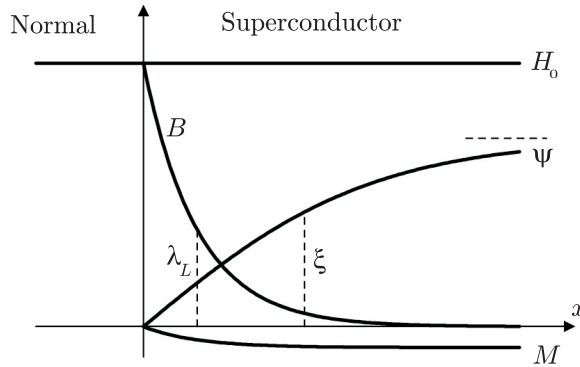
$$\vec{H}_i = \vec{H}_0 + \vec{H}_d = \vec{H}_0 - \mathcal{N}_z \vec{M} = \vec{H}_0 + D\vec{H}_i, \quad D \equiv \frac{\mathcal{N}_z}{4\pi} = \frac{1}{3} \quad (\text{sphere}) \quad (4)$$

implying

$$\vec{H}_i = \frac{\vec{H}_0}{1-D}, \quad \mathcal{G} = \mathcal{G}_S + \mathcal{G}_M = -\frac{H_c^2}{8\pi} + \frac{H_0^2}{8\pi(1-D)} \quad (5)$$

The internal field H_i is **larger** than the applied field and becomes equal the critical one, when the applied field is $H_0 = (1-D)H_c = \frac{2}{3}H_c$. This condition is not necessarily critical, since the global free energy of the superconducting sphere is still negative (as long as $H_0 < \sqrt{1-D}H_c$). A detail discussion of the *intermediate state* of the superconductor, when $(1-D)H_c < H_0 < H_c$, may be found in Landau and Lifshits, *Electrodynamics of continuous media* (Volume 8, 2nd Edition, page 189). In the intermediate range of the applied field, local thermodynamic instabilities are going to destroy superconductivity in parts of the sphere such that the effective D is reduced sufficiently to sustain superconductivity in the remaining parts. The assumption that the superconducting domain takes the form of a prolate ellipsoid with radius $a < R$ and constant height $2R$ (the largest volume for a certain value of D) is the most obvious one, but this configuration turns out to be thermodynamical unstable (the field in the normal part of the sphere is smaller than H_c near the end points of the ellipsoid). Nevertheless, domains of superconductivity are going to be present as long as $H_0 < H_c$.

27.2 Energy of normal-superconducting interfaces



(a) To start with we consider the limit of $\kappa \rightarrow 0$ or $\lambda_L \ll \xi$. Then $B = 0$ for $x > 0$ and according to (27.41) the wave function, which vanishes at $x = 0$ and saturates at Ψ_0 at large x , is

$$\Psi(x) = \Psi_0 \psi(x) = \Psi_0 \tanh\left(\frac{x}{\sqrt{2}\xi}\right) \quad (1)$$

The free energy density, the Ginzburg–Landau energy is, (27.27),

$$\mathcal{F} = \Psi_0^2 \int_0^L \frac{dx}{L} \left[\alpha \psi^2 + \frac{1}{2}\beta \Psi_0^2 \psi^4 + \frac{\hbar^2}{2m^*} (\psi')^2 \right] \quad (2)$$

Here $\Psi_0^2 = -\alpha/\beta$ is the equilibrium value at large x , and the change in energy per unit area, in comparison with the homogeneous case, is

$$L\Delta\mathcal{F} = \Psi_0^2 \int_0^\infty dx \left[\alpha(\psi^2 - 1) + \frac{1}{2}\beta\Psi_0^2(\psi^4 - 1) + \frac{\hbar^2}{2m^*}(\psi')^2 \right] \quad (3)$$

Introducing $H_c^2 = 4\pi\alpha^2/\beta$, (27.35), and $\xi^2 = -\hbar^2/(2m^*\alpha)$, (27.31), then (3) may be written

$$L\Delta\mathcal{F} = \frac{H_c^2}{4\pi} \int_0^\infty dx \left[\frac{1}{2}(1 - \psi^2)^2 + \xi^2(\psi')^2 \right] = \frac{H_c^2}{4\pi} \int_0^\infty dx (1 - \psi^2)^2 \quad (4)$$

using $\psi' = (1 - \psi^2)/(\sqrt{2}\xi)$, (27.40), in the last step. Applying this relation ones more, we get

$$L\Delta\mathcal{F} = \frac{H_c^2}{4\pi} \int_0^\infty dx (1 - \psi^2) \sqrt{2}\xi\psi' = \frac{H_c^2\sqrt{2}\xi}{4\pi} \int_0^1 (1 - \psi^2) d\psi = \frac{H_c^2\sqrt{2}\xi}{4\pi} \frac{2}{3} \quad (5)$$

which energy per unit area is positive and in agreement with (27.52) [$\Delta\mathcal{G} = \Delta\mathcal{F}$ since $\vec{B} = \vec{0}$].

(b) Next we consider the opposite limit of $\xi \ll \lambda_L$, in which case $\Psi(x) \simeq \Psi_0$ and the gradient ψ' may be neglected. In this case the free energy density is

$$\mathcal{F} = \mathcal{F}_S + \mathcal{F}_M, \quad \mathcal{F}_M = \int \frac{d\vec{r}}{V} \left(\frac{B^2}{8\pi} + \frac{4e^2}{2m^*c^2} A^2 \Psi_0^2 \right) = \int \frac{d\vec{r}}{8\pi V} \left(B^2 + \frac{A^2}{\lambda_L^2} \right) \quad (6)$$

where the first term is the zero-field contribution of the homogeneous superconductor, (2) when $\psi' = 0$, and \mathcal{F}_M is the magnetic energy density in (27.27), when $\lambda_L^2 = m^*c^2/(16\pi e^2\Psi_0^2)$, (27.32), is inserted. The applied field is assumed to be parallel to the interface, i.e. along z , and $\vec{B} = \vec{H}_0$ in the normal metal [this configuration leads to the largest possible energy gain]. Assuming \vec{A} to be along the y direction, $\vec{A} = (0, A(x), 0)$, then $\vec{B} = \nabla \times \vec{A} = (0, 0, A'(x))$ for $x > 0$. According to (27.9), $B_z = B(0)e^{-x/\lambda_L}$ for $x > 0$, where $B(0) = H_0$. Hence

$$A'(x) = B(x) = H_0 e^{-x/\lambda_L} \quad \Rightarrow \quad A(x) = -\lambda_L H_0 e^{-x/\lambda_L} \quad (\rightarrow 0 \text{ for } x \rightarrow \infty) \quad (7)$$

or $[A(x)/\lambda_L]^2 = B^2(x) = H_0^2 e^{-2x/\lambda_L}$

introducing this in (6), we get (for the field energy within the superconductor)

$$L\mathcal{F}_M = \int_0^L dx \frac{2B^2(x)}{8\pi} = \int_0^\infty dx \frac{H_0^2}{4\pi} e^{-2x/\lambda_L} = \frac{H_0^2}{8\pi} \lambda_L \quad (8)$$

The magnetic free energy may also be calculated in a direct fashion

$$\mathcal{F}_M = \frac{1}{4\pi} \int \frac{d\vec{r}}{V} \left[\int \vec{H} \cdot \delta\vec{B} \right] = \frac{1}{4\pi} \int_0^\infty \frac{dx}{L} \left[\int_0^{H_0} H e^{-x/\lambda_L} dH \right] = \frac{H_0^2}{8\pi} \frac{\lambda_L}{L} \quad (9)$$

when using $\delta\vec{B} = e^{-x/\lambda_L}\delta\vec{H}$, and that the \vec{H} -field within the superconductor is the same as the applied field in the normal metal. In this free energy density \vec{B} is the independent variable. The thermodynamical potential which is at a minimum in the equilibrium state, is the one where the applied magnetic field \vec{H} is the

independent variable. The relevant thermodynamic potential to be minimized is obtained by a Legendre transformation:

$$\begin{aligned} \mathcal{G}_M &= \mathcal{F}_M - \frac{1}{4\pi} \int \frac{d\vec{r}}{V} \vec{H} \cdot \vec{B} \quad \left(= -\frac{1}{4\pi} \int \frac{d\vec{r}}{V} \left[\int \vec{B} \cdot \delta\vec{H} \right] \right) \\ &= \mathcal{F}_M - \frac{1}{4\pi} \int_0^\infty \frac{dx}{L} H_0^2 e^{-\lambda_L/x} = \mathcal{F}_M - \frac{H_0^2}{4\pi} \frac{\lambda_L}{L} = -\frac{H_0^2}{8\pi} \frac{\lambda_L}{L} \end{aligned} \quad (10)$$

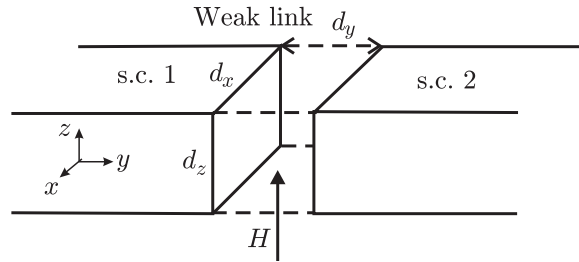
The magnetization in the superconductor is along the z axis and is determined from $\vec{B} = \vec{H} + 4\pi\vec{M}$ to be $M = M(x) = -(1 - e^{-x/\lambda_L})H_0/(4\pi)$. The allowance of the magnetic \vec{B} -field to penetrate into the superconductor gives rise to the energy density gain determined by (10) in comparison with the case of $\vec{B} = \vec{0}$ (or $\lambda_L = 0$). Based on eq. (2.6) in the note “Magnetic energy and domains”, this gain of magnetic energy density may be calculated in a direct fashion as

$$\begin{aligned} \frac{1}{V} \Delta F_M &= - \int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta\vec{H} \right] + \int \frac{d\vec{r}}{V} \left[\int \vec{M} \cdot \delta\vec{H} \right]_{\vec{B}=\vec{0}} \\ &= \int_0^L \frac{dx}{L} \int_0^{H_0} dH \left(1 - e^{-x/\lambda_L} \right) \frac{H}{4\pi} - \int_0^L \frac{dx}{L} \int_0^{H_0} dH \frac{H}{4\pi} \\ &= \int_0^\infty \frac{dx}{L} \int_0^{H_0} dH \left(-e^{-x/\lambda_L} \right) \frac{H}{4\pi} = -\frac{H_0^2}{8\pi} \frac{\lambda_L}{L} = \mathcal{G}_M \end{aligned} \quad (11)$$

[The demagnetization field $\vec{H}_d = -\mathcal{N}\vec{M}$ is neglected in all the calculations, i.e. the sample is assumed to be a thin rod along the field, see problem 27.1]. In case the applied field is equal to the critical field, $H_0 = H_{c_2}$, the interface is stable if, roughly, $2\sqrt{2}\xi H_c^2/(12\pi) - \lambda_L H_c^2/(8\pi) < 0$ or if $\kappa > 4\sqrt{2}/3$. This value is reduced when including interference between the two contributions, i.e. that λ_L becomes larger close to the surface where $|\Psi|$ is reduced.

27.3 Diffraction effects in Josephson junctions

The figure shows a weak link of normal metal (dashed lines) between two parts of a superconductor. The magnetic field \vec{H} is applied in the z direction. $\vec{B} = \vec{0}$ within the superconductors, whereas $\vec{B} = \vec{H}$ in the normal metal. The magnetic flux through the weak link is $\Phi = \mathcal{A}B = \mathcal{A}H$, where the area is $\mathcal{A} = d_x d_y$.



(a) With the choice of the Landau gauge, the vector potential within the normal metal is

$$\vec{A} = (0, xH, 0), \quad \Rightarrow \quad \nabla \times \vec{A} = (0, 0, H) = \vec{B}, \quad \nabla \cdot \vec{A} = 0 \quad (1)$$

(see also problem 25.4).

(b) The path integral, calculated at a constant x , between the two superconductors 1 and 2 is

$$\int_1^2 d\vec{s} \cdot \vec{A} = \int_0^{d_y} x H dy = H d_y x \quad (2)$$

The current density in the y direction between the two superconductors, (27.68a), is independent of z (when staying within the cross-section of the normal metal):

$$j(x) = j_0 \sin \left(\phi_2 - \phi_1 + \frac{2e}{\hbar c} \int_1^2 d\vec{s} \cdot \vec{A} \right) = j_0 \sin \left(\phi_2 - \phi_1 + \frac{4\pi}{\Phi_0} H d_y x \right) \quad (3)$$

The magnetic flux quantum is here defined, (25.51), $\Phi_0 = hc/e$, however, in much of the literature on superconductivity, the flux quantum is defined as the one applying for Cooper-pairs, i.e. $\Phi_0 = hc/e^*$. The total current is

$$\begin{aligned} J &= \int_0^{d_z} dz \int_0^{d_x} dx j(x) = d_z j_0 \left(\frac{\Phi_0}{4\pi H d_y} \right) \left[-\cos \left(\phi_2 - \phi_1 + \frac{4\pi H d_y}{\Phi_0} x \right) \right]_0^{d_x} \\ &= (d_z d_x) j_0 \frac{\Phi_0}{4\pi \Phi} \left\{ \cos(\phi_2 - \phi_1) - \cos \left(\phi_2 - \phi_1 + \frac{4\pi \Phi}{\Phi_0} \right) \right\} \end{aligned} \quad (4)$$

when introducing the total magnetic flux $\Phi = d_x d_y H$. Defining $J_0 = d_z d_x j_0$ and using the general cosine relation: $\cos(u - v) - \cos(u + v) = 2 \sin u \sin v$, we finally get

$$J = J_0 \frac{\Phi_0}{2\pi \Phi} \sin \left(\phi_2 - \phi_1 + \frac{2\pi \Phi}{\Phi_0} \right) \sin \left(\frac{2\pi \Phi}{\Phi_0} \right) \quad (5)$$

(c) At zero voltage the phases of the wave functions in the superconductors 1 and 2, ϕ_1 and ϕ_2 , are constant in time. The result (5) clearly shows that the maximum current at a certain field and zero voltage is

$$J_{\max} = J_0 \frac{\Phi_0}{2\pi \Phi} \left| \sin \left(\frac{2\pi \Phi}{\Phi_0} \right) \right| \quad (6)$$
