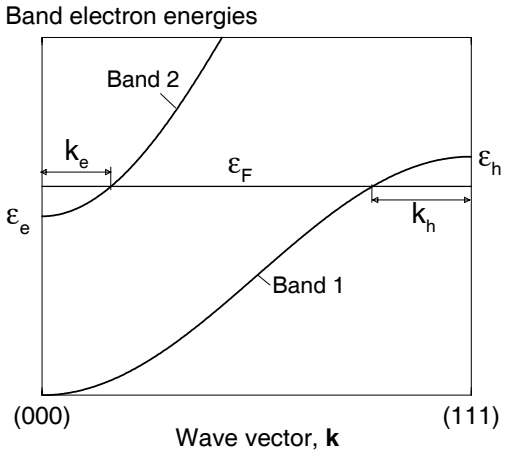
Problems in Solid State Physics II (2005-2010)

Problem 2005-I

In an fcc crystal, the Fermi surface consists of an electron-like sphere centered at (000) and a hole-like sphere around (111). The two lowest lying electronic bands are shown on the figure, and the energies are assumed to be:



Band 1, close to (111):

$$\varepsilon_h(\vec{k}) = \varepsilon_h - \frac{\hbar^2(\vec{k}-\vec{k}_{(111)})^2}{2m_h}\,.$$

Band 2, close to (000): $\varepsilon_e(\vec{k}) = \varepsilon_e + \dfrac{\hbar^2\vec{k}^2}{2m_e}\,, \quad \varepsilon_e = \varepsilon_h - \Delta\,.$

Here $\vec{k}_{(111)}$ is the position of the reciprocal lattice point (111) [the one closest to $\vec{k}$]. The system is assumed to contain two band electrons per unit cell.

1) What would happen if the energy difference $\Delta = \varepsilon_h - \varepsilon_e$ were negative?

Determine the following quantities in the zero temperature limit, when Δ is positive (and $\ll \varepsilon_F$). The results should be expressed in terms of the principal model parameters ε_h, Δ, m_e, m_h, and τ, a constant relaxation time assumed to be the same for both bands:

2) ε_F, the Fermi energy.

3) n and p, the electron and hole densities, respectively.

4) $\gamma = c_V/T$, where c_V is the specific heat per unit volume.

5) σ, the (isotropic) conductivity.

In the presence of a magnetic field B along the z axis, the xy part of the conductivity tensor for an isotropic, one-band system may be written:

$$\overline{\overline{\sigma}} = \frac{\sigma_0}{1+(\mathcal{R}B\sigma_0)^2}\begin{pmatrix} 1 & \mathcal{R}B\sigma_0 \\ -\mathcal{R}B\sigma_0 & 1 \end{pmatrix}$$

where σ_0 is the zero-field conductivity and $\mathcal{R}$ is the Hall coefficient.

6) What is the Hall coefficient of the present two-band system in the limit $|\mathcal{R}B\sigma_0| \gg 1$?

7) Calculate the electron density n, when $\Delta = 0.1$ eV, and $m_e = m_h = m$ (m is the mass of the electron).

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Problem 2005-II

The band energies of the conduction electrons in a tetragonal crystal is given by

$$\varepsilon(\vec{k}) = \frac{\hbar^2}{2m_1}\,(k_x^2 + k_y^2) + \frac{\hbar^2}{2m_2}\,k_z^2\,. \tag{1}$$

1) Describe the Fermi surface within the $\vec{k}$-space.

2) Write down the electrical conductivity tensor $\overline{\overline{\sigma}}$ (at zero magnetic field), when assuming a constant relaxation time τ. The density of the conduction electrons is n.

3) Determine the density of states $D(\varepsilon)$ of the conduction electrons.

The system may be mapped on an isotropic one by the following transformation

$$\vec{k}' = \overline{\overline{T}}\,\vec{k} = \left(k_x, k_y, \sqrt{\frac{m_1}{m_2}}\,k_z\right)\,, \qquad \overline{\overline{T}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \sqrt{\frac{m_1}{m_2}} \end{pmatrix} \tag{2}$$

The semiclassical equation of motion for $\hbar\dot{\vec{k}}$ is transformed into the equivalent one

$$\hbar\dot{\vec{k}}' = -e\,\vec{E}' - \frac{e}{c}\,\vec{v}' \times \vec{B}' \tag{3}$$

when introducing $\hbar\vec{v}' = \partial\varepsilon/\partial\vec{k}'$ and when replacing $\vec{E}$ and $\vec{B}$ by the transformed field vectors $\vec{E}'$ and $\vec{B}'$.

4) Derive the expressions for the primed vectors $\vec{v}'$, $\vec{E}'$ and $\vec{B}'$ in terms of the corresponding unprimed ones. Express the results both in terms of the Cartesian components and in terms of $\overline{\overline{T}}$ [like in eq. (2) in the case of $\vec{k}'$].

The primed conductivity tensor is defined by $\vec{j}' = -ne\langle\vec{v}'\rangle = \overline{\overline{\sigma}}'\vec{E}'$.

5) Determine the relation between $\overline{\overline{\sigma}}$ and $\overline{\overline{\sigma}}'$ (in terms of $\overline{\overline{T}}$).

In the presence of a magnetic field B along the x axis, the resistivity tensor for an isotropic ($m_1 = m_2$) system may be written:

$$\overline{\overline{\rho}} = \begin{pmatrix} \sigma_0^{-1} & 0 & 0 \\ 0 & \sigma_0^{-1} & -\mathcal{R}B \\ 0 & \mathcal{R}B & \sigma_0^{-1} \end{pmatrix} \tag{4}$$

where σ_0 is the zero-field conductivity and $\mathcal{R} = -(nec)^{-1}$ is the Hall coefficient.

6) Determine the resistivity tensor in the present, more general case ($m_1 \neq m_2$). What is the resulting Hall coefficient?

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Problem 2005-III

We shall consider a semimetal where there is an equal concentration n of electrons with mass m_e and holes of mass m_h, i.e. $p = n$. The equation-of-motion for the electrons is

$$m_e \dot{\vec{v}}_e = -e\left(\vec{E} + \frac{\vec{v}_e}{c} \times \vec{B}\right) - m_e \frac{\vec{v}_e}{\tau}\,, \tag{1}$$

when assuming the Drude model. The semimetal is placed in a constant magnetic field, applied along the z axis, and a time-dependent, circularly polarized electric field, applied perpendicular to the magnetic one:

$$\vec{B} = B\,\hat{z}, \qquad \vec{E} = E\,e^{-i\omega t}\,(\hat{x} + i\,\hat{y}) \tag{2}$$

(B and E are constants and $\hat{\alpha}$ is the unit vector along the α axis).

1) Show that $\vec{v}_e = v_e e^{-i\omega t}(\hat{x} + i\,\hat{y})$ is a solution of (1) in the presence of the fields given by (2), and derive the expression for the constant v_e.

2) Show that the frequency-dependent conductivity of this system, with $p = n$, is

$$\sigma(\omega) = i\frac{e^2 n(m_e + m_h)\left(\omega + \frac{i}{\tau}\right)}{m_e m_h \left(\omega - \omega_e + \frac{i}{\tau}\right)\left(\omega + \omega_h + \frac{i}{\tau}\right)}\,, \tag{3a}$$

where

$$\omega_e = \frac{eB}{m_e c}\,, \qquad \omega_h = \frac{eB}{m_h c}\,. \tag{3b}$$

3) Use this result (3) to determine the zero-frequency conductivity $\sigma(0)$, when the magnetic field $B = 0$.

4) Determine the frequency-dependent conductivity $\sigma(\omega)$ in the limit $(\omega_e, \omega_h) \gg \omega \gg 1/\tau$.

5) Derive the dispersion relation, $\omega = \omega(q)$, for the transverse light waves in this medium from the relation $\omega^2\epsilon(\omega) = c^2q^2$, when assuming $(\omega_e, \omega_h) \gg \omega \gg 1/\tau$ and $\epsilon(\omega) \gg 1$.

6) Calculate the velocity of these "Alfvén" waves in the case of $B = 10$ kG, $n = 10^{19}$ cm^{-3}, and $m_e = m_h = 9 \times 10^{-28}$ g.

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Problem 2006: The Ising model in a transverse field

In the non-interacting case the Hamiltonian of any single site in the crystal is

$$\mathcal{H}_1 = -\Gamma\,\sigma^x - \mu_B H\,\sigma^z\,, \qquad \Gamma > 0 \tag{1}$$

where σ^α are the Pauli spin-operators, $[\sigma^x, \sigma^y] = 2i\sigma^z$. In the Heisenberg representation the equation of motion of an operator A is

$$\frac{dA}{dt} = \frac{i}{\hbar}\,[\mathcal{H}, A] \tag{2}$$

1) Determine the equation of motion for σ^z $\left(\text{calculate } \dfrac{d^2\sigma^z}{dt^2}\right)$.
The site is in equilibrium with the surroundings of temperature $T = 1/(k_B\beta)$. The density of sites in the crystal is $n = N/V$, and the field is assumed to be $H = H_\omega(t) = H_0 e^{-i\omega t}$.

2) Show that the (non-interacting) frequency-dependent susceptibility is

$$\chi_0(\omega) \equiv n\mu_B \frac{\langle\sigma^z(t)\rangle - \langle\sigma^z\rangle}{H_\omega(t)}\Big|_{H_\omega\to 0} = n\mu_B^2 \frac{4\Gamma\,\tanh(\beta\Gamma)}{4\Gamma^2 - (\hbar\omega)^2} \tag{3}$$

where $\langle\sigma^z(t)\rangle$ is the thermal average of the time-dependent operator at $H_\omega = 0$, and $\langle\sigma^z\rangle$ is the same, when neglecting the time-dependent part of $\sigma^z(t)$.

We now turn to the interacting case, where the Hamiltonian is

$$\mathcal{H} = -J \sum_{<ij>} \sigma_i^z \sigma_j^z + \sum_i \mathcal{H}_1(i)\,, \qquad J > 0 \tag{4}$$

$<ij>$ denotes the sum over all distinct z nearest-neighbour pairs of sites.

3) In the paramagnetic phase $n\mu_B\langle\sigma_i^z(t)\rangle = \chi(\omega)H_\omega(t)$. Show that, within the mean-field approximation, the susceptibility in the interacting case is

$$\chi(\omega) = \frac{\chi_0(\omega)}{1 - \chi_0(\omega)\frac{zJ}{n\mu_B^2}} \tag{5}$$

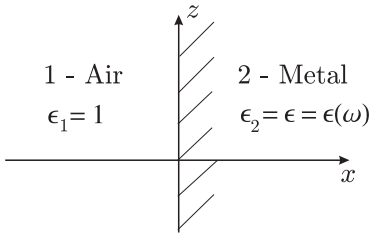
4) Make use of $\chi(0)$ for deriving an equation, which determines the Curie temperature $T_{\rm C}$. Find the condition that this equation has a solution and make a sketch of $T_{\rm C}$ as a function of $\Gamma \geq 0$.

5) Determine the excitation energies $\hbar\omega$, i.e. the resonance energies at which $\chi(\omega)$ diverges, when $T \geq T_{\rm C}$. Sketch the excitation energies as functions of $T \geq T_{\rm C}$ (and, if you have time, make a guess of what happens with the excitations below $T_{\rm C}$).

(opgavesættet er slut)

Problem 2007: Surface plasmons

We are going to consider surface plasmons propagating on an y–z interface between a simple metal at $x > 0$ and air at $x < 0$. The dielectric constant of air is $\epsilon_1 = 1$ and the conductivity tensor of the metal is assumed to be (at $k \ll k_F$)



$$\sigma = \sigma(\vec{k}, \omega) = \frac{ne^2\tau}{m} \frac{1}{1 - i\omega\tau} \tag{1}$$

1) Determine the dielectric constant of the metal $\epsilon_2 = \epsilon = \epsilon(\omega)$ in terms of the cyclic plasma frequency ω_p in the limit of $\omega\tau \gg 1$.

2) In the case of no external charges (or currents), the solution of the Maxwell equations is assumed to be of the form

$$\vec{E} = \begin{cases} \vec{E}_1 = A \left(1, 0, \dfrac{i\lambda}{k}\right) \; e^{\lambda x} \, e^{i(kz - \omega t)} & , \quad x < 0 \\ \vec{E}_2 = A \left(\dfrac{1}{\epsilon}, 0, \dfrac{i\lambda}{k}\right) e^{\epsilon\lambda x} \, e^{i(kz - \omega t)} & , \quad x > 0 \end{cases} \tag{2}$$

Show that this solution fulfills the boundary conditions at the $x = 0$ interface, $\vec{E}_1 \times \hat{\vec{x}} = \vec{E}_2 \times \hat{\vec{x}}$ and $\vec{D}_1 \cdot \hat{\vec{x}} = \vec{D}_2 \cdot \hat{\vec{x}}$, and that $\nabla \cdot \vec{E} = 0$ for $x \neq 0$. What are the necessary conditions on λ and ϵ, if this solution should be characterized as a surface (interface) wave?

3) Show that $\nabla \times \nabla \times \vec{E} = -\nabla^2 \vec{E}$, when $x \neq 0$. In this case the remaining Maxwell equations lead to the "wave equation"

$$\nabla^2 \vec{E} = \frac{1}{c^2} \frac{\partial^2 \vec{D}}{\partial t^2} \,, \qquad x \neq 0 \tag{3}$$

Use this equation to determine λ and k as functions of ω, ϵ, and c, and state the condition which ϵ has to fulfill.

4) Derive the final relation between $(kc)^2$ and ω^2 in terms of ω_p (when $\omega\tau \gg 1$). What are the simplified relations in the two limits $kc \ll \omega_p$ and $kc \gg \omega_p$. Make a sketch of ω as a function of kc.

5) Determine the relation between λ and k in the limit of $kc \gg \omega_p$, and describe the polarization of the surface wave in this limit. – In potassium metal the density of the conduction electrons is $n = 1.33 \cdot 10^{22}$ cm^{-3}. Calculate the plasma frequency, the wave number $k = k_p$ at which value $kc = \omega_p$, and the ratio between this k_p and the Fermi wave number k_{F} in potassium.

(opgavesættet er slut)

Problem 2008: Thermodynamics of a superconductor

We are going to consider a type 1 superconductor. The sample, in the shape of a long thin needle, is placed in a uniform field H_0 applied along the direction of the needle. Neglecting surface effects ($\lambda \approx 0$ and $\xi \approx 0$ compared with the dimensions of the sample), the superconductor is in a uniform state and the differential of its Gibbs free energy is

$$dG = -SdT - V\mathbf{M} \cdot d\mathbf{H}_0 \tag{1}$$

where S is the entropy, T is the temperature, $\mathbf{M}$ is the magnetization, and V is the volume of the superconductor.

1) Explain why the free energy may be written

$$G = G_s(T, H_0) = \frac{V}{8\pi}\left[H_0^2 - H_c^2(T)\right] + G_n(T) \tag{2}$$

where $H_c(T)$ is the critical field of the superconductor. $G_n(T)$ is the free energy of the metal in the normal state, which is assumed to be unaffected by the applied field.

2) Empirically, the critical field is determined from its zero temperature value $H_c(0)$ according to

$$H_c(T) = H_c(0)\left(1 - t^2\right), \quad t = \frac{T}{T_c} \tag{3}$$

where T_c is the critical temperature. Show that this expression for the critical field predicts the heat capacity at zero field to be

$$C_s = \frac{V}{2\pi T_c} H_c^2(0)\left(3t^2 - 1\right)t + C_n, \qquad (t \leq 1) \tag{4}$$

where C_n is the heat capacity of the normal metal.

3) The BCS-theory predicts the energy gain of the superconducting state at zero temperature to be

$$U = G_s(0,0) - G_n(0) = -\sum_{\vec{k}} \frac{(E_{\vec{k}} - |\xi_{\vec{k}}|)^2}{2E_{\vec{k}}} \tag{5}$$

Here $\xi_{\vec{k}} = \varepsilon_{\vec{k}} - \varepsilon_F$ is the energy of the band electrons relatively to the Fermi energy ε_F, and $E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \Delta^2}$, where Δ is the BCS energy gap. Show that

$$U = -\frac{1}{4} V D(\varepsilon_F) \Delta^2 \tag{6}$$

when $\Delta \ll \varepsilon_F$. Here $D(\varepsilon)$ is the density of states per unit volume of the band electrons. **Hints:** (i) The summation in (5) only involves the different $\vec{k}$ states – there is no σ-sum over two different spin states. (ii) Because $\Delta \ll \varepsilon_F$, the

term in the $\vec{k}$-sum is only non-zero, when $\xi_{\vec{k}} \approx 0$ or $\varepsilon_{\vec{k}} \approx \varepsilon_F$, and the density of states $D(\varepsilon_k)$ stays approximately constant at $D(\varepsilon_F)$. (iii) Finally,

$$\int_0^\infty \frac{\left(\sqrt{x^2+1}-x\right)^2}{\sqrt{x^2+1}} dx = \frac{1}{2} \tag{7}$$

4) The relation between the BCS energy gap and the transition temperature is $\Delta = \alpha\, k_B T_c$, where $\alpha = \pi/e^\gamma \simeq 1.764$. Use this relation for calculating the ratio

$$\frac{C_s - C_n}{C_n}, \quad T = T_c \tag{8}$$

when assuming that $T_c \ll T_F$ is so small that only the normal metallic electrons contribute to C_n (i.e. that the phonon contributions may be neglected).

5) Make a sketch of the heat capacity as a function of temperature, from slightly above T_c to zero temperature, based on the results above (neglecting phonon contributions); i.e., assume a certain behaviour of the heat capacity of the normal metal and show the corresponding relative variation of the heat capacity of the superconductor.

The density of band electrons in Al metal is $n = 3 \times 6.02 \cdot 10^{22}$ cm^{-3} and $T_c = 1.18$ K. Use these numbers for calculating ε_F, Δ, and $H_c(0)$ in the case of aluminium using estimates deriving from the free-electron model whenever needed. Notice, there is a misprint in Marder's equation (6.33). It should read:

$$D\left(\mathcal{E}_F\right) = \frac{3}{2}\frac{n}{\mathcal{E}_F} = 4.11 \times 10^{-2} [n \cdot \text{Å}^3]^{1/3} \text{eV}^{-1} \text{Å}^{-3} \tag{6.33}$$

(opgavesættet er slut)

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

The energies $\varepsilon(\vec{k})$ of the electrons in one particular band in a cubic crystal are assumed to be described by the tight-binding model, i.e.

$$\varepsilon(\vec{k}) = E_0 \left[3 - \cos(ak_x) - \cos(ak_y) - \cos(ak_z)\right], \tag{1}$$

where a is the cubic lattice parameter (or lattice spacing). (k_x, k_y, k_z) are the components of $\vec{k}$ along the three cubic axes of the lattice, and E_0 is a positive constant.

1) Find the energy minimum $\varepsilon_{\min}$ and maximum $\varepsilon_{\max}$ of the band (the answer should include both the energies and the corresponding $\vec{k}$). Determine the threshold value of the Fermi energy $\varepsilon_{\rm F}$, where the Fermi surface starts to touch the boundaries of the (first) Brillouin zone.

There are electrons placed in other bands contributing to the total conductivity $\sigma_{\rm tot}$. Here we are going to discuss only the separate contribution from the electrons in the band determined by eq. (1). The other bands only serve the purpose that the number of electrons placed in the present band may be varied in a continuous way. What is the basic rule, within the semiclassical approximation, which allows us to consider the separate conductivity σ_i due to the ith band, and how is $\sigma_{\rm tot}$ determined in terms of the different σ_i?

2) Show that the effective conductivity mass m^* of the cubic system, introduced by eq. (17.50) in Marder, is determined by:

$$\frac{m_0}{m^*} = \frac{m_0}{3n}\int [d\vec{k}] f_{\vec{k}} {\rm Tr}(\mathbf{M}^{-1}) = 1 - \frac{\langle\varepsilon\rangle}{3E_0}, \qquad m_0 = \frac{\hbar^2}{E_0 a^2}, \tag{2}$$

where

$$\langle\varepsilon\rangle = \frac{1}{n}\int [d\vec{k}] f_{\vec{k}} \varepsilon(\vec{k}), \qquad n = \int [d\vec{k}] f_{\vec{k}}\,, \tag{3}$$

and $f_{\vec{k}}$ is the Fermi function at the energy $\varepsilon(\vec{k})$.

3) In this question we shall consider the limit $\varepsilon(\vec{k}) \leq \varepsilon_{\rm F} \ll E_0$ and $T \ll T_{\rm F}$. Write down a simplified expression for $\varepsilon(\vec{k})$ valid in this limit. Determine $\varepsilon_{\rm F}$ and $\langle\varepsilon\rangle$ in terms of the model parameters (E_0 and a) and the density n of the electrons (charge $-e$), and write down the corresponding expression for the conductivity based on eq. (2), when assuming a constant relaxation time τ.

4) Find $\langle\varepsilon\rangle$ and σ in the case where $n = 2/a^3$. Determine the conductivity in the limit $0 < \varepsilon_{\max} - \varepsilon_{\rm F} \ll E_0$ to the same accuracy as obtained in the previous question (apply arguments rather than calculations). The Fermi surface supports closed but no open orbits, when $\varepsilon_{\rm F}$ is lying in two different intervals. Specify the two intervals and the corresponding Hall coefficients $\mathcal{R}$.

(opgavesættet er slut)

Problem 2010: Magnetic properties of band electrons

We are going to consider the electrons in a single band of a metallic crystal. The energies $\varepsilon_{\vec{k}}$ of the band electrons are assumed to lead to the following density of states per unit volume

$$D_0(\varepsilon) = \frac{1}{V}\sum_{\vec{k},\sigma}\delta(\varepsilon-\varepsilon_{\vec{k}}) = \frac{2}{V}\sum_{\vec{k}}\delta(\varepsilon-\varepsilon_{\vec{k}}) = \begin{cases} D & 0<\varepsilon<W \\ 0 & \varepsilon<0\ ,\ W<\varepsilon \end{cases} \tag{1}$$

σ is the spin variable which takes on two values $\uparrow$ or $\downarrow$. The density of electrons occupying the band is $n_0 = N/V$, where N is the number of unit cells in the volume V.

1) What is the value of the constant D in terms of the density n_0 and the bandwidth W? What is the Fermi energy ε_F^0 of the present system?

The coulomb interaction between the electrons leads to spin dependent exchange effects because of the Pauli principle. Assuming that most of the spin independent contributions are accounted for by $\varepsilon_{\vec{k}}$, a simplified version of the total Hamiltonian is

$$\mathcal{H} = \sum_{\vec{k}}\varepsilon_{\vec{k}}\left(\hat{n}_{\vec{k}\uparrow}+\hat{n}_{\vec{k}\downarrow}\right) + \frac{U}{N}\sum_{\vec{k},\vec{k}'}\hat{n}_{\vec{k}\uparrow}\,\hat{n}_{\vec{k}'\downarrow} + \mu_B H\sum_{\vec{k}}\left(\hat{n}_{\vec{k}\uparrow}-\hat{n}_{\vec{k}\downarrow}\right) \tag{2}$$

in the presence of a field H applied along the z axis. Here $\hat{n}_{\vec{k}\sigma} = 0$ or 1 is the operator for the number of electrons in the state $|\vec{k},\sigma\rangle$. When applying the mean-field approximation this Hamiltonian may be written

$$\mathcal{H} \cong \mathcal{H}_{\rm MF} = \mathcal{E}_0 + \sum_{\vec{k},\sigma}E_{\vec{k}\sigma}\hat{n}_{\vec{k}\sigma}, \qquad E_{\vec{k}\sigma} = \varepsilon_{\vec{k}} + \Delta_\sigma \tag{3}$$

2) Find the energies $\Delta_\uparrow$, $\Delta_\downarrow$ and $\mathcal{E}_0$. Express the results in terms of the parameters introduced by Eq. (2) and the spin-up and spin-down electron densities $n_\uparrow$ and $n_\downarrow$, where

$$n_\sigma = \frac{1}{V}\sum_{\vec{k}}\langle\hat{n}_{\vec{k}\sigma}\rangle = \frac{1}{V}\sum_{\vec{k}}f_{\vec{k}\sigma} \tag{4}$$

$\langle\hat{n}_{\vec{k}\sigma}\rangle$ is the thermal expectation value of $\hat{n}_{\vec{k}\sigma}$ and is equal to the Fermi function $f_{\vec{k}\sigma}$. How is $f_{\vec{k}\sigma}$ determined in the present mean-field approximation (write down the expression for the Fermi function and the general condition that determines the chemical potential μ)?

3) Evaluate the spin-dependent density of states

$$D_\sigma(\varepsilon) = \frac{1}{V}\sum_{\vec{k}}\delta(\varepsilon-E_{\vec{k}\sigma}) \tag{5}$$

in terms of W, n_0 and Δ_σ. Calculate the magnetic susceptibility

$$\chi = \lim_{H\to 0}\left(\frac{M}{H}\right), \qquad M = \mu_B(n_\downarrow - n_\uparrow) \tag{6}$$

in the zero temperature limit, when assuming U to be small compared to W.

4) The energy density at zero temperature is

$$\frac{\mathcal{E}}{V} = \frac{1}{V}\langle\mathcal{H}\rangle = \frac{1}{4}n_0(W+U) + \frac{1}{4}n_0(W-U)\left(\frac{M}{\mu_B n_0}\right)^2 - MH \tag{7}$$

The zero-temperature susceptibility is going to diverge when U approaches a critical value U_c. What is the critical value U_c? Write a short discussion of the properties of the system in the two different cases, $U < U_c$ and $U > U_c$. Try to answer questions like: What is the ground state and the corresponding energy density? What is the zero-temperature value of the magnetization M? Make a sketch of the spin-dependent densities of states (when $U > U_c$). What about the conductivity? What happens if we start to heat the system?

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Condensed Matter Physics 2
Skriftlig eksamen - April 2011

2-timers skriftlig prøve. Sædvanlige hjælpemidler er tilladte (bøger, noter og lommeregner). Opgaverne må gerne besvares med blyant.

Problem 1: Ferromagnet. Atoms with spin $s = \frac{1}{2}$ are placed on an fcc lattice with lattice constant a (primitive lattice vectors with length $\frac{a}{\sqrt{2}}$) and volume V. The atomic spin at the ith site $\vec{s}_i$ interacts with its neighbours as described by the Heisenberg Hamiltonian:

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J(i,j)\,\vec{s}_i \cdot \vec{s}_j \tag{1}$$

$J(i,j) = J_1 > 0$, if i and j are nearest neighbours
$J(i,j) = J_2 > 0$, if i and j are next-nearest neighbours
$J(i,j) = 0$, if i and j are not nearest or next-nearest neighbours

a) Find the ground state energy (the internal energy at zero temperature) of this spin system in terms of J_1, J_2, a, and V.

b) Show that the present spin system and the simple Ising model discussed by Marder in Section 24.4 become equivalent when applying the mean-field approximation. (Hint: assume the presence of an infinitesimal magnetic field along the z axis).

c) Utilize this equivalence for determining the mean-field value for the ordering temperature T_C of the present spin system.

Problem 2: Non-interacting spin-dimer system. The lattice describing the system has a basis that contains two identical atoms 1 and 2 with spins $\vec{s}_1$ and $\vec{s}_2$. The spins have $s = \frac{1}{2}$ and are coupled with each other. Any other spin interactions between different pairs or "dimers" are neglected. Hence, the spin Hamiltonian is

$$\mathcal{H} = -J\sum_{i=1}^{N} \vec{s}_1(i)\cdot\vec{s}_2(i) - g\mu_B\vec{H}\cdot\sum_{i=1}^{N}\left[\vec{s}_1(i)+\vec{s}_2(i)\right] \tag{2}$$

in the presence of a magnetic field $\vec{H}$. The density of spins is twice the number of unit cells per unit volume, i.e. $n = 2N/V$.

a) Determine the eigenenergies for a single spin dimer in terms of J and H (choose the z axis to be parallel with $\vec{H}$).

b) What is the magnetic susceptibility $\chi = \frac{\partial M}{\partial H}\big|_{H\to 0}$ of this system, if the interaction J is neglected?

c) Determine χ in the temperature range where $k_B T \ll |J|$ in the two cases $J > 0$ and $J < 0$ (use arguments rather than calculations in your answer).

(the problems are continuing on next page)

Problem 3: Anisotropic band electrons. The band energies of the conduction electrons in a crystal with orthorhombic symmetry are given by

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2} + \frac{\hbar^2 k_z^2}{2m_3} \tag{3}$$

where the x, y, and z axes are parallel with each one of the three orthorhombic lattice vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$. The density of the conduction electrons is n.

a) Describe the constant energy surface (Fermi surface) within reciprocal space.

b) Write down the electrical conductivity tensor $\overline{\overline{\sigma}}$ (at zero magnetic field) when assuming a constant relaxation time τ.
Use this result for determining the direction of the current density $\vec{j}$ when an electric field $\vec{E}$ is applied in a direction which is perpendicular to the z axis and makes an angle of 45° with the x axis.

c) The density of states for the anisotropic band electrons is the same as for free electrons, if the electron mass is replaced by an effective mass m^*. Determine m^* in terms of the three band masses m_1, m_2, and m_3.
The low-temperature specific heat is $c_V = \gamma T$. Derive the expression for the Sommerfeld constant γ in terms of the three band masses and the density n.

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