Condensed Matter Physics 2

Skriftlig eksamen - April 2011

Answer to Problem 1: Ferromagnet

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

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

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

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

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

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

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

$$T_C = \underline{\left(3J_1 + \tfrac{3}{2}J_2\right)/k_B} \qquad (a3)$$

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

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

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

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

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

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

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

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

$$\chi = (g\mu_B)^2 \frac{2N}{V} \frac{s(s+1)}{3k_BT} = \underline{\frac{n(g\mu_B)^2}{4k_BT}} \qquad (a6)$$

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

$$\begin{aligned} \chi_1 &= (g\mu_B)^2 \frac{N}{V} \frac{S(S+1)}{3k_BT} = \underline{\frac{n(g\mu_B)^2}{3k_BT}} \qquad (J > 0) \\ \chi_0 &= \underline{0} \qquad (J < 0) \end{aligned} \qquad (a7)$$

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

Answer to Problem 3: Anisotropic band electrons

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

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

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

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

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

c) Introducing a new vector variable

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

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

$$\begin{aligned} D(\varepsilon) =& \frac{2}{(2\pi)^3}\int d\vec{k}\,\delta\big(\varepsilon - \varepsilon(\vec{k})\big) = \left(\frac{m_1m_2m_3}{m^3}\right)^{\frac{1}{2}} \frac{2}{(2\pi)^3}\int d\vec{k}'\,\delta\big(\varepsilon - \varepsilon(\vec{k}')\big) \\ =& \left(\frac{m_1m_2m_3}{m^3}\right)^{\frac{1}{2}} \frac{\sqrt{2m^3\varepsilon}}{\hbar^3\pi^2} = \frac{\sqrt{2(m^*)^3\varepsilon}}{\hbar^3\pi^2}, \quad \underline{m^* = (m_1m_2m_3)^{\frac{1}{3}}} \end{aligned} \qquad (a11)$$

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

$$\gamma = \underline{\frac{k_B}{\hbar^2}\left(\frac{\pi^2}{9}m_1m_2m_3n\right)^{\frac{1}{3}}} \qquad (a12)$$