Magnetism in materials

solutions Week 08

1. The dependence of the resistivity (ρ) on temperature (T), including the Kondo effect, is written as:

$$\rho(T) = \rho_0 - \mu \ln(T) + aT^5$$

where ρ_0 is the residual resistivity, a is a constant independent of temperature, and μ is proportional to the concentration of magnetic impurities. It has been found that the electrical resistivity of dilute magnetic alloys shows a minimum at a characteristic temperature. Use the above formula to find how the minimum of the electrical resistivity behaves as a function of impurity concentration.

The following figure depicts the variation of resistivity of Cu diluted by Fe (the numbers next to the plots show the impurity concentration). Can you qualitatively see if the minimum of the resistivity shows the same behavior as you have found out?

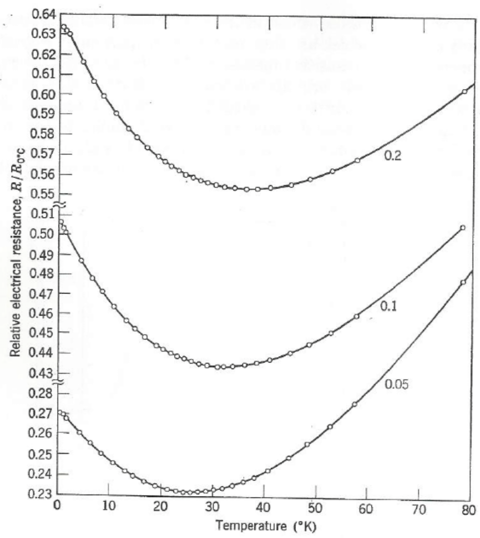

Figure 1: Electrical resistivity of Cu with Fe as solute. The nominal atomic concentration of Fe is indicated on each curve. (D.K.C. MacDonald, Thermoelectricity, Dover, 2006).

Solution The resistivity minimum can be determined by setting the derivative of resistivity with respect to temperature equal to zero:

$$\frac{d\rho(T)}{dT} = -\frac{\mu}{T} + 5aT^4 = 0$$

which leads to:

$$T_{\min} = \left(\frac{\mu}{5a}\right)^{\frac{1}{5}}.$$

The temperature at which the electrical resistivity reaches a minimum varies as the one-fifth power of the concentration of magnetic impurities. This observation aligns with experimental findings, where qualitatively, $T_{\min}$ decreases as the impurity concentration decreases.

2. Consider a system composed of 2 ions and 2 electrons, described by the Hubbard model:

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma}) + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

where $c^\dagger_{i\sigma}$ denotes the electron creation operator at site i, and $\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ represents the number operator. Determine the ground state energy and wavefunction of the system. Discuss the behavior of the ground state energy as $U/t \to 0$ and $U/t \to \infty$.

Hint: Assume that ((due to some symmetry reasons) the ground state is symmetric with one spin-up and one spin-down electron on each site, leading to a wavefunction of the form:

$$|\psi\rangle = a(c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow} c^\dagger_{2\downarrow})|0\rangle + b(c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} + c^\dagger_{2\uparrow} c^\dagger_{1\downarrow})|0\rangle$$

Solution Using the ground state wavefunction form:

$$|\psi\rangle = a(c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow} c^\dagger_{2\downarrow})|0\rangle + b(c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} + c^\dagger_{2\uparrow} c^\dagger_{1\downarrow})|0\rangle$$

and asserting $\hat{H}|\psi\rangle = E|\psi\rangle$ leads to two equations:

$$(E - U)a + 2tb = 0$$

and

$$2ta + Eb = 0$$

Solving for E, we obtain two solutions for energy, with the lower energy representing the ground state energy:

$$E_0 = \frac{1}{2}(U - \sqrt{U^2 + 16t^2})$$

and for the ground state wavefunction, $\frac{a}{b} = -\frac{E_0}{2t}$.

In the limit $U/t \to 0$,

$$E_0 \approx -2t + \frac{U}{2} - \frac{U^2}{16t^2} + \cdots$$

and in the limit $t/U \to 0$,

$$E_0 \approx -\frac{4t^2}{U} + \cdots$$

In both cases, we perform a binomial expansion of $\sqrt{U^2 + 16t^2}$, one by assuming $U \ll t$ and the other by assuming $t \ll U$.

3. Show that the density of states at the Fermi energy levels in one dimension is given by

$$g(E_F) = \frac{n}{2E_F} = \frac{2m}{\hbar^2 \pi k_F}$$

Show that the q-dependent susceptibility of the electron gas in one dimension is given by

$$\chi_{\mathbf{q}} = \chi_P \frac{k_F}{q} \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \tag{1}$$

where $\chi_P = \frac{g^2 \mu_0 \mu_B^2}{4} g(E_F)$ is the Pauli susceptibility

Solution Considering a sample of length L, each wavevector occupies in k-space a "volume" $\frac{2\pi}{L}$, so calling N the number of states with wavevector $|k_0| < k$, accounting for the two possible spin states

$$dN = \frac{2L}{\pi} dk \tag{2}$$

and normalizing per unit length

$$dn = \frac{2}{\pi} dk \tag{3}$$

so that

$$n = \int_0^{k_F} \frac{2}{\pi} dk = \frac{2}{\pi} k_F \tag{4}$$

for a free electron gas

$$E = \frac{\hbar^2 k^2}{2m} \tag{5}$$

$$\sqrt{\frac{m}{2E}} \frac{dE}{\hbar} = dk \tag{6}$$

$$g(E) = g(k) \frac{dk}{dE} = \frac{1}{\pi\hbar} \sqrt{\frac{2m}{E}} \tag{7}$$

$$n = \int_0^{E_F} g(E) dE = \frac{\sqrt{2m}}{\pi\hbar} 2\sqrt{E_F} \tag{8}$$

so

$$g(E) = \frac{n}{2\sqrt{E_F}} \frac{1}{\sqrt{E}} \tag{9}$$

$$g(E_F) = \frac{n}{2E_F} = \frac{2m}{\hbar^2 \pi k_F} \tag{10}$$

When a spatially varying field of the kind $\mathbf{H}(\mathbf{r}) = \mathbf{H_q} \cos(\mathbf{q} \cdot \mathbf{r})$ is applied, first order perturbation theory gives two different wavefunctions for the electron with wavevector $\mathbf{k}$ and spin pointing parallel $\psi_{\mathbf{k}+}$ and antiparall $\psi_{\mathbf{k}-}$ to the field, The magnetization given by electrons with such wavevector is found to be

$$M_{\mathbf{k}}(\mathbf{r}) = \frac{g\mu_0\mu_B}{2}(|\psi_{\mathbf{k}+}|^2 - |\psi_{\mathbf{k}-}|^2) \tag{11}$$

$$= \frac{g^2\mu_0\mu_B^2 m H_q \cos(\mathbf{q}\cdot\mathbf{r})}{\hbar^2 L}\left[\frac{1}{(\mathbf{k}+\mathbf{q})^2 - k^2} + \frac{1}{(\mathbf{k}-\mathbf{q})^2 - k^2}\right] \tag{12}$$

and integrating over all the occupied states

$$M(\mathbf{r}) = M_q \cos(\mathbf{q}\cdot\mathbf{r}) \tag{13}$$

with

$$M_q = \frac{g^2\mu_0\mu_B^2 m H_q}{\hbar^2}\int_{|\mathbf{k}|<k_F} g(k)\left[\frac{1}{(k+q)^2 - k^2} + \frac{1}{(k-q)^2 - k^2}\right] dk \tag{14}$$

$$\int_{|\mathbf{k}|<k_F} g(k)\left[\frac{1}{(k+q)^2 - k^2} + \frac{1}{(k-q)^2 - k^2}\right] dk = \tag{15}$$

$$= 2\int_{-k_F}^{k_F} \frac{g(k)}{(k+q)^2 - k^2} dk \tag{16}$$

$$= \int_{-k_F}^{k_F} \frac{1}{\pi q(q+2k)} dk \tag{17}$$

$$= \frac{1}{2q\pi}[\ln|q + 2k_F||_{-k_F}^{k_F} \tag{18}$$

$$= \frac{1}{2q\pi}\ln\left|\frac{q+2k_F}{q-2k_F}\right| \tag{19}$$

The q-dependent susceptibility is given by $\chi_{\mathbf{q}} = M_{\mathbf{q}}/H_{\mathbf{q}}$, so that

$$\chi_{\mathbf{q}} = \frac{g^2\mu_0\mu_B^2 m}{2q\hbar^2\pi}\ln\left|\frac{q+2k_F}{q-2k_F}\right| \tag{20}$$

$$= \chi_P \frac{k_F}{q}\ln\left|\frac{q+2k_F}{q-2k_F}\right| \tag{21}$$