Assignments to Condensed Matter Theory I
Sheet 12

G. Cuniberti (Phy 4.1.29)
A. Donarini (Phy 3.1.24)

Room H35
Mon 24.07 (h 10.15)

sheet online: http://www-MCG.uni-R.de/teaching/

Problem set: Ferromagnetism

We apply in this exercise sheet the mean field theory to two classical Hamiltonian describing the ferromagnetic properties of ionic magnetic crystals and metallic magnetism. Despite its roughness the mean field theory gives in these two examples already correct physical results.

12.1. Heisenberg model of ionic ferromagnets

Let us consider the Heisenberg Hamiltonian:

$$H = -2\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$

where $\mathbf{S}_i$ is the spin operator for the ion on site i of the christal lattice and J_{ij} is the strength of the interaction between the magnetic moment of the ions on sites i and j. The interaction is generally short range and in first approximation we can truncate it so that it is non-zero only for nearest neighbours:

$$J_{ij} = \begin{cases} J_0 & \text{if } i \text{ and } j \text{ are neighbours} \\ 0 & \text{otherwise} \end{cases}$$

(a) Can you guess the orientation of the spin in the equilibrium energy configuration depending on the sign of J_0 ?

(b) Write the mean field Hamiltonian for the Heisenberg model using the mean field assumption:

$$\langle \mathbf{S}_i \rangle = \langle S_z \rangle \mathbf{e}_z$$

where $\mathbf{e}_z$ is the vector of length 1 in the z direction. Rearrange the result in terms of the average magnetic moment $\mathbf{m}$:

$$\mathbf{m} = 2nJ_0\langle S_z \rangle \mathbf{e}_z$$

where n is number of neighbours.

(c) Calculate the canonical partition function for the mean field Hamiltonian Z_{MF} assuming for simplicity that the ions have spin $S = 1/2$.
Hint: Z_{MF} is written as:

$$Z_{\mathrm{MF}} = \mathrm{Tr}[e^{-\beta H_{\mathrm{MF}}}]$$

and the trace is taken over all the possible configurations with fixed number of ions N in the system.

Note: Since we are dealing with a lattice theory we can work in the canonical ensemble.

(d) Write the self-consistency equation for the average magnetic moment $m = |\mathbf{m}|$ in terms of minimization of free energy.

Note: Remember the definition of the free energy $F = -\frac{1}{\beta}\ln Z$.

(e) Express the self-consistency equation in terms of the normalized magnetization $\alpha = \frac{m}{nJ_0}$ and the parameter $b = nJ_0\beta$. For which values of b there is a ferromagnetic solution? Can you give the critical temperature? Which is the magnetization at zero temperature? Could you guess the result without calculating it?

(f) Solve numerically the self-consistency equation and make a plot of the magnetization as a function of the temperature.

12.2. Stoner model of metallic ferromagnets

The Stoner model is applied to those materials for which the magnetism is generated by the conduction electrons. They are typically transition metals in which the conduction band is formed by the narrower d or f orbitals. For this reason it is reasonable to introduce for this systems a model Hubbard Hamiltonian.

(a) Consider the effective Hamiltonian for a system of interacting electrons written in first quantization:

$$H = -\sum_i \frac{\nabla_i^2}{2m} + \sum_{ij} U\delta(\mathbf{r}_i - \mathbf{r}_j)$$

and write it in second quantization in the position and in the momentum basis. The former results in the Hubbard Hamiltonian presented in class.

(b) Apply the Hartree-Fock approximation on this Hamiltonian keeping in mind that we are looking for ferromagnetic solutions. That is parametrize the spin up and spin down populations:

$$\langle c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}'\uparrow}\rangle = \delta_{\mathbf{k}\mathbf{k}'}\bar{n}_{\mathbf{k}\uparrow}, \quad \langle c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}'\downarrow}\rangle = \delta_{\mathbf{k}\mathbf{k}'}\bar{n}_{\mathbf{k}\downarrow}$$

and assume that the average populations $\bar{n}_{\mathbf{k}\uparrow}$ and $\bar{n}_{\mathbf{k}\downarrow}$ of spin up and down electrons respectively can have different values.

(c) Write the the self-consistency conditions:

$$\bar{n}_\sigma = \frac{1}{V}\sum_{\mathbf{k}} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_{\mathrm{MF}}$$

for the spin up and down respectively. V is the volume of the crystal.
`Hint:` At zero temperature you should obtain:

$$\bar{n}_\uparrow = \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\,\theta\left(\mu - \frac{\hbar^2 k^2}{2m} - U\bar{n}_\downarrow\right)$$

for one spin component and similarly for the other. Here θ is the Heaviside function $(\theta(x \geq 0) = 1,\, \theta(x < 0) = 0)$. Extend the result to finite temperatures.

(d) The average spin up and down densities are connected by the self-consistency conditions just derived. Assume for the moment the $T = 0$ condition and write explicitly the system of coupled equation in $\bar{n}_\uparrow$ and $\bar{n}_\downarrow$ represented by the self-consistency equations.
`Hint:` It could be useful to introduce spin resolved Fermi momenta defined as:

$$\frac{\hbar^2}{2m} k_{\mathrm{F}\uparrow}^2 + U\bar{n}_\downarrow = \mu$$
$$\frac{\hbar^2}{2m} k_{\mathrm{F}\downarrow}^2 + U\bar{n}_\uparrow = \mu$$

(e) Rewrite the self-consistent problem in terms of the variables:

$$\zeta = \frac{\bar{n}_\uparrow - \bar{n}_\downarrow}{\bar{n}_\uparrow + \bar{n}_\downarrow}$$
$$\gamma = \frac{8\pi^{2/3} m U (\bar{n}_\uparrow + \bar{n}_\downarrow)^{1/3}}{3^{2/3}\hbar^2}$$

The physical meaning of ζ is to quantify the excess magnetization since $-1 \leq \zeta \leq 1$. We can call the system *ferromagnetic* when $|\zeta| = 1$ and paramagnetic when $\zeta = 0$. For which values of γ are these special cases $(|\zeta| = 0,\, 1)$ obtained? Can you give a physical interpretation of the result?