

Quantentheorie II

Prof. Milena Grifoni

Dr. Andrea Donarini

Blatt 9

1. Stoner model of metallic ferromagnets

The Stoner model is applied to those materials for which the magnetism is generated by the itinerant conduction electrons. They are typically transition metals in which the conduction band formed by the d or f orbitals is narrow in energy. The associated high density of states at the Fermi energy implies a strong screening of the electron-electron interaction. It is thus reasonable to describe these systems by a free electron Hamiltonian with contact interaction.

- a • Consider the effective Hamiltonian for a system of interacting electrons written in first quantization:

$$H = - \sum_i \frac{\hbar^2}{2m} \Delta_i + \sum_{i \neq j} \frac{U}{2} \delta(\mathbf{r}_i - \mathbf{r}_j)$$

and write it in second quantization in the position and in the momentum basis.

(3 Points)

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

$$\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma'} \rangle = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} n_{\mathbf{k}\sigma},$$

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

(3 Points)

- c • Prove that the self-consistency conditions:

$$N_\sigma = \sum_{\mathbf{k}} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle_{\text{MF}}$$

for the spin up and down respectively have, at zero temperature and in the thermodynamic limit, the form

$$n_\uparrow = \int \frac{d\mathbf{k}}{(2\pi)^3} \theta \left(\varepsilon_F - \frac{\hbar^2 k^2}{2m} - U n_\downarrow \right)$$

for one spin component and similarly for the other. Here θ is the Heaviside function ($\theta(x \geq 0) = 1$, $\theta(x < 0) = 0$) and $n_\sigma \equiv \sum_{\mathbf{k}} \frac{n_{\mathbf{k}\sigma}}{V}$, where V is the volume occupied by the system and ε_F is the Fermi energy. *Hint:* In the thermodynamic limit you can use the substitution

$$\sum_{\mathbf{k}} \rightarrow V \int \frac{d\mathbf{k}}{(2\pi)^3}$$

(4 Points)

- d The average spin up and down densities are connected by the self-consistency conditions just derived. Prove that the relations are:

$$\frac{\hbar^2}{2m}(6\pi^2 n_\uparrow)^{2/3} + U n_\downarrow = \varepsilon_F$$
$$\frac{\hbar^2}{2m}(6\pi^2 n_\downarrow)^{2/3} + U n_\uparrow = \varepsilon_F$$

- e Prove that the self-consistent problem can be written, in terms of the variables

$$\zeta = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}$$
$$\gamma = \frac{2mU(n_\uparrow + n_\downarrow)^{1/3}}{(3\pi^2)^{2/3}\hbar^2},$$

in the form

$$(1 + \zeta)^{2/3} - (1 - \zeta)^{2/3} = \gamma\zeta.$$

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?

Frohes Schaffen!