Quantum Theory of Condensed Matter

Prof. John Schliemann
Dr. Andrea Donarini

Mo 10:15, 5.0.21
We H33, 10:15

Sheet 4

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:

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

and write it in second quantization in the position and in the momentum basis. *Hint:* Remember that, due to the Pauli exclusion principle, you cannot create 2 fermions with the same quantum numbers.

b) Apply the Hartree-Fock approximation on the Hamiltonian written in the momentum basis, *i.e.*

$$\begin{aligned} c^\dagger_{\mathbf{k+q}\sigma}c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{p}\sigma'}c_{\mathbf{k}\sigma} \approx\ & \langle c^\dagger_{\mathbf{k+q}\sigma}c_{\mathbf{k}\sigma}\rangle c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{p}\sigma'} + c^\dagger_{\mathbf{k+q}\sigma}c_{\mathbf{k}\sigma}\langle c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{p}\sigma'}\rangle \\ & -\langle c^\dagger_{\mathbf{k+q}\sigma}c_{\mathbf{p}\sigma'}\rangle c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{k}\sigma} - \langle c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{k}\sigma}\rangle c^\dagger_{\mathbf{k+q}\sigma}c_{\mathbf{p}\sigma'} \\ & -\langle c^\dagger_{\mathbf{k+q}\sigma}c_{\mathbf{k}\sigma}\rangle\langle c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{p}\sigma'}\rangle + \langle c^\dagger_{\mathbf{k+q}\sigma}c_{\mathbf{p}\sigma'}\rangle\langle c^\dagger_{\mathbf{p-q}\sigma'}c_{\mathbf{k}\sigma}\rangle, \end{aligned}$$

keeping in mind that we are looking for ferromagnetic solutions. That is, parametrize the spin up and spin down populations:

$$\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma'}\rangle = \delta_{\mathbf{kk}'}\delta_{\sigma\sigma'}\bar{n}_{\mathbf{k}\sigma},$$

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:

$$\bar{n}_\sigma = \int \frac{d\mathbf{k}}{(2\pi)^3}\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle_{\mathrm{MF}}$$

for the spin up and down respectively. *Hint:* At zero temperature you should obtain:

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

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

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

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!