University of Regensburg Summer Term 17

Quantum theory of condensed matter I

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	Thu	10:00 - 12:00	H33
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Sheet 11

Stoner model for metallic ferromagnets

The Stoner model provides a simple mean field description of the ferromagnetism in transition metals. In such metals the conduction band is very narrow since as it formed by weakly coupled d or f orbitals. The associated high density of states at the Fermi energy implies strong screening of the electron-electron interactions already at unusually short length scales. This motivates one to replace the resulting short-range interaction with the contact interaction $\hat{V}_c$ considered in Sheet 9.

1. We consider the effective Hamiltonian $\hat{H} = \hat{T} + \hat{V}_c$ for spin-1/2 conduction electrons in a 3D parabolic band. The kinetic part $\hat{T} = \sum_{\mathbf{k},\sigma} \xi_k \, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$, where $\xi_k = \hbar^2 k^2/2m$, $\sigma = \uparrow, \downarrow$ labels the spin projection on (an arbitrarily chosen) z-axis, and $\mathbf{k}$ label three-dimensional momenta in a normalization volume $\mathcal{V}$, so that $\mathcal{V}^{-1} \sum_{\mathbf{k}} \leftrightarrow (2\pi)^{-3} \int d^3k$. Start with the general form for electron-electron interaction, $\hat{V}_{\text{e-e}} = (1/2) \int d\mathbf{r} \int d\mathbf{r}' \sum_{\sigma,\sigma'} \psi^\dagger_\sigma(\mathbf{r}) \psi^\dagger_{\sigma'}(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_\sigma(\mathbf{r})$, and demonstrate using the Pauli exclusion principle that in the case of contact interaction, $V(\mathbf{r} - \mathbf{r}') = U\delta(\mathbf{r} - \mathbf{r}')$, $\hat{V}_{\text{e-e}}$ reduces to

$$\hat{V}_c = U \int d\mathbf{r} \; \hat{\rho}_\uparrow(\mathbf{r}) \hat{\rho}_\downarrow(\mathbf{r}) = \frac{U}{\mathcal{V}} \sum_{\mathbf{q}} \hat{\rho}_{\mathbf{q}\uparrow} \hat{\rho}_{-\mathbf{q}\downarrow}$$

where $\hat{\rho}_\sigma(\mathbf{r}) = \psi^\dagger_\sigma(\mathbf{r}) \psi_\sigma(\mathbf{r}) = \mathcal{V}^{-1} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \hat{\rho}_{\mathbf{q}\sigma}$ and $\hat{\rho}_{\mathbf{q}\sigma} = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}$ are the density operators for a given spin projection σ in the real and momentum space, respectively. **(1 point)**

2. Apply the mean field approximation to $\hat{H}$ keeping in mind that we are looking for (homogeneous in space) ferromagnetic solutions. Similarly to the Hartree-Fock approximation, we expect non-zero mean field values only for diagonal in σ and k combinations of creation and annihilation operators

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

but now we assume that the spin up and spin down populations $\bar{n}_{\mathbf{k}\uparrow}$ and $\bar{n}_{\mathbf{k}\downarrow}$ can in general be *different*.

Write down the corresponding mean field Hamiltonian $\hat{H}_{\text{MF}}$ and find its spectrum. Observe that the potential energies of spin-down and spin-up states for a given momentum $\mathbf{k}$ are in general different. Find the difference and observe that it is independent of $\mathbf{k}$. At the same time, unlike in usual single-particle problems, the mean field spectrum is a functional of the state of the entire system. Indeed, in order to find the energy of a particular eigen state, we need to know

$$\bar{n}_\sigma = V^{-1} \sum_k \bar{n}_{\mathbf{k}\sigma} = \int \frac{d\mathbf{k}}{(2\pi)^3} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle,$$

while calculation of $\bar{n}_\sigma$ requires the knowledge of the spectrum, temperature T, etc.. Therefore, it is necessary to search for a self-consistent solution which requires derivation and analysis of a nonlinear equation for $\bar{n}_\sigma$. **(2 points)**

3. Derive the self-consistency conditions for the ground state of the system (T=0). In this case, all $\{k, \sigma\}$ states below the Fermi energy ϵ_F are filled, while all other states are empty. You should obtain

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

for one spin component and similar equation for the other. Here $\theta(x)$ is the Heaviside function. Generalize the above equation to finite temperatures. **(2 points)**

4. For the $T = 0$ case, find the system of coupled equations for $\bar{n}_\uparrow$ and $\bar{n}_\downarrow$ represented by the above self-consistency equations. Hint: It could be useful to introduce spin resolved Fermi momenta defined as:

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

Write the self-consistency equation in terms of $\bar{n}_\sigma$, and then re-express it in terms of variables

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

You should obtain the following equation

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

Plot the left-hand side of the above equation together with the right-hand side taken at $\gamma = 4/3$ and at $\gamma = 2^{2/3}$. **(3 points)**

5. You can infer from the plot that at $\gamma < 4/3$ the only solution is $\zeta = 0$, meaning that spin polarization is absent. The system is thus paramagnetic. In the region $4/3 < \gamma < 2^{2/3}$, corresponding i.e. to a stronger interaction strength U or larger densities $\bar{n}_\uparrow + \bar{n}_\downarrow$, there are solutions with both $0 < |\zeta| < 1$ (weak ferromagnet) and $\zeta = 0$. The latter is in fact unstable (how would you prove it?). For γ approaching $2^{2/3}$ from below, the spin polarization approaches one. Finally, for $\gamma > 2^{2/3}$ the above self-consistency equation becomes not applicable.

   Find out what what happens at $\gamma > 2^{2/3}$ and how the self-consistency equation should be modified in this case (Hint: Return back to items 3. and 4. and consider the case of full spin polarization). Derive the condition for the strong ferromagnetism when only possible states are fully polarized states with $|\zeta| = 1$. What in general determines the direction of spin polarization? If you don't know the answer, search for phase transitions, order parameter, and spontaneous symmetry breaking .... Which symmetry is broken in a ferromagnet, with respect to a paramagnet? What is the order parameter? Illustrate the spectrum and occupation of states for all three cases of a weak and strong ferromagnet as well as a paramagnet. **(4 points)**

Frohes Schaffen!