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Problem Set 9: Stoner transition

Let us discuss the phase transition of normal metals from a para- to a ferromagnetic state. We assume that the itinerant electrons screen the Coloumb potential so that the interaction is exponentially suppressed beyond a distance of a lattice constant. Thus, we start restrict our investigation of metallic magnetism to the following Hamiltonian, with only the on-site repulsive part of the Coulomb interaction, that reads

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}.$$
 (1)

Exercise 1. Mean-field theory

(a) Show that

$$H_{\rm int} = U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} = -\frac{2U}{3} \sum_{i} \mathbf{S}_i^2 + \frac{U}{2} \sum_{i} n_i, \qquad (2)$$

where we use the electronic spin operator $\mathbf{S}_i = \frac{1}{2} c_{i,\sigma}^{\dagger} \boldsymbol{\sigma}_{\sigma,\sigma'} c_{i,\sigma'}$.

- (b) Expand the Hamiltonian around the mean-field value of the spin operator via $\delta \mathbf{S}_i = \mathbf{S}_i \langle \mathbf{S}_i \rangle$, where the mean-field value describes the magnetic ordering in the system with $\mathbf{M}_i = -\frac{4U}{3} \langle \mathbf{S}_i \rangle$.
- (c) Consider a ferromagnetic state, $\mathbf{M}_{\mathbf{k}} = \mathbf{M}_0 \,\delta_{\mathbf{k},\mathbf{0}}$, with the spin polarization along the z axis, $\mathbf{M}_0 = M_0 \,\mathbf{e}_z$. Show that the mean-field Hamiltonian including the chemical potential reads $(V = N^d)$

$$H_{\rm MF} = \frac{3}{8U} V |M_0|^2 + \sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k}} + \frac{1}{2} M_0 + \mu \right) c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} + \left(\epsilon_{\mathbf{k}} - \frac{1}{2} M_0 + \mu \right) c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k}\downarrow}.$$
(3)

Now, we calculate the ground-state energy $E_0(M_0, \mu, \epsilon_{\uparrow}, \epsilon_{\downarrow})$ at zero temperature, where the spin-up (spin-down) states are filled up to the energies ϵ_{\uparrow} (ϵ_{\downarrow}).

- (d) Rewrite the energy density E_0/V using the one-particle density of states (DOS) $\rho(\epsilon)$.
- (e) Extremize the energy density with respect to the set of parameters $(M_0, \mu, \epsilon_{\uparrow}, \epsilon_{\downarrow})$ for fixed density. We can conclude from this set of equations that the polarization is $M_0 = \epsilon_{\downarrow} - \epsilon_{\uparrow}$ (for $\rho(\epsilon_{\uparrow,\downarrow}) \neq 0$) and the chemical potential equals $\mu = -\frac{1}{2}(\epsilon_{\downarrow} + \epsilon_{\uparrow})$. Argue that there is a finite magnetization above a critical value $U > U_c$, and express U_c through the DOS, $\rho(\epsilon)$.

Exercise 2. Hubbard-Stratonovich approach

Let us now explicitly use a Hubbard–Stratonovich decoupling and expand the action around its classical solution. We will consider the leading-order fluctuations, neglecting the effect of any spatial and temporal dependence of the fluctuations, and try to detect a phase transition into a magnetically ordered state.

(a) We focus on the spin channel described by $H_{\text{int}} \approx -U \sum_i (S_i^z)^2$. Write down the field integral representation of this Hamiltonian and decouple the quartic term by introducing a bosonic field $m_i(\tau)$. After integrating out the fermionic states, show that the system has the following partition sum

$$\mathcal{Z} = \mathcal{Z}_0 \int \mathcal{D}[m] e^{-S[m]},$$

$$S[m] = \frac{1}{4} U \int_0^\beta d\tau \Big[\sum_{\mathbf{p}} |m_{\mathbf{p}}|^2 \Big] - \operatorname{Tr} \Big[\ln \Big(1 - \frac{1}{2} U \sigma_z \hat{m} \hat{G}_0 \Big) \Big], \tag{4}$$

with matrices \hat{m} and \hat{G}_0 in spin-momentum space. Here, \mathcal{Z}_0 is the partition function of the non-interacting electron gas.

- (b) Find the solution of the saddle-point equation for S[m]. We assume that the solution is homogeneous and not polarized. Expand the action up to leading order (fourth order) in the fluctuations around its classical solution. Verify that the odd terms in the field $m_i(\tau)$ vanish by the symmetry under the transformation $m \to -m$.
- (c) Show that contributions from the quadratic and quartic part of the expansion can be collected in an effective action for the bosonic field that reads

$$S_{\text{eff}}[m] = \frac{1}{2} \sum_{q} v_2(q) |m_q|^2 + \frac{1}{4N\beta} \sum_{q_i} v_4(\{q_i\}) \prod_{i=1}^4 m_{q_i} \delta_{\sum_i q_i, 0}, \qquad (5)$$

where $v_2(q) = \frac{U}{2}(1 - U\Pi_q)$ with the polarization function $\Pi_q = -\frac{1}{\beta N} \sum_k G_{0,k} G_{0,k+q}$. *Remark:* No explicit computation of the traces, respectively of $v_{2/4}(q)$, is needed.

(d) Let us consider the frequency- and momentum-independent contribution, $\Pi_q \to \nu_0$ and $v_4(\{q_i\}) \to u = v_4(0)\beta N$, and also neglect any spatial/temporal dependence of the magnetic field. Then, the action exhibits a phase transition at a critical point U_c . Determine U_c in this simplified case.

Remark: The polarization function Π_q can be approximated at small frequencies $|\omega_n|/|\mathbf{q}v_f|$ as follows: $\Pi_q \approx \Pi_{0,\mathbf{q}} - \nu_0 \frac{|\omega_n|}{v|\mathbf{q}|}$ with $v = c v_f$ (c depends on the dimension). The static susceptibility $\Pi_{0,\mathbf{q}}$ at small \mathbf{q} reads $\Pi_{0,\mathbf{q}} \approx \nu_0 [1 - \xi^2 \mathbf{q}^2 + ...]$, where $\xi \sim 1/k_f$.

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