Advanced Theoretical Condensed Matter Physics — SS11

Exercise 5

(Please return your solutions by sTues. 31.05.2011)

We have seen in the previous exercise sheet that given a strong enough on-site Coulomb interaction U we can expect that our Hubbard model to undergo a transition to a ferromagnetic groundstate. This is the so-called "Stoner criterion" for the occurence of a ferromagnetic groundstate. In the first part of this exercise sheet we will see more clearly how the *Ansatz* of Stoner leads naturally to the Hubbard interaction, and how we can derive diagrams from it. However, we know that perturbation theory breaks down for a sufficiently strong interaction strength; how can perturbative calculations be extended? One way is to select only certain diagrams which can be iterated to any arbitrary order; these diagrams can then be "resummed" to yield a finite value for physical quantities. We will do an elementary version of this process in the second exercise.

5.1. Excitations above the Ferromagnetic Groundstate I: Zeroth Order Diagrams
We start from a noninteracting Hamiltonian, given generically as

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu)\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} \tag{1}$$

where the dispersion is for the moment independent of spin variables. Stoner's *Ansatz* has its roots already early on in the ideas of ferromagnetism of Weiss. He postulated that an externally applied magnetic field will not only influence the magnetization of the system directly, but also induce a local *molecular field* M which adds to the external field H.

$$\bar{H} = H + \lambda M \tag{2}$$

where $\bar{H}$ is the effective magnetic field on the system, H is the externally applied field, and $M = \mu_B(n_\uparrow - n_\downarrow)$ (here μ_B = Bohr magneton, $n_{\uparrow,\downarrow}$ =density of spin up and down electrons respectively, $n_\sigma = \frac{1}{V}\sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}$ and total electron density $n = n_\uparrow + n_\downarrow$) is the local molcular field, and λ a *phenomenological* coupling constant. Stoner's idea was to write the previously spin independent dispersion $\epsilon_{\mathbf{k}} \to \epsilon_{\mathbf{k}\sigma} \equiv \epsilon_{\mathbf{k}} - \mu_\sigma$, where the *spin-dependent* chemical potential $\mu_\sigma \equiv \mu + \sigma\mu_B\bar{H}$, and $\sigma = \pm 1$ signifies the different spin orientations.

a) Setting $H = 0$ in (2) and using the definition of M, μ_σ and the Fourier transform $\frac{1}{\sqrt{L}}\sum_i \hat{c}^\dagger_{i\sigma} e^{i\mathbf{k}\cdot\mathbf{r}}$ show that we can write (1) as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int} \tag{3}$$

where $\mathcal{H}_{int} = -V\lambda\mu_B^2(n_\uparrow - n_\downarrow)^2$ and subsequently show that in coordinate space

$$\mathcal{H}_{int} = -\frac{NU}{2} + U\sum_i n_{i\uparrow}n_{i\downarrow} - 2U\sum_{i\neq j} S_i^z S_j^z \tag{4}$$

Use the fact that $n_\sigma = \frac{1}{V} \sum_i n_{i\sigma}$ and that due to the Pauli principle $n_{i\sigma}^2 = n_{i\sigma}$. The spin operator S_i^z is defined as $S^z = \sum_i S_i^z = \frac{1}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})$.

We neglect the first term in (4) since it is a simple constant shift of the energy, and we also neglect the third term since it is negligible for uncorrelated sites and nonmagnetic electrons. We therefore see that Stoner's *Ansatz* yields, from the noninteracting Hamiltonian, a *Hubbard* Hamiltonian with an on-site Hubbard interaction term.

We would now like to calculate the *spin-spin* correlation function again, as in the previous exercise sheet, but using a diagrammatic method. Remind yourselves of the definition of the correlation function in the Matsubara formalism, which in our notation shall look like

$$\langle T_\tau \hat{A}(\tau)\hat{B}(\tau')\rangle = \sum_{n=0}^{\infty} (-1)^n \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \langle T_\tau [\mathcal{H}_{int}(\tau_1) \cdots \mathcal{H}_{int}(\tau_n) \hat{A}(\tau)\hat{B}(\tau')]\rangle_{0,\text{con-dis}} \quad (5)$$

where the subscript refers to all connected and distinct diagrams. We will also need the spin operator, which is the same as defined in the previous sheet, but which we write down here once again to keep the sheet self-contained. We need the spin operator

$$\hat{\mathbf{s}}^\alpha(\mathbf{q}) = \frac{1}{2} \sum_{\mathbf{k}} \sum_{\sigma\sigma'} \hat{c}_{\mathbf{k}\sigma}^\dagger \sigma_{\sigma\sigma'}^\alpha \hat{c}_{\mathbf{k}+\mathbf{q}\sigma'}$$

and in this sense we define our correlation function

$$\chi^{\alpha\beta}(\mathbf{q}, i\nu) = \frac{1}{V} \int_0^\beta d\tau \, e^{i\nu\tau} \langle T_\tau \hat{\mathbf{s}}^\alpha(\mathbf{q}, \tau)\hat{\mathbf{s}}^\beta(-\mathbf{q}, 0)\rangle \quad (6)$$

and

b) Write the U term in (4) in momentum space to obtain

$$\mathcal{H}_{int} = \frac{U}{L} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}'\downarrow}^\dagger \hat{c}_{\mathbf{k}'+\mathbf{q}\downarrow} \hat{c}_{\mathbf{k}-\mathbf{q}\uparrow} \quad (7)$$

We will use this form of the interaction Hamiltonian to write down our diagrammatic expansion. To simplify the calculational process, first write (6) in the form

$$\chi^{\alpha\beta} = \frac{1}{4V} \sum_{\sigma\sigma'} \sum_{\rho\rho'} \sigma_{\sigma\sigma'}^\alpha \sigma_{\rho\rho'}^\beta \sum_{N=0}^{\infty} T^{(N)} \quad (8)$$

and work with $T^{(N)}$. Using Wick's theorem, calculate first $T^{(0)}$ and show that one obtains for $\chi_0^{\alpha\beta}(\mathbf{q}, i\nu) \equiv \chi^{\alpha\beta}(q)$ the expression

$$\chi_0^{\alpha\beta}(q) = \frac{1}{4V} \sum_{\sigma\sigma'} \sigma_{\sigma\sigma'}^i \sigma_{\sigma'\sigma}^j \Gamma_{\sigma\sigma'}(q) \quad (9)$$

where

$$\Gamma_{\sigma\sigma'}(q) \equiv -\beta^{-1} \sum_k \mathcal{G}_\sigma^{(0)}(k) \mathcal{G}_{\sigma'}^{(0)}(k+q) = \Gamma_{\sigma'\sigma}(-q), \quad q \equiv (\mathbf{q}, i\nu) \quad (10)$$

Use the fact that we work in a diagonal basis, i.e., the free Green's function $\mathcal{G}^{(0)}(\mathbf{k}\sigma; \mathbf{k}'\sigma') \propto \mathcal{G}(\mathbf{k}\sigma)\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}$. Here

$$\mathcal{G}_\sigma^{(0)}(\mathbf{k}, i\nu) \equiv \mathcal{G}(k) = \frac{1}{i\nu - \epsilon_\mathbf{k} - \mu_\sigma}$$

We see that the splitting into 2 energy bands in the system is also to be seen in the structure of the Green's function itself.

Figure 1: Zeroth order transverse sus. diagram

Figure 2: Zeroth order longitudinal sus. diagram

(10) looks very much like the expression we obtained when we calculated the density-density correlation bubble on exercise sheet 2. However, (10) still has free spin indices. As we shall see below, different combinations of the spin variable will correspond to different sets of diagrams.

c) From the explicit form of the Pauli matrices and the fact that $\sigma^{\pm} = \frac{1}{2}(\sigma^x \pm i\sigma^y)$ one sees that

$$\sigma^{\alpha}_{\uparrow\downarrow} = \delta_{\alpha+}, \quad \sigma^{\alpha}_{\downarrow\uparrow} = \delta_{\alpha-}, \quad \sigma^{\alpha}_{\uparrow\uparrow} = -\sigma^{\alpha}_{\downarrow\downarrow} = \delta_{\alpha z} \tag{11}$$

Use (11) and show that the zeroth order diagrams would correspond to the functions

$$\chi^{+-}_0(q) = \frac{1}{4V}\Gamma_{\uparrow\downarrow}(q) = \chi^{-+}_0(-q)$$

$$\chi^{zz}_0(\pm q) = \frac{1}{4V}(\Gamma_{\uparrow\uparrow}(q) + \Gamma_{\downarrow\downarrow}(q))$$

The zeroth order *transversal* susceptibility $\chi^{+-}_0(q)$ corresponds to the single bubble diagram, as shown in Fig. 1 with the spin configuration illustrated. On the other hand, the *longitudinal* susceptibility is given by the sum of the diagrams as shown in Fig. 2. As expected, we see that the *transverse* spin susceptibility has the form of the "bubble", which is quite similar to the density-density correlation function we calculated on exercise sheet 3. The *longitudinal* susceptibility, however, corresponds also to "bubble" diagrams, but with a different spin configuration.

5.2. Excitations above the Ferromagnetic Groundstate II: Resummation of Diagrams

In this exercise we will extend our work in the previous exercise and compute the diagrams corresponding to 1st order in the interaction strength U. We shall consequently see that the these basic diagrams can then be resummed up to an arbitrary high order N, and this is the usual way one deals with strong interaction strengths.

a) Repeat the steps for the calculation of the zeroth order susceptibility $\chi^{ij}_0(q)$ in 1b) up to 1st order (refer to (5) !). Use Wick's theorem, sum over the relevant momentum variables, and finally Fourier transform into $(\mathbf{q}, i\nu)$ variables. Show that one obtains the expression

$$T^{(1)}(\sigma\sigma', \rho\rho'; q) = \frac{U}{L}\Gamma_{\sigma\sigma'}(q)\Gamma_{\rho'\rho}(q)\left(\delta_{\uparrow\sigma}\delta_{\downarrow\rho} - \delta_{\downarrow\sigma}\delta_{\uparrow\rho}\right)\left(\delta_{\downarrow\sigma'}\delta_{\uparrow\rho'} - \delta_{\uparrow\sigma'}\delta_{\downarrow\rho'}\right) \tag{12}$$

b) We can write (12) in the form

$$T^{(N)} = T^{(N)}_{\text{ladder}}(q)\delta_{\uparrow\downarrow,\sigma\sigma'}\delta_{\downarrow\uparrow,\rho\rho'} + T^{(N)}_{\text{ladder}}(-q)\delta_{\downarrow\uparrow,\sigma\sigma'}\delta_{\uparrow\downarrow,\rho\rho'}$$
$$+ T^{(2N-1)}_{\text{chain}}(q)(\delta_{\uparrow\uparrow,\sigma\sigma'}\delta_{\downarrow\downarrow,\rho\rho'} + \delta_{\downarrow\downarrow,\sigma\sigma'}\delta_{\uparrow\uparrow,\rho\rho'})$$

where the factors $T_{\text{ladder}}^{(N)}(\pm q)$ and $T_{\text{chain}}^{(2N-1)}(q)$ can be figured out by chaining together the fundemental diagram elements in Figs. 1 and 2 where N increases with the increasing power of the interaction line U. What are the expressions $T_{\text{ladder}}^{(N)}(\pm q)$ and $T_{\text{chain}}^{(2N-1)}(q)$ respectively?

c) Using the scalar expressions obtained in b) and the expressions for the zeroth order susceptibilities obtained in 1.c) together with (8) show that we have, finally

$$\chi^{+-}(q) = \frac{1}{4V}\Gamma_{\uparrow\downarrow}\left[1 - \frac{U}{L}\Gamma_{\uparrow\downarrow}\right]^{-1} = \chi^{-+}(-q) \tag{13}$$

$$\chi_{zz}(\pm q) = \frac{1}{4V}\left\{\Gamma_{\uparrow\uparrow} + \Gamma_{\downarrow\downarrow} + 2\frac{U}{L}\Gamma_{\uparrow\uparrow}\Gamma_{\downarrow\downarrow}\left[1 - \left(\frac{U}{L}\right)^2\Gamma_{\uparrow\uparrow}\Gamma_{\downarrow\downarrow}\right]^{-1}\right\} \tag{14}$$

Hint: If you are having problems visualizing the resummation process, the individual terms in the sum is illustrated below. Try to separate out the appropriate recurring elements. Note that the recurring elements may not be those illustrated in Figs. 1 and 2