Homework #9 — Phys625 — Spring 2002
Deadline: Thursday, April 25, 2002.
Turn in homework in the class or put it in the box on the door of Phys 2314 by 10 a.m.

Victor Yakovenko, Associate Professor
Office: Physics 2314
Phone: (301)-405-6151
E-mail: yakovenk@physics.umd.edu
Web page: http://www2.physics.umd.edu/˜yakovenk/teaching/phys625.spring2002

Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of the textbook.
Equation numbers without period, like (5), refer to the equations of this homework.

Generalized Susceptibilities at Finite Temperature (Ch. IV)

1. *Analytical continuation from Matsubara to real frequencies*

Read the handouts: §123 from *Statistical Physics, Part 1* by Landau and Lifshitz (Volume 5 of the Theoretical Physics Course), which introduces the generalized susceptibility, and 3.3.1 from *Quantum Theory of Many-Body Systems* by Zagoskin, which introduces the Kubo formula. In the first hangout, carefully study the first three pages; the rest is optional.

(a) [**4 points**] The dynamical susceptibility $\chi(\omega)$ is given by the Kubo formula [see Eqs. (3.73) and (3.77) of Zagoskin]:

$$\chi(\omega) = i\int_0^\infty dt\, e^{i\omega t}\langle[\hat{A}(t),\hat{B}(t)]\rangle_T, \tag{1}$$

where t and ω are the real time and frequency, $\hat{A}(t)$ and $\hat{B}(t)$ are the operators in the Heisenberg representation, and the averaging is performed over the Gibbs distribution with the temperature T. Notice the similarity with Eq. (36.2) for the retarded Green's function, except Eq. (1) has commutator instead of anticommutator.

The Matsubara susceptibility $\chi_M(i\omega_n)$ is defined as

$$\chi_M(i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\, e^{i\omega_n\tau}\langle\mathcal{T}_\tau \hat{A}_M(\tau),\hat{B}_M(\tau)\rangle_T, \tag{2}$$

where τ and $i\omega_n$ are the Matsubara time and frequency, $\hat{A}(\tau)$ and $\hat{B}(\tau)$ are the operators in the Matsubara representation, and $\mathcal{T}_\tau$ is chronological ordering with respect to τ. Notice the similarity with Eq. (37.3) for the Matsubara Green's function.

Prove that

$$\chi(i\omega_n) = \chi_M(i\omega_n), \tag{3}$$

thus $\chi(\omega)$ can be obtained from $\chi_M(i\omega_n)$ by analytical continuation from the discrete points $i\omega_n$ on the positive imaginary semi-axis of complex ω to the real axis of ω.

Notice the similarity between Eqs. (3) and (37.12). In order to prove Eq. (3), use the method of formal expansion over a complete set of exact energy eigenstates, similar to §36 and $37. If you cannot solve this problem, go to the next part.

(b) [**4 points**] Consider the case where the operators $\hat{A}$ and $\hat{B}$ are bilinear in creation and destruction operators:

$$\hat{A}(t) = \sum_{kl} A_{kl}e^{-i(E_k-E_l)t}\hat{a}_k^+\hat{a}_l, \qquad \hat{B}(t) = \sum_{kl} B_{kl}e^{-i(E_k-E_l)t}\hat{a}_k^+\hat{a}_l. \tag{4}$$

where A_{kl} and B_{kl} are the matrix elements of $\hat{A}$ and $\hat{B}$ between the energy eigenstates k and l.

Substituting Eq. (4) into Eq. (1) and performing the thermal averaging for non-interacting particles, show that

$$\chi(\omega) = \sum_{kl} A_{kl}B_{lk}\frac{f(E_l)-f(E_m)}{\omega - E_l + E_k + i0}, \tag{5}$$

where $f(E)$ is the thermal Fermi or Bose distribution function.

Notice the similarity between Eq. (5) and Eq. (5) of HW8, provided the indices k and l represent the momenta $\mathbf{p}$ and $\mathbf{q}$. It is clear that Eq. (5) can be obtained from Eq. (5) of HW8 by the analytical continuation $i\Omega_n \to \omega + i0$.

2. *Electron spin resonance (ESR)*

Let us consider a 3D electron gas with the Fermi momentum p_F in a magnetic field. Here we consider only the effect of the magnetic field on the electron spins and ignore the orbital effect.

Suppose a magnetic field B_0 is applied along the z axis. First, the field B_0 is considered to be finite and *not* a small perturbation. The energies of electrons with spins up and down (relative to the z axis) experience the Zeeman split:

$$\varepsilon_\uparrow(\mathbf{p}) = p^2/2m - \mu_B B_0, \qquad \varepsilon_\downarrow(\mathbf{p}) = p^2/2m + \mu_B B_0. \tag{6}$$

Suppose an additional small magnetic field $\mathbf{B}_\perp(t)$ rotates in the (x, y) plane:

$$B_x(t) = B_\perp \cos\omega t, \qquad B_y(t) = B_\perp \sin\omega t. \tag{7}$$

The field (7) produces the following perturbation in the Hamiltonian:

$$\hat{H}_1(t) = -\mu_B\, \hat{\mathbf{s}}_\perp \cdot \mathbf{B}_\perp(t) = -\mu_B(B_\perp e^{i\omega t}\hat{\psi}_\downarrow^+\hat{\psi}_\uparrow - B_\perp e^{-i\omega t}\hat{\psi}_\uparrow^+\hat{\psi}_\downarrow), \tag{8}$$

where $\hat{\mathbf{s}} = \hat{\psi}_\alpha^+ \boldsymbol{\sigma}_{\alpha,\beta}\hat{\psi}_\beta$ is the spin operator of electrons, and $\boldsymbol{\sigma}_{\alpha,\beta}$ are the Pauli matrices.

(a) [**4 points**] Using Eq. (5), calculate the dynamical susceptibility $\chi_\perp(\omega)$ with respect to $\mathbf{B}_\perp$, which is defined as

$$s_\perp = \chi_\perp(\omega)\, \mathbf{B}_\perp. \tag{9}$$

How does $\chi_\perp(\omega)$ depend on temperature? What is the resonance frequency? Does the resonance exist for positive and negative ω, i.e. for $\mathbf{B}_\perp(t)$ rotating clockwise and counterclockwise?

Calculate the total spectral weight of absorption (dissipation) of energy (see Eq. (123.11)):

$$\int_0^\infty \frac{d\omega}{2\pi}\, 2\omega\, \mathrm{Im}\chi(\omega). \tag{10}$$

(b) [**4 points**] Now let us consider the case where $\mathbf{B}_\perp = 0$, and B_0 is considered as a (static) perturbation:

$$s_z = \chi_z B_0. \tag{11}$$

Calculate χ_z. Does it depend on temperature?

3. *Transition temperature of the Peierls instability*

Let us consider an external potential $U(\mathbf{r})$ acting as a perturbation on electrons:

$$\hat{H}_1 = \int d^3r\, U(\mathbf{r})\hat{n}(\mathbf{r}). \tag{12}$$

Then, the density response function

$$n(\mathbf{q}) = \chi(\mathbf{q})\, U(\mathbf{q}) \tag{13}$$

is given by Eq. (8) of HW8. According to Eq. (3), the static susceptibility is equal to both $\chi_M(i\omega_n = 0)$ and $\chi(\omega = 0)$. Eq. (13) could be also written at a finite frequency ω, but here we are interested in the static case.

Let us consider 1D electron gas with the Fermi momentum k_F. In the following calculations, use the linearized dispersion law for electrons.

(a) [**4 points**] Using Eq. (8) of HW8, calculate the response function χ in Eq. (13) at $q = 2k_F$ at temperature T for noninteracting electrons.

(b) [**4 points**] Suppose electron interact with an amplitude g. Considering the following series of diagrams:

where the circle represents the interaction vertex g, calculate the renormalized susceptibility χ at $q = 2k_F$. Determine the temperature T_c where χ diverges. Interpret the result.

4. [**6 points**] *Transition temperature of superconducting transition*

Let us consider response of a (3D) electron gas to a fictitious perturbation h that creates electron pairs with the opposite momenta:

$$\hat{H}_1 = \int \frac{d^3k}{(2\pi)^3}\, h\, \psi_\uparrow^+(\mathbf{k})\psi_\downarrow^+(-\mathbf{k}) + \text{H.c.} \tag{14}$$

In principle, we could take h to be a function of $\mathbf{k}$ and the total momentum of the electron pair, and give h a more complicated spin structure (see §54). However, here we consider only the simplest case of the singlet s-wave pairing, where h is a constant.

Let us define the (static) response function to the perturbation (14) as follows:

$$\langle \psi_\uparrow^+(\mathbf{k})\psi_\downarrow^+(-\mathbf{k})\rangle = \chi\, h. \tag{15}$$

Then, for electron interacting with the amplitude g, the generalized susceptibility is given by the following sequence of diagrams:

Notice that arrows are parallel in this figure, whereas they are antiparallel in the previous figure.

Determine the temperature T_c where χ diverges. Interpret the result. Does the divergence occur for positive or negative g (repulsion or attraction)? Compare with the Peierls instability.