PHZ 7428 Fall 2004 – Homework 4

Due by 12 noon on Thursday, December 16.

Answer both questions. Please write neatly and include your name on the front page of your answers. You must also clearly identify all your collaborators on this assignment. To gain maximum credit you should explain your reasoning and show all working.

This homework is designed to lead you through some of the basics of itinerant magnetism in systems of interacting electrons. The first question deals with the homogeneous electron gas, while the second concerns electrons in a strong periodic potential.

1. *Magnetic susceptibility of the homogeneous electron gas.* In this question, we consider a gas of free electrons, i.e., a translationally invariant system of electrons experiencing a zero (or at least spatially uniform) single-particle potential. This gas is subjected to a magnetic field $\mathbf{H}(\mathbf{r},t)$, which perturbs the Hamiltonian through the Zeeman coupling:

$$\hat{H}'(t) = -\int d^3\mathbf{r}\ \hat{\mathbf{m}}(\mathbf{r})\cdot\mathbf{H}(\mathbf{r},t),$$

where

$$\hat{\mathbf{m}}(\mathbf{r}) = -\frac{g\mu_B}{2}\sum_{\sigma,\sigma'}\hat{\psi}^\dagger_\sigma(\mathbf{r})\,\boldsymbol{\sigma}_{\sigma,\sigma'}\,\hat{\psi}_{\sigma'}(\mathbf{r}) \tag{1}$$

is the magnetization-density operator. Here, $\sigma^\alpha_{\sigma,\sigma'}$ $(\alpha = x,\, y\, z)$ is a Pauli matrix, $\mu_B = e\hbar/(2mc)$ is the Bohr magneton and $g \approx 2$ is the electron g factor. Note the overall sign of the right-hand side of Eq. (1), which many authors (including Mahan) get wrong.

The perturbation's effect is characterized by the magnetic susceptibility $\chi_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',t')$, defined through

$$\delta\langle\hat{m}_\alpha(\mathbf{r},t)\rangle = \sum_\beta\int d^3\mathbf{r}'\int_{-\infty}^{\infty}dt'\ \chi_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',t')H_\beta(\mathbf{r}',t').$$

(a) By applying the Kubo formula, show that the susceptibility is

$$\chi_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',t') = \frac{i}{\hbar}\theta(t-t')\langle[\hat{m}_\alpha(\mathbf{r},t),\hat{m}_\beta(\mathbf{r}',t')]\rangle.$$

(b) In an isotropic system, the susceptibility satisfies $\chi_{\alpha\beta} = \frac{1}{2}\delta_{\alpha,\beta}\chi_{-+}$, where the transverse susceptibility is

$$\chi_{-+}(\mathbf{r},t,\mathbf{r}',t') = \frac{i}{\hbar}\theta(t-t')\langle[\hat{m}_-(\mathbf{r},t),\hat{m}_+(\mathbf{r}',t')]\rangle, \qquad \hat{m}_\pm = \hat{m}_x \pm i\hat{m}_y.$$

Show that the spatial Fourier transform of the transverse susceptibility has a Matsubara version

$$\begin{aligned}\chi_{-+}(\mathbf{q},\tau) &= \frac{(g\mu_B)^2}{\hbar V}\sum_{\mathbf{k},\mathbf{k}'}\langle T_\tau c^\dagger_{\mathbf{k}\downarrow}(\tau+\eta)c_{\mathbf{k}+\mathbf{q}\uparrow}(\tau)c^\dagger_{\mathbf{k}'\uparrow}(\eta)c_{\mathbf{k}'-\mathbf{q}\downarrow}(0)\rangle,\\ &= \frac{(g\mu_B)^2}{\langle\hat{S}(\beta\hbar,0)\rangle_0\,\hbar V}\sum_{\mathbf{k},\mathbf{k}'}\langle T_\tau c^\dagger_{\mathbf{k}\downarrow}(\tau+\eta)c_{\mathbf{k}+\mathbf{q}\uparrow}(\tau)c^\dagger_{\mathbf{k}'\uparrow}(\eta)c_{\mathbf{k}'-\mathbf{q}\downarrow}(0)\,\hat{S}(\beta\hbar,0)\rangle_0,\end{aligned}$$

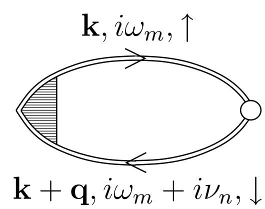
where η is a positive infinitesimal and $\langle \cdots \rangle_0$ indicates a thermal average with respect to the Hamiltonian H_0 for noninteracting electrons.

(c) Assume for the moment that the electrons are noninteracting. Apply Wick's theorem to the right-hand side of Eq. (2), and hence conclude by comparison with the calculation of the noninteracting polarization function $\Pi^{(0)}(\mathbf{q}, i\nu_n)$ that

$$\chi^{(0)}_{-+}(\mathbf{q}, i\nu_n) = -\frac{(g\mu_B)^2}{V} \sum_{\mathbf{k}} \frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{i\hbar\nu_n + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}}.$$

(d) Use the result of part (c) to obtain the noninteracting version of the $T = 0$ uniform, static susceptibility χ_0 (known as the Pauli susceptibility). Also, identify the region of $(\mathbf{q}, \omega)$ space within which the system dissipates energy due to magnetic excitations. What is the nature of these excitations?

In the presence of electron-electron interactions, the transverse susceptibility can be written diagrammatically

$\chi_{-+}(\mathbf{q}, i\nu_n) =$ 

Here, a double line represents a fully dressed electron Green's function, an open circle is a bare spin vertex (i.e., $\frac{1}{2} g\mu_B \sigma^{\pm}$), and the filled triangle represents the fully dressed vertex. Note that, unlike the case of the screened Coulomb interaction, $\chi_{-+}(\mathbf{q}, i\nu_n)$ does not contain a sum of 2, 3, 4, ... bubbles connected by Coulomb interaction lines. The reason is that an arbitrary Feynman diagram in the expansion of $\chi_{-+}(\mathbf{q}, i\nu_n)$ contains exactly two spin vertices, which give a nonzero result when traced over spin indices only if they are associated with the same bubble.

The diagrammatic equation above translates into

$$\chi_{-+}(\mathbf{q}, i\nu_n) = -\frac{(g\mu_B)^2}{\beta\hbar^2 V} \sum_{\mathbf{k},m} \Gamma(\mathbf{k}, i\omega_m, \mathbf{k}{+}\mathbf{q}, i\omega_m{+}i\nu_n) G_\uparrow(\mathbf{k}, i\omega_m) G_\downarrow(\mathbf{k}{+}\mathbf{q}, i\omega_m{+}i\nu_n), \quad (2)$$

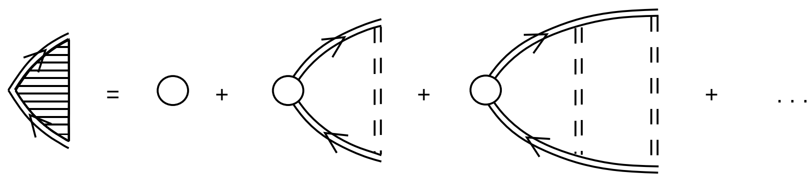
where Γ is the dimensionless vertex function.

In the self-consistent Hartree-Fock approximation, we set $\Gamma = 1$ and

$$G_\sigma(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - \tilde{\omega}_k}. \quad (3)$$

Let us denote the corresponding transverse susceptibility $\chi^{\mathrm{HF}}_{-+}(\mathbf{q}, i\nu_n)$.

(e) In order to go beyond Hartree-Fock, we will approximate the full vertex by a sum of ladders in which the rungs are the RPA screened Coulomb interaction (represented by double dashed lines):



Write down the algebraic equation corresponding to the diagrammatic equation above.

(f) The equation for the vertex function still cannot be solved in closed form, so we will make the additional approximation of replacing the effective interaction by $V_{\mathrm{RPA}}(\mathbf{0},0) = 4\pi e^2/q_{\mathrm{TF}}^2$. Show that this yields

$$\Gamma(\mathbf{k}, i\omega_m, \mathbf{k}{+}\mathbf{q}, i\omega_m{+}i\nu_n) = \left[1 + \frac{4\pi e^2}{\beta\hbar^2 q_{\mathrm{TF}}^2 V} \sum_{\mathbf{k}',p} G_\uparrow(\mathbf{k}', i\omega_p) G_\downarrow(\mathbf{k}'{+}\mathbf{q}, i\omega_p{+}i\nu_n)\right]^{-1}, \tag{4}$$

independent of $\mathbf{k}$ and $i\omega_m$.

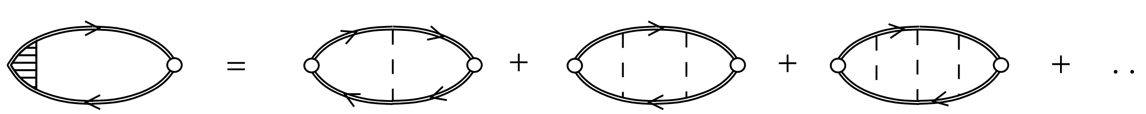
(g) In order to make further progress, let us substitute the Hartree-Fock form [Eq. (3)] for G in Eq. (4). Hence show that the right-hand side of Eq. (4) can be written compactly in terms of $\chi_{-+}^{\mathrm{HF}}(\mathbf{q}, i\nu_n)$.

(h) Now substitute Eq. (3) and the results of the previous parts into Eq. (2) to show that within our approximation scheme (let's call it the Thomas-Fermi approximation)

$$\chi_{-+}^{\mathrm{TF}}(\mathbf{q}, i\nu_n) = \frac{\chi_{-+}^{\mathrm{HF}}(\mathbf{q}, i\nu_n)}{1 - \chi_{-+}^{\mathrm{HF}}(\mathbf{q}, i\nu_n)/[2N(0)(g\mu_B)^2]}.$$

This result assumes that the Fermi-surface density of states $N(0)$ is the same in the noninteracting, Hartree-Fock, and Thomas-Fermi approximations. You may take this to be the case.

An alternative way of proceeding is to approximate the transverse susceptibility by the sum of ladder diagrams with unscreened interaction rungs (dashed lines):



This sum is closely related to the local field correction to the RPA polarization calculated by Hubbard, and it yields

$$\frac{1}{\chi_{-+}^{\mathrm{H}}(\mathbf{q}, i\nu_n)} = \frac{1}{\chi_{-+}^{(0)}(\mathbf{q}, i\nu_n)} - \frac{G(\mathbf{q})V(\mathbf{q})}{(g\mu_B)^2}$$

with

$$G(\mathbf{q}) = \frac{1}{2}\frac{|\mathbf{q}|^2}{|\mathbf{q}|^2 + q_{\mathrm{TF}}^2}.$$

(i) Show that in both the Thomas-Fermi and Hubbard approximations, the net effect of electron-electron interactions is to enhance the susceptibility. Compare the Pauli susceptibilities χ_0^{TF} and χ_0^{H} with $\chi_0^{(0)}$.

2. *Magnetic susceptibility of lattice electrons.* An over-simplified (but fiendishly difficult to solve!) alternative to the homogeneous electron gas as a description of electrons in a metal is the Hubbard model for electrons confined to a lattice of N sites:

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}, \tag{5}$$

where $\epsilon_{\mathbf{k}}$ is the band energy, $\hat{n}_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$, and

$$c_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j} c_{\mathbf{k}\sigma}$$

destroys an electron in a "Wannier state" localized about lattice site j. (Wannier states on different lattice sites are orthogonal.) The second term in Eq. (5) approximates the screened Coulomb potential by an interaction U between up and down electrons on the same lattice site j. It can be re-expressed

$$U \sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} = \frac{U}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} c_{\mathbf{k}'\downarrow}.$$

(a) Calculate the susceptibility of the Hubbard model following the same steps as in the Thomas-Fermi approximation for the homogeneous electron gas, with the differences that you should (i) use N in place of the volume V, (ii) use U instead of $V_{\mathrm{RPA}}(\mathbf{0}, 0)$, and (iii) sum only over wavevectors lying in the first Brillouin zone. Show that

$$\chi_{-+}(\mathbf{q}, i\nu_n) = \frac{\chi^{\mathrm{HF}}_{-+}(\mathbf{q}, i\nu_n)}{1 - U\chi^{\mathrm{HF}}_{-+}(\mathbf{q}, i\nu_n)/[(g\mu_B)^2]}.$$

where

$$\chi^{\mathrm{HF}}_{-+}(\mathbf{q}, i\nu_n) = -\frac{(g\mu_B)^2}{N} \sum_{\mathbf{k}} \frac{n_F(\hbar\tilde{\omega}_{\mathbf{k}}) - n_F(\hbar\tilde{\omega}_{\mathbf{k}+\mathbf{q}})}{i\hbar\nu_n + \hbar\tilde{\omega}_{\mathbf{k}} - \hbar\tilde{\omega}_{\mathbf{k}+\mathbf{q}}}.$$

(b) As the interaction strength U is increased, it is possible for $\chi_{\alpha\beta}(\mathbf{q}, \omega)$ to diverge, signaling an instability of the paramagnetic phase towards magnetic ordering. This instability normally occurs first in the static susceptibility. Use the result of the previous part to write down the "Stoner criterion" for the interaction strength U at which $\chi_{\alpha\beta}(\mathbf{q}, 0)$ diverges.

(c) Provide a simplified version of the Stoner criterion for the instability towards ferromagnetism ($\mathbf{q} = \mathbf{0}$).