FIP10604 – Text 13 — MAGNETISM IN METALS II:
MAGNETIC EXCITATIONS

Elementary excitations in the FM phase of metals

In Text 12, we studied the paramagnetic response and the establishment of magnetic order in metals within the Hartree-Fock approximation. As we did in the case of localized magnetic moments (Text 07), we can study more rigorously excitations from the magnetically ordered ground state.

Starting with FM order, elementary excitations involve **spin deviations**. As in the case of localized spins, the operator that creates a spin deviation at a lattice site i (relative to *up* ordering) is S_i^-. Since in metals the magnetic moments are carried by electrons, the operator that creates a spin-deviation is naturally written in terms of fermionic operators,

$$S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow} \, . \tag{1}$$

The corresponding annihilation operator is

$$S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow} \, . \tag{2}$$

In wave-vector space, we have

$$S_{\mathbf{q}}^- = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}\uparrow} \, , \qquad S_{\mathbf{q}}^+ = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}\downarrow} \, . \tag{3}$$

Note that the two spin operators in this last equation are **not** a pair of creation and annihilation operators. $S_{\mathbf{q}}^-$ creates an **extended** spin deviation, with a spatial modulation characterized by the wave vector $\mathbf{q}$. The corresponding annihilation operator is its Hermitian conjugate, i.e,

$$\left(S_{\mathbf{q}}^-\right)^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}\downarrow} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}-\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}\downarrow} = S_{-\mathbf{q}}^+ \, . \tag{4}$$

The general theory of interacting many-body systems indicates that a spectrum of elementary excitations is given by the poles of an appropriate Green's function (GF). The retarded GF describing the propagation of a spin deviation is

$$\mathcal{G}(\mathbf{q}, t) = -\mathrm{i}\,\theta(t) \langle [S_{-\mathbf{q}}^+(t), S_{\mathbf{q}}^-(0)] \rangle \, , \tag{5}$$

whose time Fourier transform will be denoted as $\mathcal{G}(\mathbf{q}, \omega)$.

The Matsubara version is

$$\tilde{\mathcal{G}}(\mathbf{q}, \tau) = \langle \hat{T}_\tau S_{-\mathbf{q}}^+(\tau) S_{\mathbf{q}}^-(0) \rangle \, , \tag{6}$$

where $\hat{T}_\tau$ is the time-ordering operator in the *imaginary-time* axis. The corresponding Fourier transform is $\tilde{\mathcal{G}}(\mathbf{q}, \nu_n)$, involving **bosonic** Matsubara frequencies $\nu_n = 2n\pi T$, for integer n, because each spin operator is composed by two fermionic ones. The Matsubara GF is more appropriate to a perturbative formalism. In the end, one can obtain the retarded GF by analytic continuation in the complex-frequency plane:

$$\tilde{\mathcal{G}}(\mathbf{q}, \nu_n) \underset{\mathrm{i}\nu_n \to \omega + \mathrm{i}\eta}{\longrightarrow} \mathcal{G}(\mathbf{q}, \omega) \ , \ \eta \to 0^+ \ . \tag{7}$$

Using Eqs. (3) and (4) into (6), we have

$$\tilde{\mathcal{G}}(\mathbf{q}, \tau) = \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} \langle \hat{T}_\tau \, c^\dagger_{\mathbf{k}'\uparrow}(\tau) \, c_{\mathbf{k}'+\mathbf{q}\downarrow}(\tau) \, c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow}(0) \, c_{\mathbf{k}\uparrow}(0) \rangle \ . \tag{8}$$

Zeroth order (non-interacting system)

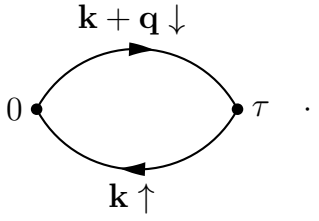
In the absence of interaction, the average on the right-hand side of Eq. (8) satisfies **Wick's theorem**, allowing it to be decomposed into averages involving pairs of operators (single-particle GF's), with conservation of particle number and spin. There is only one possibility for such a decomposition:

$$\tilde{\mathcal{G}}^0(\mathbf{q}, \tau) = -\frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} \tilde{G}^0_{\mathbf{k}\uparrow}(-\tau) \, \tilde{G}^0_{\mathbf{k}+\mathbf{q}\downarrow}(\tau) \, \delta_{\mathbf{k}'\mathbf{k}} \ , \tag{9}$$

where $\tilde{G}^0_{\mathbf{k}\sigma}(\tau)$ is the zeroth-order approximation to the one-electron GF

$$\tilde{G}_{\mathbf{k}\sigma}(\tau) = -\langle \hat{T}_\tau \, c_{\mathbf{k}\sigma}(\tau) \, c^\dagger_{\mathbf{k}\sigma}(0) \rangle \ . \tag{10}$$

Equation (9) corresponds to a simple-loop Feynmann diagram,

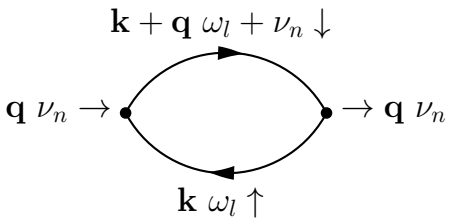


. (11)

The "time" Fourier transform yields

$$\tilde{\mathcal{G}}^0(\mathbf{q}, \nu_n) = -\frac{T}{N} \sum_{\mathbf{k}, \omega_l} \tilde{G}^0_{\mathbf{k}\uparrow}(\omega_l) \, \tilde{G}^0_{\mathbf{k}+\mathbf{q}\downarrow}(\omega_l + \nu_n) \ , \tag{12}$$

where T is the temperature, and $\omega_l = (2l+1)\pi T$ (for l integer) are **fermionic** Matsubara frequencies. The corresponding diagram is



. (13)

Using the explicit form of the zeroth-order one-electron GF, $\tilde{G}^0_{\mathbf{k}\sigma}(\omega_l) = [\mathrm{i}\omega_l - \varepsilon_{\mathbf{k}\sigma} + \mu]^{-1}$, it follows that

$$\begin{aligned}\tilde{\mathcal{G}}^0(\mathbf{q},\nu_n) &= -\frac{T}{N}\sum_{\mathbf{k},\omega_l}\frac{1}{(\mathrm{i}\omega_l - \varepsilon_{\mathbf{k}\uparrow}+\mu)\,(\mathrm{i}\omega_l + \mathrm{i}\nu_n - \varepsilon_{\mathbf{k}+\mathbf{q}\downarrow}+\mu)} \\ &= -\frac{T}{N}\sum_{\mathbf{k}}\frac{1}{\mathrm{i}\nu_n + \varepsilon_{\mathbf{k}\uparrow} - \varepsilon_{\mathbf{k}+\mathbf{q}\downarrow}}\sum_{\omega_l}\left[\tilde{G}^0_{\mathbf{k}\uparrow}(\omega_l) - \tilde{G}^0_{\mathbf{k}+\mathbf{q}\downarrow}(\omega_l+\nu_n)\right] \\ &= \frac{1}{N}\sum_{\mathbf{k}}\frac{\bar{n}_{\mathbf{k}+\mathbf{q}\downarrow} - \bar{n}_{\mathbf{k}\uparrow}}{\mathrm{i}\nu_n - (\varepsilon_{\mathbf{k}+\mathbf{q}\downarrow} - \varepsilon_{\mathbf{k}\uparrow})}\,, \end{aligned} \tag{14}$$

where $\bar{n}_{\mathbf{k}\sigma}$ is the average number of electrons in the state $\mathbf{k}$ with spin σ, here given by the Fermi function of the corresponding energy, and we have used the identity[1]

$$\frac{1}{\beta}\sum_n \frac{e^{\mathrm{i}\omega_n 0+}}{\mathrm{i}\omega_n - \varepsilon} = -\oint_C \frac{dz}{2\pi\mathrm{i}}\,\frac{e^{z\,0+}\,f(z)}{z-\varepsilon} = f(\varepsilon)\,. \tag{15}$$

Performing the analytic continuation to real frequencies, we obtain

$$\mathcal{G}^0(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}}\frac{\bar{n}_{\mathbf{k}+\mathbf{q}\downarrow} - \bar{n}_{\mathbf{k}\uparrow}}{\omega - (\varepsilon_{\mathbf{k}+\mathbf{q}\downarrow} - \varepsilon_{\mathbf{k}\uparrow}) + i\eta}\,, \quad \eta\to 0^+\,. \tag{16}$$

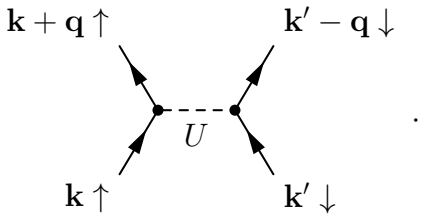
This GF has poles for $\omega = \varepsilon_{\mathbf{k}+\mathbf{q}\downarrow} - \varepsilon_{\mathbf{k}\uparrow}$, which allows us to interpret the elementary excitations (at $T = 0$) as the creation of electron-hole pairs **with spin flipping**, known as *Stoner excitations*. This is the only possible type of spin excitation in a non-interacting system.

Including the interaction between electrons

The interaction Hamiltonian (see Text 12) is

$$\mathcal{H}_I = \frac{U}{N}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow}\,. \tag{17}$$

This can be diagrammatically represented as

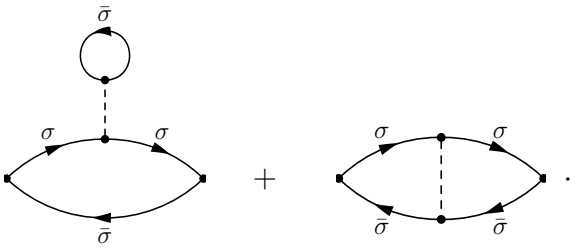


. (18)

[1] For more details see lecture notes of FIP10601: Text 15, Eq. (13) and related comments.

It may be viewed as a "scattering" process between two electrons of opposite spins.

The only way to insert these internal vertices in the diagrams of $\tilde{\mathcal{G}}$ is either attached to one of the lines and having an internal G^0-line closed upon itself, or with each vertex on one of the G^0 lines. The first order diagrams for these two cases (with the notation $\bar{\sigma} \equiv -\sigma$) are



(19)

The first diagram, when summed to all numbers of *tadpoles*, renormalizes the non-interacting GF to the HF one. It is actually the Hartree approximation, since there is no exchange term for an interaction between two electrons with opposite spins. From here on, we omit all tadpole insertions, implicitly assuming that $\tilde{G}^0$ lines are HF GF's.

The simplest series that begins with the second diagram in Eq. (19) contain all the *ladder* contributions, i.e., all loop diagrams having multiple **parallel** (non-crossing) U-lines. To sum such a series, we should notice that a U-line may be collapsed to a point, since U is local (independent of wave vector) and "instantaneous" (independent of frequency). Thus, the two sectors separated by the U-line (or point) in the first-order diagram are equal, and equivalent to the single loop. This will also happen to sectors between two U-lines at higher orders. Therefore we have a geometric series

$$\tilde{\mathcal{G}} = \tilde{\mathcal{G}}^0 + \tilde{\mathcal{G}}^0 U \tilde{\mathcal{G}}^0 + \tilde{\mathcal{G}}^0 U \tilde{\mathcal{G}}^0 U \tilde{\mathcal{G}}^0 + \cdots \tag{20}$$

If we restrict ourselves to this series we have the so-called *Random-Phase Approximation* (RPA). It is the same denomination encountered when studying the density-density GF, which describes particle-hole and plasmon excitations in the non-magnetic state. In that case the U-lines connect (horizontally) two loops. But the same series is reproduced when the U-lines are collapsed, except that each simple loop has the same spin all around, and terms of odd order in U have negative signs.[2] In our present case the RPA should rather be called HF-RPA, since we have included the Hartree-Fock corrections.

Formal summation of the HF-RPA series results in the expression

$$\tilde{\mathcal{G}}(\mathbf{q}, \nu_n) = \frac{\tilde{\mathcal{G}}^0(\mathbf{q}, \nu_n)}{1 - U\tilde{\mathcal{G}}^0(\mathbf{q}, \nu_n)} \,, \tag{21}$$

whose real-frequency version is

$$\mathcal{G}(\mathbf{q}, \omega) = \frac{\mathcal{G}^0(\mathbf{q}, \omega)}{1 - U\mathcal{G}^0(\mathbf{q}, \omega)} \,. \tag{22}$$

[2] See the section "Collective excitations" in the same text referred to in footnote 1.

The spectrum of magnetic excitations is given by the poles of $\mathcal{G}(\mathbf{q},\omega)$, that is, zeros of the denominator in the right-hand side of last equation. Using the explicit form of $\mathcal{G}^0(\mathbf{q},\omega)$, Eq. (16), the frequencies $\omega(\mathbf{q})$ of elementary excitations can be obtained from the equality

$$\frac{U}{N}\sum_{\mathbf{k}}\frac{\bar{n}_{\mathbf{k}+\mathbf{q}\downarrow}-\bar{n}_{\mathbf{k}\uparrow}}{\omega(\mathbf{q})-(\varepsilon_{\mathbf{k}+\mathbf{q}\downarrow}-\varepsilon_{\mathbf{k}\uparrow})}=1\ , \tag{23}$$

Remembering that the energies have the HF form,

$$\begin{aligned}\varepsilon_{\mathbf{k}\uparrow}&=\varepsilon_{\mathbf{k}}+\frac{1}{2}nU-\frac{1}{2}UM\ ,\\ \varepsilon_{\mathbf{k}\downarrow}&=\varepsilon_{\mathbf{k}}+\frac{1}{2}nU+\frac{1}{2}UM\ ,\end{aligned} \tag{24}$$

with $M=n_\uparrow-n_\downarrow$, the difference of energies appearing in the denominator of Eq. (23) is

$$\varepsilon_{\mathbf{k}+\mathbf{q}\downarrow}-\varepsilon_{\mathbf{k}\uparrow}=UM+\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}\ . \tag{25}$$

This shows that there is a gap $\Delta=UM$ for Stoner excitations in the limit $q\to 0$. On the other hand, we can see that $\omega(\mathbf{q})=0$ at $\mathbf{q}=\mathbf{0}$ is a solution, since Eq. (23) becomes

$$\frac{U}{N}\sum_{\mathbf{k}}\frac{\bar{n}_{\mathbf{k}\uparrow}-\bar{n}_{\mathbf{k}\downarrow}}{UM}=1\ . \tag{26}$$

Assuming a parabolic band (with effective mass m^*) and the limit $T\to 0$, we have $|\mathbf{k}|=k_{F\uparrow}$ (note that the Fermi surfaces for spin *up* and *down* have different radii due the energy shifts $\mp UM$). So, the Stoner excitations are distributed between the energies

$$\begin{aligned}E_{\min}&=UM+\frac{q^2}{2m^*}-\frac{k_{F\uparrow}q}{m^*}\ ,\\ E_{\max}&=UM+\frac{q^2}{2m^*}+\frac{k_{F\uparrow}q}{m^*}\ .\end{aligned} \tag{27}$$

In the thermodynamic limit, these solutions are continuous. This implies that they also exist in the interacting system, even though they are poles of $\mathcal{G}^0$, because between every two "successive" poles the function $\mathcal{G}^0(\mathbf{q},\omega)$ varies from $-\infty$ to ∞, thus crossing the point that satisfies the condition $U\mathcal{G}^0(\mathbf{q},\omega)=1$.

The branch of solutions that starts at $\omega=0$ has $\omega\sim\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}$, and it can be shown that for small q one has a dispersion relation of the type $\omega=Dq^2$. This branch of solutions is identified with **magnons** for a metallic system.

Fig. 1 shows schematically the spectrum of elementary magnetic excitation (one spin deviation). We see the continuum of Stoner excitations and the magnon branch. The former can be interpreted as scattering states of an electron and a hole with opposite spins, while the latter correspond to bound states of these pairs. In the region where the two types of

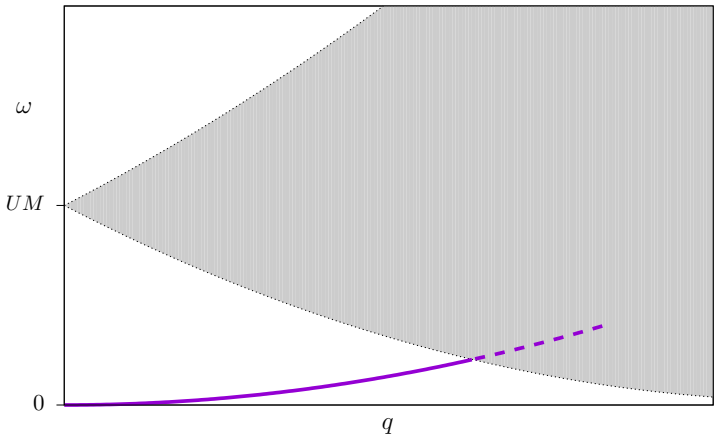


Figure 1: Magnetic excitation spectrum of a metal, showing the continuum of Stoner excitations (for $q < k_{F\uparrow} - k_{F\downarrow}$) and the magnon branch.

excitations coincide in energy, the poles of $\mathcal{G}(\mathbf{q}, \omega)$ develop a nonzero imaginary part, indicating the instability (finite lifetime) of magnon excitations, which decay into scattering states.

When the product UM is large (compared to T), the low-temperature behavior is dominated by magnons. The magnon dispersion relation with the same form as for insulating systems implies that we have the same behavior of magnetization and specific heat at low temperatures (c_m or $\Delta M \sim T^{3/2}$).

Dynamic susceptibility

Linear Response Theory tells us that if a physical system is subjected to a perturbation of the type $\mathcal{H}_1 = B\, f(t)$, where B is an observable of the system and $f(t)$ is a time-dependent external "force", and if the response is measured by the average value of an observable A, then the *response function* (or generalized susceptibility) is given by a Green's function of the operators A and B.[3] Applying this general theory to our case, we assume an applied field perpendicular to the z axis, representing it as a combination of H^+ and H^- in the same way as x and y spin components are written in terms of S^+ and S^-. Then, the Zeeman part of the Hamiltonian can be written as

$$\mathcal{H}_1 = -2 \sum_{\mathbf{q}} S^-_{\mathbf{q}} H^+(-\mathbf{q}, t) \; . \tag{28}$$

Measuring the response by the average value $\langle S^+_{-\mathbf{q}}(t) \rangle$ (and taking into account the g-factor 2 between magnetic moment and spin), we have

$$2\langle S^+_{-\mathbf{q}}(\omega) \rangle = \chi^{+-}(\mathbf{q}, \omega) H^+(-\mathbf{q}, \omega) \tag{29}$$

[3] For more details see lecture notes of FIP10601: Text 16.

with

$$\chi^{+-}(\mathbf{q},\omega) = 2\mathcal{G}(\mathbf{q},\omega). \tag{30}$$

Thus, magnetic-excitation energies correspond to poles of the dynamic susceptibility. Generalizing to any components, one has a tensor that is a complex function, usually separated in real and imaginary parts as $\boldsymbol{\chi}(\mathbf{q},\omega) = \boldsymbol{\chi}'(\mathbf{q},\omega) + \mathrm{i}\boldsymbol{\chi}''(\mathbf{q},\omega)$. Experimentally, the imaginary part is associated with the absorption spectrum, since energy is absorbed from the electromagnetic field to create excitations. In particular, $\boldsymbol{\chi}''(\mathbf{q},\omega)$ has sharp peaks at frequencies $\omega = \omega(\mathbf{q})$ corresponding to magnon excitations. In the static limit (which is, in practice, also the uniform limit in space) there is no energy absorption, and the susceptibility is **real**.

We must mention that it is also possible to evaluate the *longitudinal* susceptibility χ^{zz}. The Green's function involves two S^z operators, being related to the density-density GF (mentioned above), but the RPA series has loops with well-defined (alternating) spin states.

AF (or SDW) phase

So far we focused on elementary excitations from the FM ground state. Let us briefly comment on the case of non-uniform magnetic order, which, as we saw earlier, is associated to a spin-density wave. At the end of Text 12 we analyzed the nature of the SDW state, identifying two situations. When the SDW opens a gap on the whole Fermi surface, the ordered state is insulating, and we have magnon behavior as previously studied for such systems. However, if a reconstructed Fermi surface remains, the situation is quite complex. The absence of long-range spin polarization does not clearly separate the regions of Stoner excitations and magnons (there is no *Stoner gap*). Hence, magnons are always *damped*.

Shortcomings of Hartree-Fock approximation

We finish this analysis of *band magnetism* with some critical comments about the approximations described here.

The HF approximation presents typical shortcomings of mean-field approaches. These weaknesses are partially corrected by inclusion of RPA (correct behavior of c_m and ΔM for $T \to 0$), mainly for the FM case. By treating the electrons as independent, with interactions partially accounted for through an effective field, the HF approach fails to take into account an important effect of strong Coulomb interaction which is **correlated** behavior among the electrons. When correlations are very important, as happens with systems approaching conditions for a metal-insulator transition (*Mott transition*), we enter the domain of the so-called *strongly correlated electronic systems*. For such systems the HF approach fails even in qualitative aspects, and cannot be improved by perturbative corrections as RPA. More sophisticated theoretical methods have been developed to deal with these systems, but their study is beyond the scope of this course. A brief introduction to some of the relevant problems and models in this context will be given in Text 14.