FIP10604 – Text 12 — Magnetism in metals I:
Static susceptibility and magnetic order

So far, our study of magnetic properties of solids has been restricted to **localized magnetic moments**, associated to transition-metal or rare-earth ions with partially occupied electronic shells. The discussion of exchange interactions assumed that these ions were in insulating compounds. Here we will begin to study magnetic properties of metallic solids.

There are few monoatomic metallic solids that exhibit magnetic order. Basically, we can list Cr, Mn, Fe, Co and Ni among transition metals. Within the rare-earth series there appear Gd, Tb, Dy, Ho, Er and Tm. Although the second group present ordering temperatures comparable to those observed in insulators, and magnetic moments per atom consistent with the expected values for isolated atoms, the same is not true for the first one.

A noticeable characteristic of the three ferromagnetic transition metals (Fe, Co and Ni) is to present high Curie temperatures (above 1000 K for Fe and Co; slightly above 600 K for Ni). Another remarkable feature is that the magnetic moment per atom at low temperatures, as determined from magnetization measurements, is significantly smaller than the expected contribution from unpaired electron spins in the atom: $2.2\,\mu_B$, $1.7\,\mu_B$, and $0.6\,\mu_B$, instead of $4\,\mu_B$, $3\,\mu_B$, and $2\,\mu_B$, respectively for Fe, Co and Ni. Moreover, *nonmagnetic* metals (those without spontaneous magnetic order) have paramagnetic susceptibilities that do not follow Curie's law, but are essentially **independent of temperature**.

These observations indicate that it is not possible to describe the magnetism in metals from spin Hamiltonians as we did for insulators. One must take into account that charge degrees of freedom are not frozen in metals, which makes it necessary to address the problem with focus on the existence of conduction electrons that carry **itinerant magnetic moments**.

As in the case of insulators, magnetic properties of metals also have their origin in the Coulomb interaction associated with the effect of fermionic statistics. Here, however, we cannot reformulate the problem in terms of an effective interaction between spins. We must work with a system of electrons moving in the lattice potential and interacting with each other. From this general picture we will try to select what is relevant to magnetic properties. Initially, the problem will be addressed from the opposite limit with respect to the insulating case, i.e., a conduction band. Later, we will analyze more complex situations, including the coexistence of itinerant and localized moments, which is relevant, for example, in the case of rare earth metals mentioned above.

We begin by reviewing the **paramagnetism** of conduction electrons, as a preliminary step to introducing interactions between these electrons and investigating their effect on magnetic behavior.

Review: Pauli paramagnetism

Let us consider a single conduction band of **non-interacting** electrons, with individual energies $\varepsilon_{\mathbf{k}}$, to which we apply a magnetic field of magnitude H. We choose the field direction as the z axis.

We know that the electron spin gives rise to an intrinsic magnetic moment

$$\boldsymbol{\mu} = 2\mathbf{S} . \tag{1}$$

Note that we continue to "define" the magnetic moment as **parallel** to the spin (no minus sign) and to take $\mu_B = 1$, but we explicitly include the spin g-factor ($g = 2$). Any component of $\mathbf{S}$ has eigenvalues $\pm 1/2$ ($\hbar = 1$). Therefore, the electron energies with the magnetic field turned on are

$$\varepsilon_{\mathbf{k}\pm} = \varepsilon_{\mathbf{k}} \mp H , \tag{2}$$

where $\pm$ as a subscript refers to the spin eigenvalues $\pm 1/2$, for which we also use $\uparrow$ and $\downarrow$.

The zero-field density of states (DOS), $D(\varepsilon)$, can still be used for $\varepsilon_{\mathbf{k}}$, allowing to write the magnetization as

$$M = n_\uparrow - n_\downarrow = \int d\varepsilon \, D(\varepsilon) \left[f(\varepsilon - H) - f(\varepsilon + H) \right] , \tag{3}$$

where $f(\varepsilon) = \{\exp[(\varepsilon - \mu)/T] + 1\}^{-1}$ is the Fermi function.

Up to first order in H, and for low temperatures ($T \ll T_F$), we have

$$M = 2H \int d\varepsilon \, D(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) \simeq 2D(\varepsilon_F)H , \tag{4}$$

with the usual notation for *Fermi energy* and *Fermi temperature*. Therefore, the paramagnetic susceptibility of an electron gas, also known as *Pauli susceptibility*, is

$$\chi_P = 2D(\varepsilon_F) . \tag{5}$$

It is **independent of temperature** as long as the condition $T \ll T_F$ is fulfilled.

Actually, this is not the full story. We assumed that the magnetic field acts only on the electron's spin, but it also couples to the electron's charge. This yields the Lorentz force in the classical limit, and Landau levels in a quantum-mechanical solution. Quantization of energy states in Landau levels changes the DOS, and introduces a diamagnetic contribution called *Landau susceptibility*, χ_L. Without developing any details, we just quote the result for free electrons, which is $\chi_L = -\chi_P/3$. Under appropriate conditions, the lattice effect is absorbed into the electron's effective mass m^*. In this case, χ_L has an extra factor $(m_e/m^*)^2$. Except for semiconductors, which tend to have $m* \ll m_e$, the paramagnetic part is dominant. Henceforth, when we refer to *paramagnetic* susceptibility it is implied that the diamagnetic correction is already included.

It is interesting to compare the orders of magnitude of paramagnetic susceptibilities in metals and insulators. Still using the independent-electron approximation as a reference, for a total electron density n in a single band we have $D(\varepsilon_F) \sim n/\varepsilon_F$, which means that $\chi_P \sim 1/T_F$. Note that χ_P corresponds to a Curie-law form with the temperature "frozen" at T_F. Therefore, χ_P is two or three orders of magnitude **smaller** than the Curie susceptibility at room temperature. In other words, paramagnetism in metals is much weaker than in insulators, and can even compete with the diamagnetic effect of closed atomic shells. Indeed, the net susceptibility of some metals, such as copper, silver and gold, is diamagnetic. This seems to contradict what was said at the end of the previous paragraph, but it is not the case. There we where comparing paramagnetism an diamagnetism of conduction electrons only, while here we are also taking into account the diamagnetism of closed-shell electrons localized in the ions.

The fact that χ_P is independent of temperature reflects the correlation of spin orientations among the conduction electrons caused by Pauli's principle. It is easy to verify from Eq. (4), but taking the opposite limit in temperature, that the paramagnetic susceptibility of metals would satisfy Curie's law if $T \gg T_F$, since in this regime the electrons would not be restricted to the lowest energy states, and the aforementioned spin correlations would tend to disappear. Only in such a nonphysical limit would conduction electrons behave like **independent** magnetic moments.

Interacting system

We know that effects of interaction between electrons are more important, and may lead to instabilities of the Fermi-liquid state, when the conduction band is narrow. As already mentioned, the only mono-atomic metallic solids that present magnetic order are some transition metals (Cr, Mn, Fe, Co and Ni) and certain rare earths. In these metals, the Fermi level lies in a region of high density of states, mainly of 3d or 4f character, despite some hybridization with s states. The usual model to study interacting electrons in narrow bands is the Hubbard model, which considers a *tight-binding* band with intra-site repulsive interaction. It is described by the Hamiltonian

$$\mathcal{H} = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \, . \tag{6}$$

This same Hamiltonian was used in Text 05 to obtain exchange interactions in insulators, in the limit $U \gg t_{ij}$. Here we assume that the interaction is not strong enough to suppress the metallic state.

Using the relationship

$$c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k}\sigma}^\dagger \, , \tag{7}$$

we can rewrite the Hubbard Hamiltonian in Bloch representation:

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} c_{\mathbf{k}'-\mathbf{q},\downarrow}^{\dagger} c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} \ . \tag{8}$$

Hartree-Fock approximation

It is well known that exact solutions for many-body problems like the one described by Eq. (8) do not exist. The simplest approach is to use the Hartree-Fock (HF) approximation, which assumes independent-electron states. The operator product in the interaction term is then rewritten (like in a mean-field approximation) as

$$c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} c_{\mathbf{k}'-\mathbf{q},\downarrow}^{\dagger} c_{\mathbf{k}'\downarrow} \simeq \langle c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} \rangle c_{\mathbf{k}'-\mathbf{q},\downarrow}^{\dagger} c_{\mathbf{k}'\downarrow} + \langle c_{\mathbf{k}'-\mathbf{q},\downarrow}^{\dagger} c_{\mathbf{k}'\downarrow} \rangle c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} - \langle c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} \rangle \langle c_{\mathbf{k}'-\mathbf{q},\downarrow}^{\dagger} c_{\mathbf{k}'\downarrow} \rangle \ . \tag{9}$$

Among the possible decoupling schemes, we have chosen averages that conserve particle number and spin. Given the nature of HF states, the average values in Eq. (9) are nonzero only for $\mathbf{q} = \mathbf{0}$. Substituting into Eq. (8), and dropping an additive constant coming from the last term of Eq. (9), we obtain the HF Hamiltonian

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma}^{\mathrm{HF}} n_{\mathbf{k}\sigma} \ , \tag{10}$$

where

$$\varepsilon_{\mathbf{k}\sigma}^{\mathrm{HF}} = \varepsilon_{\mathbf{k}} + \frac{U}{N} \sum_{\mathbf{k}'} \langle n_{\mathbf{k}'\bar{\sigma}} \rangle = \varepsilon_{\mathbf{k}} + U n_{\bar{\sigma}} \ . \tag{11}$$

Our notation for the spin subscript is such that $\bar{\sigma} = \downarrow$ when $\sigma = \uparrow$ and vice versa. Note that $n_{\bar{\sigma}}$ in the last term is a global average value (density). For simplicity, an n with a site or wave-vector subscript is an operator, otherwise it is a density.

Equation (11) shows that the interaction in HF approximation is equivalent to an applied magnetic field, since it produces an energy shift that depends on the spin orientation. This can be better seen if we use the relations

$$n = n_{\uparrow} + n_{\downarrow} \ , \qquad M = n_{\uparrow} - n_{\downarrow} \ , \tag{12}$$

where n is the electron density and M is the magnetization. We can then write

$$n_{\uparrow} = \frac{1}{2}(n + M) \ , \qquad n_{\downarrow} = \frac{1}{2}(n - M) \ , \tag{13}$$

and the electron energies take the form

$$\varepsilon_{\mathbf{k}\pm}^{\mathrm{HF}} = \varepsilon_{\mathbf{k}} + \frac{1}{2}nU \mp \frac{1}{2}UM \ , \tag{14}$$

with the already mentioned correspondence $(+,-) \rightarrow (\uparrow,\downarrow)$. Equation (14) puts into evidence the effect of interaction as an overall energy shift $(nU/2)$ plus an effective magnetic field $UM/2$ [see Eq. (2) for comparison].

Generalizing what we did for the paramagnetic case with applied field, Eqs. (12) become

$$n = \int d\varepsilon\, D(\varepsilon)\left[f(\varepsilon + nU/2 - UM/2) + f(\varepsilon + nU/2 + UM/2)\right] ,$$

$$M = \int d\varepsilon\, D(\varepsilon)\left[f(\varepsilon + nU/2 - UM/2) - f(\varepsilon + nU/2 + UM/2)\right] . \tag{15}$$

Considering that n is **fixed** and that this set of equations must be solved for a given temperature, these equations determine the chemical potential μ (which appears in the Fermi functions) and the magnetization M as functions of temperature.

PM susceptibility

We begin by investigating the possibility of still having a paramagnetic system at all temperatures, despite the presence of interactions. In the absence of spontaneous magnetization, the susceptibility must be obtained applying a weak external field (linear response). The resulting effective field is

$$H^{\text{eff}} = \frac{1}{2}UM + H . \tag{16}$$

Following the standard procedure for an effective field, i.e.,

$$M = \chi H = \chi_P H^{\text{eff}} , \tag{17}$$

the last two equations allow to isolate the susceptibility,

$$\chi = \frac{\chi_P}{1 - \frac{1}{2}U\chi_P} = \frac{\chi_P}{1 - D(\varepsilon_F)U} , \tag{18}$$

where the second equality involves using Eq. (5). For $D(\varepsilon_F)U < 1$, we see an **enhanced** paramagnetic response as the effect of electron-electron interactions.

Instability of the PM state

For $D(\varepsilon_F)U > 1$, Eq. (18) shows an instability of the PM state, since the susceptibility becomes negative. The assumed magnetization is uniform, which means that the stable state should be **FM order**.

Another way to visualize this is through the introduction of a small spin polarization of the electron system (uniform magnetization), evaluating the energy change with respect to the PM state. Starting with the PM condition $n_\uparrow = n_\downarrow = n$, we switch a fraction δn

of spin-down electrons to spin up. This fraction of electrons occupies an energy range of width $\delta\varepsilon$ around the Fermi level, so that we end up with

$$n_\uparrow = \frac{n}{2} + \delta n \ , \quad n_\downarrow = \frac{n}{2} - \delta n \ , \quad \delta n = D(\varepsilon_F)\delta\varepsilon \ , \tag{19}$$

The change in kinetic energy (at $T = 0$) is

$$\frac{\Delta K}{N} = \int_{\varepsilon_F}^{\varepsilon_F + \delta\varepsilon} \varepsilon D(\varepsilon)d\varepsilon - \int_{\varepsilon_F - \delta\varepsilon}^{\varepsilon_F} \varepsilon D(\varepsilon)d\varepsilon = D(\varepsilon_F)(\delta\varepsilon)^2 \ , \tag{20}$$

while the interaction energy changes by

$$\frac{\Delta E_{\text{int}}}{N} = U\left(\frac{n}{2} + \delta n\right)\left(\frac{n}{2} - \delta n\right) - U\left(\frac{n}{2}\right)^2 = -U(\delta n)^2 \ . \tag{21}$$

Therefore, the total energy change can be written as

$$\frac{\Delta E}{N} = D(\varepsilon_F)(\delta\varepsilon)^2[1 - D(\varepsilon_F)U] \ . \tag{22}$$

One can see that this energy difference is positive (the PM state is stable) for $D(\varepsilon_F)U < 1$, and is negative (the PM state is **unstable** against FM order) for $D(\varepsilon_F)U > 1$. This latter condition is known as the *Stoner criterion* for ferromagnetism.

Metals of the *iron group* are characterized by the presence of a hybrid 4s-3d band. The presence of atomic d states, which are quite localized, leads to the formation of a narrow band, consequently with a high DOS. The atomic 3d levels being partially filled in Fe, Co and Ni (configurations $[\text{Ar}]3\text{d}^{n_d}4\text{s}^2$, with $n_d = 6$, 7 and 8, respectively) implies that the Fermi level falls in this high-DOS region. This is consistent with the observation that these metals are ferromagnetic at room temperature.

Ordered FM phase

As we discussed above, if the Stoner criterion is satisfied the system displays FM order in the ground state. A critical temperature $T_C > 0$ is then expected to exist at which a transition to the PM phase takes place. This means that a reduction of the magnetization with increasing temperature should be observed, similarly to what we have seen for insulators.

$M(T)$ is evaluated by solving Eqs. (15) for each T value. The second of those equations can be represented graphically, as we did in the case of localized spins (but now the function at the right-hand side is not a Brillouin function). Once more, the left-hand side is represented by a straight line of unit slope ($M = M$), while the right-hand side is a nontrivial function of M, which vanishes at $M = 0$, and is limited by the maximum values $M = \pm n$. If the first derivative of this function is smaller than 1, the only point of contact with the straight line is at $M = 0$; if it is larger than 1, there is an intersection for $M > 0$. Therefore, the

critical temperature corresponds to the first derivative exactly equal to 1. Expanding the right hand side in powers of M, we obtain

$$M = MU \int d\varepsilon\, D(\varepsilon) \left[-\frac{\partial f}{\partial \varepsilon} \right]_{T_c} + \mathcal{O}(M^3) . \tag{23}$$

Thus, the equation that determines T_C is

$$U \int d\varepsilon\, D(\varepsilon) \left[-\frac{\partial f}{\partial \varepsilon} \right]_{T_c} = 1 . \tag{24}$$

The Fermi function is evaluated with the Hartree-Fock energies for $M = 0$, i.e., $\varepsilon + \frac{1}{2}nU - \mu$. But $\mu(T = 0) = \varepsilon_F = \varepsilon_F^0 + nU$, where ε_F^0 is the Fermi energy of the non-interacting system. We have $D(\varepsilon_F) = D(\varepsilon_F^0)$ since the HF energies are **rigidly** displaced. Unlike an insulating system, the magnetization at $T = 0$ is not saturated (i.e., independent of the applied field), unless the relative displacement of the spin-up and down bands is very large, caused by a very intense Coulomb interaction. We have two qualitatively different situations:

1. **U is very large, so that the top of the spin-up band is below the Fermi level:** In this case, $M(0)$ is saturated. Furthermore, there is a gap $\Delta = UM$ for spin-flip excitations, leading to deviations $\Delta M(T) = M(0) - M(T)$ that follow an exponential law, $\Delta M(T) \sim \exp(-\Delta/T)$. Among the 3d (pure) metals, this is the case of Ni (Fig. 1) and Co.
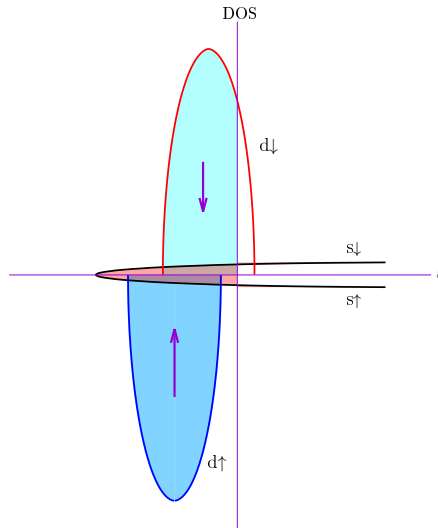
Figure 1: Schematic representation of the density of states for the spin-polarized bands in Ni. The Fermi level is at the origin of the energy axis. The band occupations correspond to $n_{d\uparrow} = 5$ (the d↑ band is placed completely below the Fermi level), $n_{d\downarrow} \simeq 4.4$, $n_s \simeq 0.6$ (without polarization), implying that $M \simeq 0.6\,\mu_B/$at, as mentioned before.

2. U **is not strong enough to cause a gap:** There are states with both spin orientations in the vicinity of the Fermi level, implying that $M(0)$ is not saturated (spins can be flipped by an applied field). Furthermore, the variation $\Delta M(T)$ is no longer exponential, but follows a power law, which in HF is $\Delta M(T) \sim T^2$. Iron (Fe) falls into this category, but the experimentally observed behavior is $\Delta M(T) \sim T^{3/2}$ (spin waves?!).

Nonuniform magnetic order

To verify the existence of other types of magnetic ordering we follow the same procedure as for localized spins, looking for divergences in the static wave-vector-dependent susceptibility $\chi(\mathbf{q})$.

With a position-dependent external field, the HF solution leads to the effective field

$$H^{\text{eff}}(\mathbf{q}) = H(\mathbf{q}) + \frac{1}{2}UM(\mathbf{q}) , \tag{25}$$

which reproduces Eq. (16) in the uniform case. By the usual procedure, we obtain the PM susceptibility

$$\chi(\mathbf{q}) = \frac{\chi^0(\mathbf{q})}{1 - \frac{1}{2}U\chi^0(\mathbf{q})} . \tag{26}$$

According to our previous discussion of susceptibility an correlation functions for a generic magnetic system (Text 09), the static susceptibility in the non-interacting limit can be obtained through the relation

$$\chi^0_{ij} = 4 \int_0^\beta d\tau \langle S_i^z(\beta)S_j^z(\tau)\rangle , \tag{27}$$

where $\beta = 1/T$, the average is at zero applied field, and the factor 4 appears because we included $g = 2$. Our choice of the z component does not imply any loss of generality for an isotropic system in the PM phase.

In wave-vector space, Eq. (28) becomes

$$\chi^0(\mathbf{q}) = 4 \int_0^\beta d\tau \langle S_{\mathbf{q}}^z(\beta)S_{-\mathbf{q}}^z(\tau)\rangle . \tag{28}$$

Using the relationships

$$S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) , \quad n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} , \quad c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k}\sigma}^\dagger , \tag{29}$$

we have

$$S_{\mathbf{q}}^z = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} (c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}\uparrow} - c_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}\downarrow}) . \tag{30}$$

From the single-particle form of the unperturbed HF Hamiltonian, time-dependent creation and annihilation operators are simply written as

$$
\begin{aligned}
c_{\mathbf{k}\sigma}^{\dagger}(\tau) &= \mathrm{e}^{\varepsilon_{\mathbf{k}}\tau} c_{\mathbf{k}\sigma}^{\dagger} , \\
c_{\mathbf{k}\sigma}(\tau) &= \mathrm{e}^{-\varepsilon_{\mathbf{k}}\tau} c_{\mathbf{k}\sigma} .
\end{aligned}
\tag{31}
$$

Therefore,

$$
\chi^{0}(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}\,\mathbf{k}'} \langle (c_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}+\mathbf{q}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow})(c_{\mathbf{k}'-\mathbf{q}\uparrow}^{\dagger} c_{\mathbf{k}'\uparrow} - c_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger} c_{\mathbf{k}'\downarrow}) \rangle \, I(\beta) ,
\tag{32}
$$

where

$$
I(\beta) \equiv \mathrm{e}^{\beta(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})} \int_{0}^{\beta} d\tau \, \mathrm{e}^{(\varepsilon_{\mathbf{k}'-\mathbf{q}}-\varepsilon_{\mathbf{k}'})\tau} = \frac{\mathrm{e}^{\beta(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})} \left[\mathrm{e}^{\beta(\varepsilon_{\mathbf{k}'-\mathbf{q}}-\varepsilon_{\mathbf{k}'})} - 1 \right]}{\varepsilon_{\mathbf{k}'-\mathbf{q}} - \varepsilon_{\mathbf{k}'}} .
\tag{33}
$$

What remains to evaluate are the average values appearing in Eq. (32), whose Hartree-Fock decoupling has the generic form

$$
\langle c_{\mathbf{k}+\mathbf{q}\,\sigma}^{\dagger} c_{\mathbf{k}\sigma} c_{\mathbf{k}'-\mathbf{q}\,\sigma'}^{\dagger} c_{\mathbf{k}'\sigma'} \rangle = \langle n_{\mathbf{k}\sigma} \rangle \langle n_{\mathbf{k}'\sigma'} \rangle \, \delta_{\mathbf{q},\mathbf{0}} + \langle n_{\mathbf{k}'\sigma} \rangle (1 - \langle n_{\mathbf{k}\sigma} \rangle)\,(1 - \delta_{\mathbf{q},\mathbf{0}}) \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}} \delta_{\sigma\sigma'} .
\tag{34}
$$

Given that $\langle n_{\mathbf{k}\sigma} \rangle = f(\varepsilon_{\mathbf{k}})$ (independent of σ), and using Eqs. (33) and (34) in Eq. (32), we obtain

$$
\chi^{0}(\mathbf{q}) = \frac{2}{N} \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}} .
\tag{35}
$$

Again, $\varepsilon_{\mathbf{k}}$ can be taken as the bare band energies, since the uniform HF displacement cancels out in the denominator, and is absorbed by the chemical potential in the Fermi functions. For $T \ll T_F$, the numerator on the right-hand side is nonzero only when the energies $\varepsilon_{\mathbf{k}}$ and $\varepsilon_{\mathbf{k}+\mathbf{q}}$ are near the Fermi level, one of them above and the other below ε_F.

Magnetic order means periodicity of the magnetization in space, so that a single non-zero Fourier component $\mathbf{M}(\mathbf{Q})$ exists, corresponding to a wave vector $\mathbf{Q}$ such that the denominator of Eq. (26) vanishes, i.e.,

$$
\frac{1}{2} U \chi^{0}(\mathbf{Q}) = 1 .
\tag{36}
$$

The ordering occurs for the wave vector that satisfies this condition at the highest temperature. When $\mathbf{Q} = \mathbf{0}$, we have FM order. For instance, it is easy to verify that Eq. (35) gives $\chi^{0}(\mathbf{0}) = \chi_P = 2D(\varepsilon_F)$ when $T \to 0$, and Eq. (36) reproduces the Stoner criterion.

When $\mathbf{Q} \neq \mathbf{0}$, the nonuniform ordering can be seen as a spatial modulation of the distribution of electron spins, which is called a *spin-density wave* (SDW). It may correspond to a simple AF (Néel) order if the lattice is sc and $\mathbf{Q} = (\pi/a, \pi/a, \pi/a)$. Experimental results for Cr yield $\mathbf{Q} \simeq 0.96\,(2\pi/a, 0, 0)$, which seems to indicate a SDW that is incommensurate with the lattice [more details in: *Eric Fawcett, Rev. Mod. Phys. 60, 209 (1988)*]. The other transition metal classified as antiferromagnetic is Mn (α phase), with $T_N \lesssim 100$ K, but it appears to present a complex, non-collinear order, probably also incommensurate.
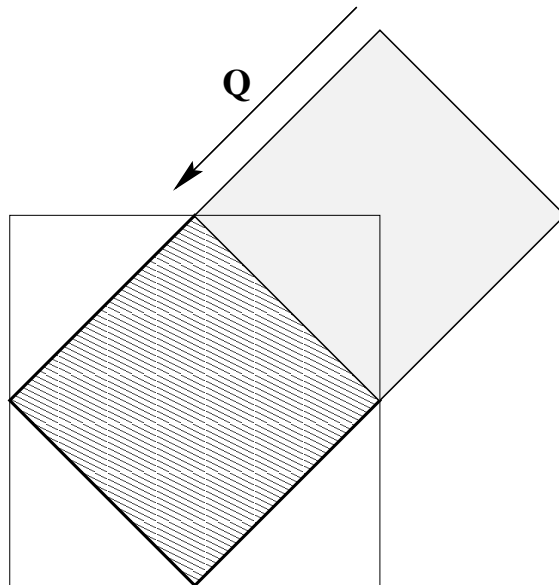
Nesting

From the form of Eq. (35) we can see that a maximum (or possibly a divergence) of $\chi^0(\mathbf{Q})$ must appear when fairly large parallel regions of the Fermi surface (FS) are relatively displaced by $\mathbf{Q}$, since all the corresponding states have the same energy. The complete coincidence of electron and hole Fermi surfaces under a displacement $\mathbf{Q}$ is called *nesting*.

A trivial nesting example is a one-dimensional electron gas. In this case, the Fermi "surface" consists of two points, that can be brought together by a wave-vector of magnitude $Q = 2k_F$. The susceptibility $\chi^0(2k_F)$ presents a logarithmic divergence, also known as *Kohn anomaly*.

A less trivial example is the tight-binding model on a square lattice ($d = 2$). For an electron density $n = 1$, i.e., half-filled band, the Fermi "surface" is a square with half the Brillouin-zone area. The vector $\mathbf{Q} = (\pi/a, \pi/a)$ causes perfect nesting (Fig. 2), leading to a **divergence** of $\chi^0(\mathbf{Q})$. This indicates an instability of the PM state against the establishment of an AF-type (Néel) SDW for any value of $U \neq 0$.

When the nesting is not perfect (which is the more realistic case), $\chi^0(\mathbf{q})$ is always finite, but can present sharp maxima. Then, the instability of the PM phase occurs for U above a finite **critical** value. It is also possible to have a nesting vector incommensurate with the lattice, as in the case of chromium that we mentioned before. A planar cut of chromium's FS (bcc lattice) is shown in Fig. 3, where $\mathbf{q}$ is the wave-vector that we denoted as $\mathbf{Q}$, for which we can see that there is nesting of more or less extensive regions of the FS.

Figure 2: Nesting of the FS on a tight-binding square lattice for $n = 1$.
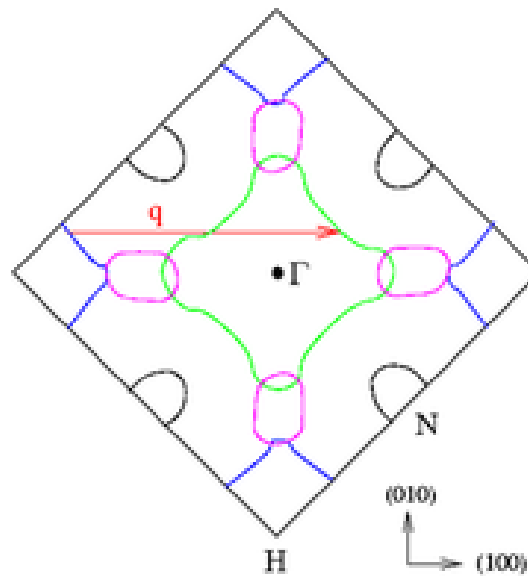
Figure 3: Fermi-surface nesting in Cr (http://www.answers.com/topic/spin-density-wave).

Nature of the SDW state

In the low-temperature region, once a SDW is established, we have essentially two scenarios:

1. **The SDW opens a gap throughout the FS:** Then the ordered system is no longer metallic, and the magnetic transition is also a *metal-insulator transition*. This is what happens in the square-lattice model.

2. **The SDW does *not* open a gap on the entire FS:** It occurs if there is partial nesting (as for Cr). The system preserves a metallic character, but gaps open up on parts of the FS, leaving (possibly several) branches of a *reconstructed* FS. This reflects the change of periodicity that occurs between the PM and ordered phases. A detailed description of such a situation tends to be quite complex, particularly when the SDW is incommensurate.