Chapter 7

Magnetic properties

Before we start to discuss the specific magnetic properties of solids, let us recall concepts that are normally taught in mechanics and in the elementary course in quantum mechanics.

We consider the simple case of a charged particle in a stationary magnetic field. Then, the Hamilton function in classical mechanics is given by

$$H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 , \tag{7.1}$$

such that the equations of motion lead to the Lorentz force. As always, the passage to quantum mechanics is made by replacing the functions $p(t)$ and $q(t)$ by operators. Let us assume further, that the magnetic field is homogeneous, such that the vector potential can be chosen as follows

$$A_i\left(\boldsymbol{x}\right) = -\frac{1}{2}\varepsilon_{ijk}\, x_j\, B_k , \tag{7.2}$$

where ε_{ijk} is the Levi-Civita symbol in three dimensions, and a summation over repeated indices is understood. Using this vector potential, we look now at the different contributions to the Hamiltonian above, where we have to recall that $\boldsymbol{p}$ and $\boldsymbol{x}$ are quantum mechanical operators.

$$\frac{1}{2m}\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\left(\hat{\boldsymbol{x}}\right)\right]^2 = \frac{1}{2m}\left[\hat{\boldsymbol{p}}^2 - \frac{e}{c}\hat{\boldsymbol{p}}\cdot\boldsymbol{A}\left(\hat{\boldsymbol{x}}\right) - \frac{e}{c}\boldsymbol{A}\left(\hat{\boldsymbol{x}}\right)\cdot\hat{\boldsymbol{p}} + \frac{e^2}{c^2}\boldsymbol{A}^2\right] , \tag{7.3}$$

where we obtain in a natural way an expansion in powers of the magnetic field, since $\boldsymbol{A} \sim \boldsymbol{B}$. For the different orders we have:

i) Free part.

$$\frac{\hat{\boldsymbol{p}}^2}{2m} + V\left(\boldsymbol{x}\right) \longrightarrow H_0 , \tag{7.4}$$

where we generalized the Hamiltonian with some external potential $V\left(\boldsymbol{x}\right)$.

ii) Linear coupling.

$$\boldsymbol{p}\cdot\boldsymbol{A} \;=\; -\frac{1}{2}\boldsymbol{p}\cdot(\boldsymbol{x}\times\boldsymbol{B}) = -\frac{1}{2}\boldsymbol{B}\cdot(\boldsymbol{p}\times\boldsymbol{x}) = \frac{1}{2}\boldsymbol{L}\cdot\boldsymbol{B}\,, \tag{7.5}$$

where $\boldsymbol{L}$ is the angular momentum. By performing the same calculation for the other linear contribution, one finally obtains

$$\frac{e}{2mc}\left(\boldsymbol{p}\cdot\boldsymbol{A}+\boldsymbol{A}\cdot\boldsymbol{p}\right) \;=\; \frac{\mu_B}{\hbar}\boldsymbol{L}\cdot\boldsymbol{B}\,, \tag{7.6}$$

where

$$\mu_B \equiv e\hbar/2mc \tag{7.7}$$

is the *Bohr magneton.* The linear coupling to the magnetic field gives rise then to a *paramagnetic* term in the Hamiltonian

$$H_1 = -\frac{\mu_B}{\hbar}\boldsymbol{L}\cdot\boldsymbol{B}\,. \tag{7.8}$$

This shows that a *magnetic moment*

$$\boldsymbol{M} = \frac{\mu_B}{\hbar}\boldsymbol{L} \tag{7.9}$$

is associated to the angular momentum (orbital motion) of a charged particle. The coupling is here paramagnetic, since the magnetic moment will tend to be aligned in the direction of the magnetic field. Furthermore, we can see from the equation above that μ_B is a magnetic moment, since $[L] = [\hbar]$, where the symbol [ ] means here units.

iii) Quadratic coupling

$$\begin{aligned}\frac{e^2}{8mc^2}\left(\boldsymbol{x}\times\boldsymbol{B}\right)^2 \;&=\; \frac{e^2}{8mc^2}\left[\boldsymbol{x}^2\boldsymbol{B}^2-(\boldsymbol{x}\cdot\boldsymbol{B})^2\right] \\ &=\; \frac{e^2\boldsymbol{B}^2}{8mc^2}\left[\boldsymbol{x}^2-\frac{(\boldsymbol{x}\cdot\boldsymbol{B})^2}{\boldsymbol{B}^2}\right]\,,\end{aligned} \tag{7.10}$$

where the term in square brackets gives the components of $\boldsymbol{x}$ in the direction perpendicular to the magnetic field:

$$\boldsymbol{x}_\perp^2 = \boldsymbol{x}^2 - \frac{(\boldsymbol{x}\cdot\boldsymbol{B})^2}{\boldsymbol{B}^2}\,. \tag{7.11}$$

The quadratic term corresponds to a *diamagnetic* term in the Hamiltonian

$$H_2 \;=\; \frac{e^2\boldsymbol{x}_\perp^2\boldsymbol{B}}{8mc^2}\cdot\boldsymbol{B}\,, \tag{7.12}$$

where a magnetic moment

$$\boldsymbol{M} \;=\; -\frac{e^2\boldsymbol{x}_\perp^2}{8mc^2}\boldsymbol{B}\,, \tag{7.13}$$

couples to the magnetic field, i.e. the diamagnetic part describes the coupling of an induced magnetic moment that opposes the applied magnetic field.

After having discussed the coupling of the charge of the electron to a magnetic field, we should consider the coupling of a magnetic field to its spin. It is described by the *Zeeman coupling*

$$H_S = -\boldsymbol{M}_S \cdot \boldsymbol{B} \; , \tag{7.14}$$

where the magnetic moment associated to the spin

$$\boldsymbol{M}_S \;=\; g_S \frac{\mu_B}{\hbar} \boldsymbol{S}$$

where

$$g_S = 2 \left[1 + \frac{\alpha}{2\pi} + \mathcal{O}\left(\alpha^2\right) \right] \; , \tag{7.15}$$

is the *gyromagnetic factor*, that can be calculated in the frame of *quantum electrodynamics*, with the *hyperfine structure constant*

$$\alpha = \frac{e}{\hbar c} \simeq \frac{1}{137} \; . \tag{7.16}$$

Since $\alpha \ll 1$, we can consider $g_S = 2$.

Once we discussed all the couplings of a magnetic field to the electron, we can go over to the situation in solids.

7.1 Pauli paramagnetism

Let us first consider the effect of a magnetic field in a metall. For this purpose, we simplify metals to a Fermi gas, a simplification that is meaningful in the case of Fermi liquids, as we discussed in Sec. 4.4.3. Furthermore, we assume the magnetic field weak enough, so that only effects linear in $\boldsymbol{B}$ are important. Then, the contributions arising from the quadratic term in $\boldsymbol{A}$ can be neglected. With respect to the contribution from H_1, we notice that $< \boldsymbol{L} >= 0$ in the ground-state of the Fermi-gas, such that, we neglect it in the limit of a weak magnetic field. Then, in the limit of a weak magnetic field, the Zeeman coupling to the spins dominates. On the basis of the arguments above, the Hamiltonian is

$$H \;=\; \sum_i \left(\frac{\boldsymbol{p}_i^2}{2m} - \frac{g_S \mu_B}{\hbar} \boldsymbol{S}_i \cdot \boldsymbol{B} \right) \; . \tag{7.17}$$

In order to proceed further, we go over to second quantization. As seen in Sec. 4.2, for a one-particle operator, we have to consider the eigenstates of the operator, in this case the spin-operator. Let us choose the spin-quantization axis in the z-direction, with the eigenstates of S^z

$$\begin{aligned} S^z \left|\uparrow\right> &= \frac{\hbar}{2} \left|\uparrow\right> , \\ S^z \left|\downarrow\right> &= -\frac{\hbar}{2} \left|\downarrow\right> \; . \end{aligned} \tag{7.18}$$

The spin-operators can be easily represented in this two dimensional space using the Pauli matrices,

$$\boldsymbol{S} = \frac{\hbar}{2} \boldsymbol{\sigma} \; , \tag{7.19}$$

with

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; , \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; , \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \; . \tag{7.20}$$

Then,

$$\sum_{i,j} f_i^\dagger < i \mid \boldsymbol{S} \mid j > f_j \quad \Longrightarrow \quad \frac{\hbar}{2} \sum_{\alpha,\beta} f_\alpha^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_\beta \; , \tag{7.21}$$

with $\alpha, \beta = \uparrow, \downarrow$. Choosing a coordinate system such that $\boldsymbol{B} \parallel \hat{z}$, we can finally write the Hamiltonian in second quantization

$$H = \sum_{\boldsymbol{k}} \left(\epsilon_{\boldsymbol{k}\uparrow} f_{\boldsymbol{k}\uparrow}^\dagger f_{\boldsymbol{k}\uparrow} + \epsilon_{\boldsymbol{k}\downarrow} f_{\boldsymbol{k}\downarrow}^\dagger f_{\boldsymbol{k}\downarrow} \right) \; , \tag{7.22}$$

where with $g_S = 2$,

$$\epsilon_{\boldsymbol{k},\sigma} \;\; = \;\; \frac{\hbar^2 \boldsymbol{k}^2}{2m} \mp \mu_B B \; . \tag{7.23}$$

The effect of the magnetic field is to shift the eigenvalues of the original system by $\pm \mu_B B$. Taking into account the chemical potential, we see that the magnetic field leads to a spin-dependent chemical potential

$$\mu \longrightarrow \mu \pm \mu_B B \; . \tag{7.24}$$

Once we obtained the Hamiltonian in a diagonal form, it is in principle possible to calculate any desired observable. We consider therefore the magnetization, that is given by the expectation values of the magnetic moments

$$\begin{aligned} M &= \frac{1}{V} < \sum_i M_i^z > = \frac{1}{V} \frac{g_S \mu_B}{\hbar} < \sum_i S_i^z > \\ &= \frac{1}{V} \frac{g_S \mu_B}{2} < \sum_{\boldsymbol{k}} \left(f_{\boldsymbol{k}\uparrow}^\dagger f_{\boldsymbol{k}\uparrow} - f_{\boldsymbol{k}\downarrow}^\dagger f_{\boldsymbol{k}\downarrow} \right) > = \mu_B \frac{N_\uparrow - N_\downarrow}{V} \; , \end{aligned} \tag{7.25}$$

where $N_{\uparrow,\downarrow}$ give the number of electrons for each spin projection. Since we are dealing with non-interacting electrons, we know already from (4.249) in Sec. 4.3.3 how the number of electrons depends on the chemical potential. Taking into account the fact that depending on the spin projection a different chemical potential has to be used, as already discussed above, and the fact that the degeneracy factor $g = 1$, when looking at each spin-projection, we have

$$\frac{N_{\uparrow,\downarrow}}{V} = \frac{1}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} (\mu \pm \mu_B B)^{\frac{3}{2}} \left[1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\mu \pm \mu_B B}\right)^2 + \cdots\right] , \tag{7.26}$$

where we just replaced in (4.249) $\mu \longrightarrow \mu \pm \mu_B B$ depending on the spin-projection. We restrict ourselves as already stated in the beginning of this section, to the limit of weak magnetic fields $\mu_B B \ll E_F$, such that we need only to expand (7.26) up to first order in B. Furthermore, as already discussed in Sec. 4.3.3, it is a good approximation to replace μ by E_F for most relevant temperatures in condensed matter physics, since the corrections are of the order of $\mathcal{O}\left(k_B T/E_F\right)^2$. Finally, let us recall the form of the density of states (4.225), such that

$$M = N(E_F)\, \mu_B B \left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{E_F}\right)^2\right] , \tag{7.27}$$

leading again to a correction in temperature of the same order as the one we already discarded, so that we should discard it also. The corresponding spin susceptibility, called in this case *Pauli susceptibility*, is obtained as

$$\chi = \frac{\partial M}{\partial B} = N(E_F)\, \mu_B , \tag{7.28}$$

where we again discarded terms of $\mathcal{O}\left(k_B T/E_F\right)^2$. Then, the characteristics of the paramagnetic response of metals is that they are temperature independent and is a direct measure of the density of states at the Fermi energy.

7.2 Ferromagnetism in the Heisenberg model

In this section we examine the opposite case to the one in the previous section, namely the case when electrons are fairly localized, such that the contributions from the kinetic part are not important in determining the magnetic state of the system.

7.2.1 The Heisenberg model

We start with a general form for the Hamiltonian, as given in (4.193),

$$\begin{aligned} H = & \sum_{\substack{i,j \\ \sigma}} f^\dagger_{i,\sigma} < i \mid T \mid j > f_{j,\sigma} \\ & + \frac{1}{2} \sum_{\substack{i,j,k,\ell \\ \sigma,\sigma'}} f^\dagger_{i,\sigma} f^\dagger_{j,\sigma'} < i,j \mid V \mid k,\ell > f_{\ell,\sigma'} f_{k,\sigma} , \end{aligned} \tag{7.29}$$

where V corresponds to the Coulomb interaction and the states $\mid i, \sigma >$ are Wannier states in a solid, where i denotes the site (or cell) where the Wannier orbital is centered on, and σ the spin state. Notice that the spin indices were chosen as in (4.289), but in principle the indices corresponding to Wannier orbitals may have up to four different values. In fact, the matrix element is explicitly given by

$$
\begin{aligned}
& < i, j \mid V \mid k, \ell > \\
& \quad = \int \mathrm{d}^3x \, \mathrm{d}^3x' \, \frac{\varphi^*_\sigma(\boldsymbol{x} - \boldsymbol{R}_i) \, \varphi^*_{\sigma'}(\boldsymbol{x}' - \boldsymbol{R}_j) \, \varphi_{\sigma'}(\boldsymbol{x}' - \boldsymbol{R}_\ell) \, \varphi_\sigma(\boldsymbol{x} - \boldsymbol{R}_k)}{\mid \boldsymbol{x} - \boldsymbol{x}' \mid} \, . \qquad (7.30)
\end{aligned}
$$

Wannier orbitals give a convenient basis for the case of rather localized electronic states. Here we consider for simplicity only the case of a single band.

In the following we restrict ourselves to matrix elements of the interaction that take into account only one- and two-center integrals. For the one-center integrals we have $i = j = k = \ell$,

$$
\frac{1}{2} \sum_{\substack{i \\ \sigma, \sigma'}} f^\dagger_{i,\sigma} f^\dagger_{i,\sigma'} < i, i \mid V \mid i, i > f_{i,\sigma'} f_{i,\sigma} \;\; = \;\; U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \, , \qquad (7.31)
$$

where we defined

$$
\hat{n}_{i,\sigma} = f^\dagger_{i,\sigma} f_{i,\sigma} \, . \qquad (7.32)
$$

Here, due to Pauli's exclusion principle $\sigma' = -\sigma$, and since the matrix element of the Coulomb interaction does not depend on spin, we can extract it defining $U \equiv < i, i \mid V \mid i, i >$. This term is the famous Hubbard interaction, a radical idealization of Coulomb interaction, that takes into account the effects of local electronic correlation. By retaining only this term and the first term in (7.29), with $-t \equiv < i \mid T \mid j >$, one obtains the *Hubbard model*, that is widely used for the description of magnetic systems, mostly antiferromagnetic ones, and more recently it became one of the most discussed models in connection with high temperature superconductivity. In the case of very localized electrons such that we can assume that the number of electrons per site does not fluctuate ($t/U \to 0$), magnetism would arise with one electron per site if we have only one band. In this case, the term obtained above cancels.

For the two center integrals we had three possibilities that we consider in the following.

i) $< i, j \mid V \mid j, i >$, $i \neq j$.

In this case, we have in general an exchange of spin between different sites:

$$
\begin{aligned}
& \frac{1}{2} \sum_{\substack{i \neq j \\ \sigma, \sigma'}} f^\dagger_{i,\sigma} f^\dagger_{j,\sigma'} < i, j \mid V \mid j, i > f_{i,\sigma'} f_{j,\sigma} \\
& \qquad\qquad = -\frac{1}{2} \sum_{\substack{i \neq j \\ \sigma, \sigma'}} J_{ij} \, f^\dagger_{i,\sigma} \, f_{i,\sigma'} \, f^\dagger_{j,\sigma'} \, f_{j,\sigma} \, . \qquad (7.33)
\end{aligned}
$$

Such an interaction term can be easily understood after seeing that the following relationship for Pauli matrices holds

$$\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta} \; = \; 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta} \; . \tag{7.34}$$

Then, we can write

$$\begin{aligned} \frac{1}{2}\sum_{\alpha,\beta} f^{\dagger}_{i,\alpha}\, f_{i,\beta}\, f^{\dagger}_{j,\beta}\, f_{j,\alpha} \; &= \; \frac{1}{4}\Big(\sum_{\alpha,\beta,\gamma,\delta} f^{\dagger}_{i,\alpha}\boldsymbol{\sigma}_{\alpha\beta} f_{i,\beta} \cdot f^{\dagger}_{j,\gamma}\boldsymbol{\sigma}_{\gamma\delta} f_{j,\delta} \\ &\qquad + \sum_{\alpha,\beta} f^{\dagger}_{i,\alpha}\, f_{i,\alpha}\, f^{\dagger}_{j,\beta}\, f_{j,\beta} \Big) \\ &= \; \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + \frac{1}{4}\hat{n}_i \hat{n}_j \; , \end{aligned} \tag{7.35}$$

where we defined the spin operator in second quantization

$$\hat{\boldsymbol{S}}_i \equiv \frac{1}{2} \sum_{\alpha,\beta} f^{\dagger}_{i,\alpha}\boldsymbol{\sigma}_{\alpha\beta} f_{i,\beta} \; , \tag{7.36}$$

and

$$\hat{n}_i \equiv \sum_{\sigma} \hat{n}_{i,\sigma} \; . \tag{7.37}$$

Then, we have for (7.33),

$$(7.33) \; = \; -\sum_{i\neq j} J_{ij} \left(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + \frac{1}{4}\hat{n}_i \hat{n}_j \right) \; , \tag{7.38}$$

where the exchange couplings J_{ij} are given by

$$J_{ij} \; = \; < i,j \mid V \mid j,i > \; , \tag{7.39}$$

whose explicit form can be obtained by replacing the corresponding indices in (7.30). In the case that the electrons are very localized like in an insulator, and having only one electron per site, the second term in (7.38) gives only a constant shift of energy, and can be discarded.

ii) $< i,j \mid V \mid i,j >$, $i \neq j$.
In this case, we have

$$\frac{1}{2} \sum_{\substack{i\neq j \\ \sigma,\sigma'}} f^{\dagger}_{i,\sigma} f^{\dagger}_{j,\sigma'} \; < i,j \mid V \mid i,j > \; f_{j,\sigma'} f_{i,\sigma} = \frac{1}{2}\sum_{i\neq j} V_{ij}\, \hat{n}_i\, \hat{n}_j \; . \tag{7.40}$$

This corresponds to density-density interactions, and again, in the cases where charge fluctuations are suppressed, this term leads only to an overall shift of the energy.

iii) $< i,i \mid V \mid j,j >$, $i \neq j$.

$$\frac{1}{2}\sum_{\substack{i\neq j\\ \sigma,\sigma'}} f^\dagger_{i,\sigma} f^\dagger_{i,\sigma'} < i,i \mid V \mid j,j > f_{j,\sigma'} f_{j,\sigma} = \frac{1}{2}\sum_{\substack{i\neq j\\ \sigma}} \tilde{t}_{ij} f^\dagger_{i,\sigma} f^\dagger_{i,-\sigma} f_{j,-\sigma} f_{j,\sigma} \; . \tag{7.41}$$

> Such a term describes pair-hopping processes of local singlet pairs. It certainly gives no contribution to magnetism and since the Coulomb repulsion is largest on-site (given by the coupling U introduced above), such processes may be important in highly excited states but not at the energy scales related to magnetism. It can be therefore, discarded in general.

From the discussion above, we see that in the cases where a local magnetic moment is present, the magnetic interaction arises from the Coulomb interaction and neglecting charge fluctuations, one obtains

$$H_H = -\sum_{i\neq j} J_{ij}\, \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j - g_S \mu_B \boldsymbol{B} \cdot \sum_i \hat{\boldsymbol{S}}_i \; , \tag{7.42}$$

the *Heisenberg model*, where we added the coupling to an external magnetic field.

7.2.2 Mean-field theory for the ferromagnetic Heisenberg model

In the same way as we proceeded in the case of the BCS Hamiltonian, we can reduce the interacting system to an effectively free theory by discarding fluctuations around a mean-field, that in this case is of magnetic nature. We introduce the identity

$$\hat{\boldsymbol{S}}_i \;=\; < \hat{\boldsymbol{S}}_i > + \left(\hat{\boldsymbol{S}}_i - < \hat{\boldsymbol{S}}_i > \right) \; , \tag{7.43}$$

into the Hamiltonian (7.42), and neglect terms quadratic in the fluctuations around the mean-field. Then, we obtain

$$H_H \;\rightarrow\; -2\sum_{i\neq j} J_{ij} \hat{\boldsymbol{S}}_i \cdot < \hat{\boldsymbol{S}}_j > - g_S \mu_B B \sum_i \hat{S}^z_i \; , \tag{7.44}$$

where we used the fact that $J_{ij} = J_{ji}$. In this way, the problem with interacting spins is reduced to a system of independent spins under the action of an effective magnetic field, i.e.

$$H_H \;\rightarrow\; -\sum_i \tilde{\boldsymbol{b}}_i \cdot \hat{\boldsymbol{S}}_i \; , \tag{7.45}$$

where

$$\tilde{\boldsymbol{b}}_i \;=\; g_S \mu_B \boldsymbol{B} + 2 \sum_{j(\neq i)} J_{ij} < \hat{\boldsymbol{S}}_j > \; . \tag{7.46}$$

Since the spins are independent, the problem is reduced to a one-spin problem, that given the magnetic field, is easily solved. Taking the spin quantization axis in the direction of the magnetic field, we have

$$H_i = -bS_i^z \ . \tag{7.47}$$

Setting $\hbar = 1$, the eigenvalues are $E_i^{(1,2)} = \pm b/2$. We can then obtain the expectation value $< S^z >$ given a temperature T as

$$< S^z > \ = \ \frac{\frac{1}{2}\,\mathrm{e}^{\beta b/2} + \left(-\frac{1}{2}\right)\,\mathrm{e}^{-\beta b/2}}{\mathrm{e}^{\beta b/2} + \mathrm{e}^{-\beta b/2}} = \frac{1}{2}\tanh\left(\frac{\beta b}{2}\right) \ , \tag{7.48}$$

where $\beta = 1/k_B T$.

Let us now assume that the external magnetic field is in the direction of the spontaneous magnetization, that we choose to be in the z-direction. Furthermore, since a ferromagnetic state forms, we set a homogeneous field for the magnetization, i.e. $< S^z >= \sigma$, such that inserting (7.46) into (7.48), we have

$$\sigma \ = \ \frac{1}{2}\tanh\left[\frac{\beta}{2}\left(g_S \mu_B B + 2J_0\,\sigma\right)\right] \ , \tag{7.49}$$

where we defined

$$J_0 \equiv \sum_{j(\neq i)} J_{ij} \ . \tag{7.50}$$

Equation (7.49) shows the selfconsistent nature of the problem.

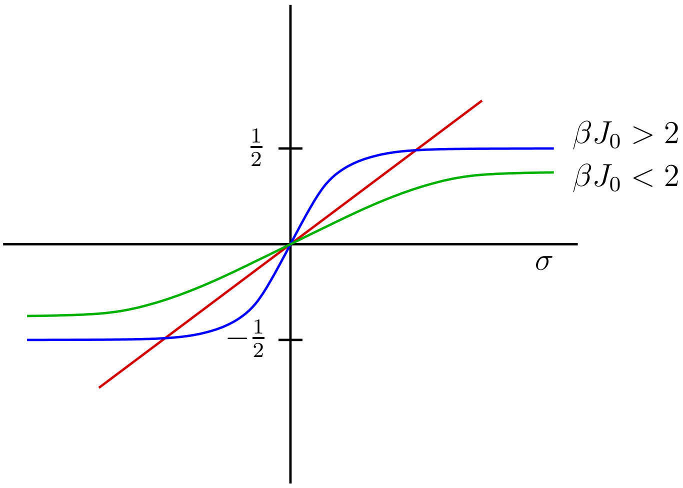

Figure 7.1: Graphical solution of the mean-field equation for the magnetization σ.

The mean-field approximation leads to a free problem, where the effective magnetic field at a given site consists of the external one and the one due to all the other spins on that site.

We consider first the case without external magnetic field. The solution of the eq. (7.49) can be found graphically as shown in Fig. 7.1 by looking at the intersection of the identity with the line corresponding to the right hand side of eq. (7.49), where we set $B = 0$. The critical temperature is given by the temperature at which the slope of the r.h.s. of (7.49) is unity, i.e.

$$1 = \frac{\beta_c J_0}{2} \; . \tag{7.51}$$

For $\beta J_0 < 2$, i.e. $T > T_c = J_0/2k_B$, the only possible solution is $\sigma = 0$, whereas for $T < T_c$ a finite value for σ is also a solution. The *critical temperature* T_c is called the *Curie temperature*.

Magnetization

In order to calculate the magnetization close to T_c, we can expand the r.h.s. of (7.49) since σ is vanishing small. Then, we have

$$\sigma \simeq \frac{\beta J_0 \sigma}{2} - \frac{1}{6} \left(\beta J_0 \sigma\right)^3 \; , \tag{7.52}$$

that leads to

$$\sigma^2 \simeq \frac{3}{4} \frac{T_c - T}{T_c} \left(\frac{T}{T_c}\right)^2 = \frac{3}{4} \frac{T_c - T}{T_c} + \mathcal{O}\left(\frac{(Tc - T)^2}{T_c^2}\right) \; , \tag{7.53}$$

such that in lowest order,

$$\sigma \simeq \sqrt{\frac{3}{4} \frac{T_c - T}{T_c}} \; , \quad (T < T_c) \; , \tag{7.54}$$

The magnetization shows *critical behavior*

$$\sigma \sim \left(T_c - T\right)^\beta \; , \tag{7.55}$$

with a critical exponent $\beta = \frac{1}{2}$. This is a result found in mean-field theory, with the same critical exponent for the order parameter as in the Ginzburg-Landau theory for superconductivity. The actual value found in computer simulations and in *renormalization group theory* for three dimensions is $\beta \simeq 0.33$.

Magnetic susceptibility

We consider now a weak external magnetic field at temperatures higher but close to T_c. By expanding the r.h.s. of (7.49) to lowest order we have,

$$\sigma \simeq \frac{\beta}{4} \left(g_S \mu_B B + 2 J_0 \, \sigma\right) \; , \tag{7.56}$$

leading to

$$\sigma = \frac{g_S \mu_B B}{4k_B} \frac{1}{T - T_c} , \tag{7.57}$$

the *Curie-Weiss law.* The magnetic susceptibility is obtained as the derivative of the magnetization with respect to the field, leading to

$$\chi = \frac{g_S \mu_B}{4k_B} \frac{1}{T - T_c} . \tag{7.58}$$

The divergence of the susceptibility is another sign of criticality, that is summarized by the relation

$$\chi \sim (T - T_c)^{-\gamma} , \tag{7.59}$$

with the critical exponent $\gamma = 1$ in mean field, the correct value being $\gamma = 1.38$. It is seen again, that although the mean-field theory captures qualitatively the critical behavior, it is not a method for a quantitative description of it.

7.2.3 Spin-waves in a ferromagnet

After having discussed the behavior of the system close to the phase transition, we focus now on the excitations of the system at temperatures $T \ll T_c$, where an ordered ferromagnetic state is present. Before we start with the treatment of the excitations in such a state, we recall some features of the $S - \frac{1}{2}$ spin algebra. In order to simplify notation, we set as in the previous section, $\hbar = 1$.

As we already discussed in Sec. 7.1, the spin-operators are connected to the Pauli matrices through (7.19), and the Pauli matrices are given by (7.20). Then, it is easy to verify that the spin operators fulfill the following algebra

$$\left[S^a , S^b \right] = i \varepsilon^{abc} S^c . \tag{7.60}$$

As seen in quantum mechanics, we can define raising and lowering operators

$$\begin{aligned} S^+ &= S^x + i S^y , \\ S^- &= S^x - i S^y , \end{aligned} \tag{7.61}$$

that obey the following commutation relations

$$\begin{aligned} \left[S^z , S^+ \right] &= S^+ , \\ \left[S^z , S^- \right] &= -S^- , \\ \left[S^+ , S^- \right] &= 2 S^z . \end{aligned} \tag{7.62}$$

Then, we can express the spin coupling in the Heisenberg Hamiltonian as follows

$$\begin{aligned} \boldsymbol{S}_i \cdot \boldsymbol{S}_j &= S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \\ &= \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z . \end{aligned} \tag{7.63}$$

Then, it is easy to see that the ground-state is the ferromagnetic one with maximal polarization $\mid 0 > = \mid \uparrow\uparrow\uparrow \cdots >$, since

$$S_i^z S_j^z \mid\uparrow\uparrow> = \frac{1}{4} \mid\uparrow\uparrow> \ , \tag{7.64}$$

whereas

$$\left(S_i^+ S_j^- + S_i^- S_j^+\right) \mid\uparrow\uparrow> = 0 \ . \tag{7.65}$$

Next we can look for an excited state, that for a periodic solid can be constructed by a coherent superposition of downturned spins:

$$\begin{aligned} \mid \boldsymbol{k} > &= \sum_j \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_j\right)\ S_j^- \mid 0 > \\ &= S^-\left(\boldsymbol{k}\right) \mid 0 > \ . \end{aligned} \tag{7.66}$$

It will be useful to consider the commutator of H_H with $S^-(\boldsymbol{k})$,

$$\begin{aligned} \left[H_H, S^-\left(\boldsymbol{k}\right)\right] &= -\sum_\ell \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_\ell\right) \sum_{i\neq j} J_{ij} \\ &\quad \times \left[\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + S_i^z S_j^z, S_\ell^-\right] \ . \end{aligned} \tag{7.67}$$

Using the commutation relations (7.62), we have

$$\begin{aligned} \left[S_i^+ S_j^-, S_\ell^-\right] &= \left[S_i^+, S_\ell^-\right] S_j^- = 2\delta_{i\ell} S_i^z S_j^- \ , \\ \left[S_i^- S_j^+, S_\ell^-\right] &= S_i^- \left[S_j^+, S_\ell^-\right] = 2\delta_{j\ell} S_i^- S_j^z \ , \\ \left[S_i^z\ S_j^z, S_\ell^-\right] &= \left[S_i^z, S_\ell^-\right] S_j^z + S_i^z \left[S_j^z, S_\ell^-\right] \\ &= -\left(\delta_{i\ell} S_i^- S_j^z + \delta_{j\ell} S_i^z S_j^-\right) \ . \end{aligned} \tag{7.68}$$

Introducing these relations into (7.67), we have

$$(7.67) = 2\sum_\ell \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_\ell\right) \sum_{i(\neq\ell)} J_{i\ell}\left(S_i^z S_\ell^- - S_i^- S_\ell^z\right) \ . \tag{7.69}$$

This means that

$$\begin{aligned} H_H\, S^-\left(\boldsymbol{k}\right) \mid 0 > &= S^-\left(\boldsymbol{k}\right)\ H_H \mid 0 > \\ &\quad +2\sum_\ell \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_\ell\right) \sum_{i(\neq\ell)} J_{i\ell}\left(S_\ell^- S_i^z - S_i^- S_\ell^z\right) \mid 0 > . \end{aligned} \tag{7.70}$$

Here we have on the one hand

$$\left(S_\ell^- S_i^z - S_i^- S_\ell^z\right) \mid 0 > = \frac{1}{2}\left(S_\ell^- - S_i^-\right) \mid 0 > \ . \tag{7.71}$$

Then, one of the summations gives

$$\sum_{\ell} \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_{\ell}\right) \sum_{i(\neq\ell)} J_{i\ell}\, S_{\ell}^{-} = J_0\, S^{-}\left(\boldsymbol{k}\right) \ , \tag{7.72}$$

where we used the definition (7.50). For the other summation we can introduce the Fourier transform of $J_{i\ell}$, since it should be a periodic function.

$$J_{i\ell} = \frac{1}{N}\sum_{\boldsymbol{k}_1} \exp\left[i\boldsymbol{k}_1\cdot\left(\boldsymbol{R}_i - \boldsymbol{R}_{\ell}\right)\right] J\left(\boldsymbol{k}_1\right) \ , \tag{7.73}$$

such that

$$\begin{aligned} \sum_{\ell} \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_{\ell}\right) \sum_{i(\neq\ell)} J_{i\ell}\, S_i^{-} &= \frac{1}{N}\sum_{\boldsymbol{k}_1}\sum_{i} \exp\left(i\boldsymbol{k}_1\cdot\boldsymbol{R}_i\right) S_i^{-}\, J\left(\boldsymbol{k}_1\right) \\ &\quad \times \sum_{\ell} \exp\left[i\left(\boldsymbol{k}-\boldsymbol{k}_1\right)\cdot\boldsymbol{R}_{\ell}\right] \\ &= J\left(\boldsymbol{k}\right)\, S^{-}\left(\boldsymbol{k}\right) \ . \end{aligned} \tag{7.74}$$

Going back to (7.70), we have

$$\begin{aligned} H_H\, S^{-}\left(\boldsymbol{k}\right) \mid 0 > &= S^{-}\left(\boldsymbol{k}\right)\, E_0 \mid 0 > \\ &\quad + J_0\, S^{-}\left(\boldsymbol{k}\right) \mid 0 > - J\left(\boldsymbol{k}\right)\, S^{-}\left(\boldsymbol{k}\right) \mid 0 > \\ &= \left[E_0 + J_0 - J\left(\boldsymbol{k}\right)\right] S^{-}\left(\boldsymbol{k}\right) \mid 0 > \ . \end{aligned} \tag{7.75}$$

This means that $S^{-}\left(\boldsymbol{k}\right) \mid 0 >$ is an eigenstate with an excitation energy $\omega_{\boldsymbol{k}} = J_0 - J\left(\boldsymbol{k}\right)$. Since $J_{ij} = J_{ji}$,

$$J\left(\boldsymbol{k}\right) = 2\sum_{m>0} \cos\left(\boldsymbol{k}\cdot\boldsymbol{R}_m\right)\, J\left(\boldsymbol{R}_m\right) \ , \tag{7.76}$$

such that

$$\omega_{\boldsymbol{k}} = 2\sum_{m>0} \left[1 - \cos\left(\boldsymbol{k}\cdot\boldsymbol{R}_m\right)\right]\, J\left(\boldsymbol{R}_m\right) \overset{k\to 0}{\longrightarrow} \sim k^2 \ . \tag{7.77}$$

The elementary excitations of a magnetic system are called *magnons*. In the case of an *antiferromagnet*, where $J < 0$, (in this case we have to restrict the range of the interaction to nearest neighbors, in order to have a well defined scheme for the ordered state; for longer range interactions, competing contributions would appear leading to *frustration*), we do not posses an explicit eigenstate for the ground-state. The so-called *Néel state* is a classical approximation and, hence the excitations above it are approximate spin-waves.