Modelo de Stoner para o Ferromagnetismo metálico

$$\begin{aligned} E_\uparrow(\boldsymbol{k}) &= E(\boldsymbol{k}) - I n_\uparrow / N \, , \\ E_\downarrow(\boldsymbol{k}) &= E(\boldsymbol{k}) - I n_\downarrow / N \, , \end{aligned} \tag{8.36}$$

$$R = \frac{n_\uparrow - n_\downarrow}{N} \, .$$

$$\begin{aligned} R &= \frac{1}{N} \sum_k f_\uparrow(\boldsymbol{k}) - f_\downarrow(\boldsymbol{k}) \\ &= \frac{1}{N} \sum_k \frac{1}{e^{[\tilde{E}(\boldsymbol{k}) - IR/2 - E_\mathrm{F}]/\not{k}T} + 1} - \frac{1}{e^{[\tilde{E}(\boldsymbol{k}) + IR/2 - E_\mathrm{F}]/\not{k}T} + 1} \, . \end{aligned}$$

$$\tilde{D}(E_\mathrm{F}) = \frac{V}{2N} D(E_\mathrm{F}) \, . \tag{8.44}$$

The condition for ferromagnetism to occur at all is then simply

$$I\tilde{D}(E_\mathrm{F}) > 1 \, . \tag{8.45}$$

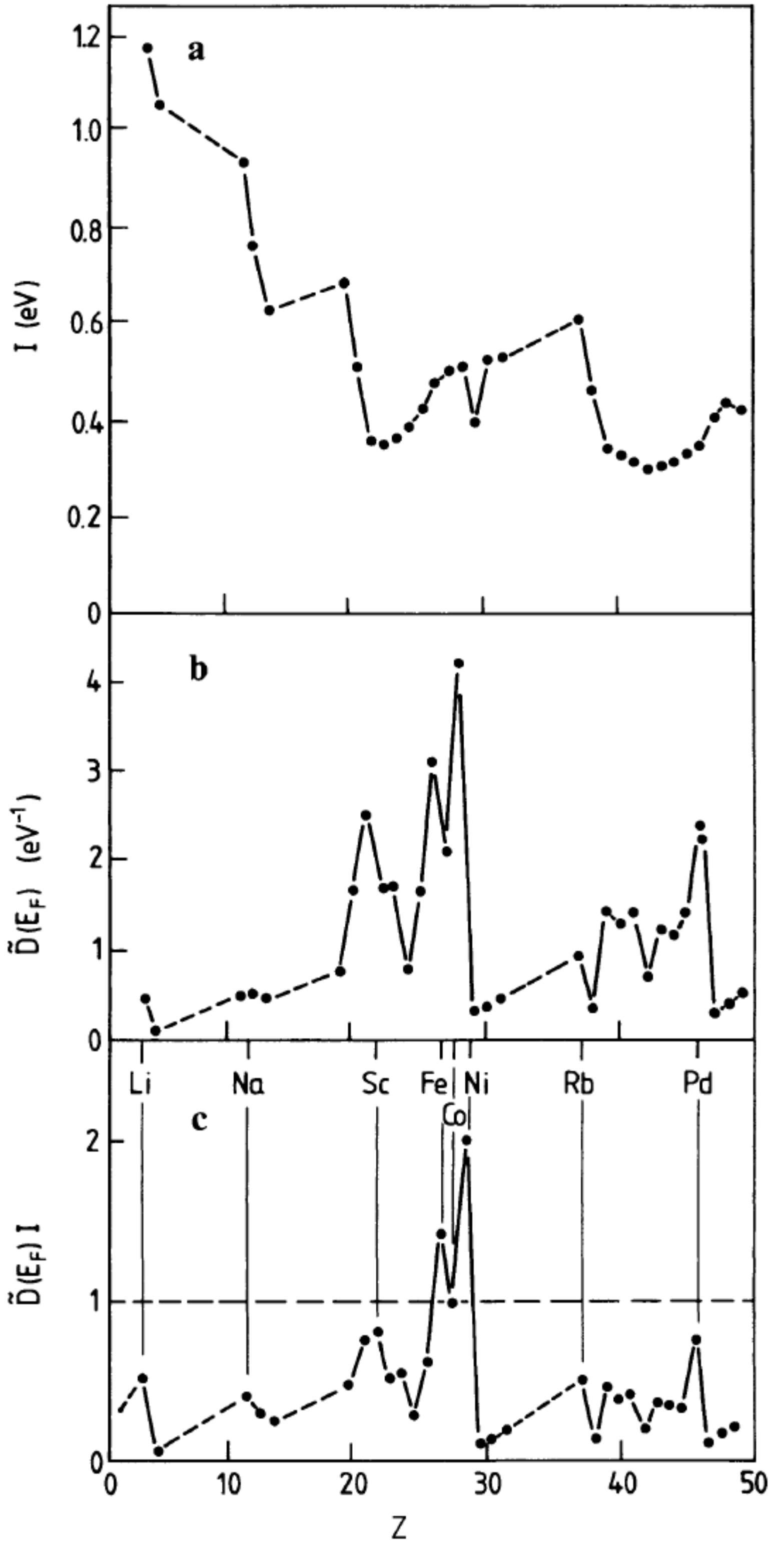

Fig. 8.5. (**a**) Integral of the exchange correlation (Stoner parameter) I as a function of the atomic number (after [8.2]). (**b**) Density of states per atom $\tilde{D}(E_{\mathrm{F}})$; (**c**) the product of the density of states $\tilde{D}(E_{\mathrm{F}})$ and the Stoner parameter I. The elements Fe, Co and Ni with values of $I\tilde{D}(E_{\mathrm{F}}) > 1$ display ferromagnetism. The elements Ca, Sc and Pd come very close to achieving ferromagnetic coupling

For the elements of the $4d$ series, the density of states and the Stoner parameter are too small to achieve the ferromagnetic state. Nevertheless, there is a considerable enhancement of the magnetic susceptibility due to the positive exchange interaction of the band electrons. For an external magnetic field B_0, (8.39) contains, in addition to the exchange splitting of $IR/2$, a splitting of $\mu_B B_0$. In a first approximation for R at $T = 0$, (8.41) then becomes

$$R = \tilde{D}(E_F)(IR + 2\mu_B B_0) \,. \tag{8.46}$$

For the magnetization M one thus obtains

$$M = \mu_B \frac{N}{V} R = \tilde{D}(E_F)\left(IM + 2\mu_B^2 \frac{N}{V} B_0\right)$$

$$M = 2\mu_B^2 \frac{N}{V} \frac{\tilde{D}(E_F)}{1 - I\tilde{D}(E_F)} B_0 \,. \tag{8.47}$$

$$\chi = \frac{\chi_0}{1 - I\tilde{D}(E_F)} \,. \tag{8.48}$$

Modelo de Stoner: Dependência com a Temperatura

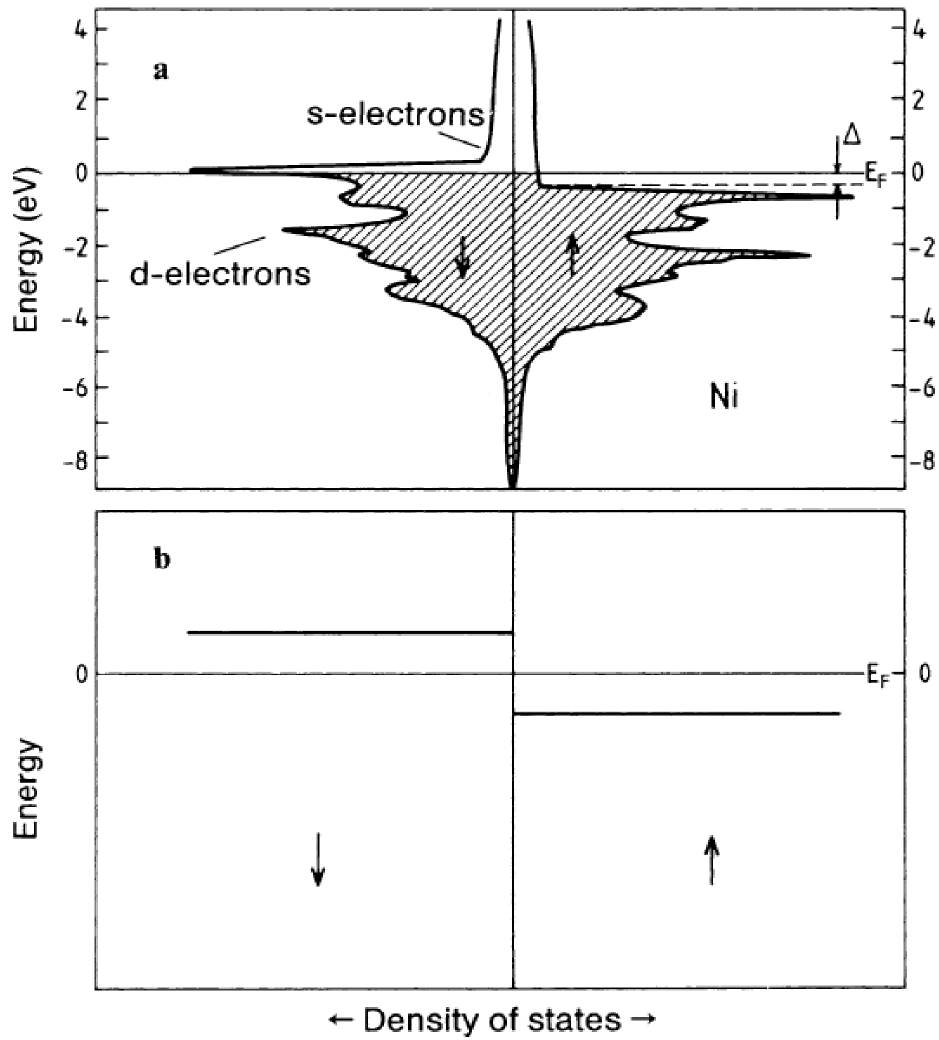

Fig. 8.6. (**a**) Calculated density of states of nickel (after [8.3]). The exchange splitting is calculated to be 0.6 eV. From photoelectron spectroscopy a value of about 0.3 eV is obtained. However the values cannot be directly compared, because a photoemitted electron leaves a hole behind, so that the solid remains in an excited state. The distance Δ between the upper edge of the *d*-band of majority spin electrons and the Fermi energy is known as the Stoner gap. In the bandstructure picture, this is the minimum energy for a spin flip process (the *s*-electrons are not considered in this treatment). (**b**) A model density of states to describe the thermal behavior of a ferromagnet

$$\tilde{D}(E) = \frac{\mu_{\mathrm{B_{eff}}}}{\mu_{\mathrm{B}}}\left[\delta(E - E_{\mathrm{F}} - \mu_{\mathrm{B}} B_0 - IR/2) + \delta(E - E_{\mathrm{F}} + \mu_{\mathrm{B}} B_0 + IR/2)\right] .$$

$$\Downarrow \tag{8.49}$$

$$R = \frac{\mu_{\mathrm{B_{eff}}}}{\mu_{\mathrm{B}}}\left(\frac{1}{\mathrm{e}^{(-\mu_{\mathrm{B}} B_0 - IR/2)/\not{k} T} + 1} - \frac{1}{\mathrm{e}^{(\mu_{\mathrm{B}} B_0 + IR/2)/\not{k} T} + 1}\right) .$$

We now look for ferromagnetic solutions to this equation, i.e., solutions with $R \geq 0$ at $B_0 = 0$. With the abbreviations $T_{\mathrm{c}} = I\mu_{\mathrm{B_{eff}}}/\mu_{\mathrm{B}} 4\not{k}$ and $\tilde{R} = \mu_{\mathrm{B}}/\mu_{\mathrm{B_{eff}}} R$, equation (8.50) becomes

$$\tilde{R} = \frac{1}{\mathrm{e}^{-2\tilde{R} T_{\mathrm{c}}/T} + 1} - \frac{1}{\mathrm{e}^{+2\tilde{R} T_{\mathrm{c}}/T} + 1} = \tanh \frac{\tilde{R} T_{\mathrm{c}}}{T} . \tag{8.51}$$

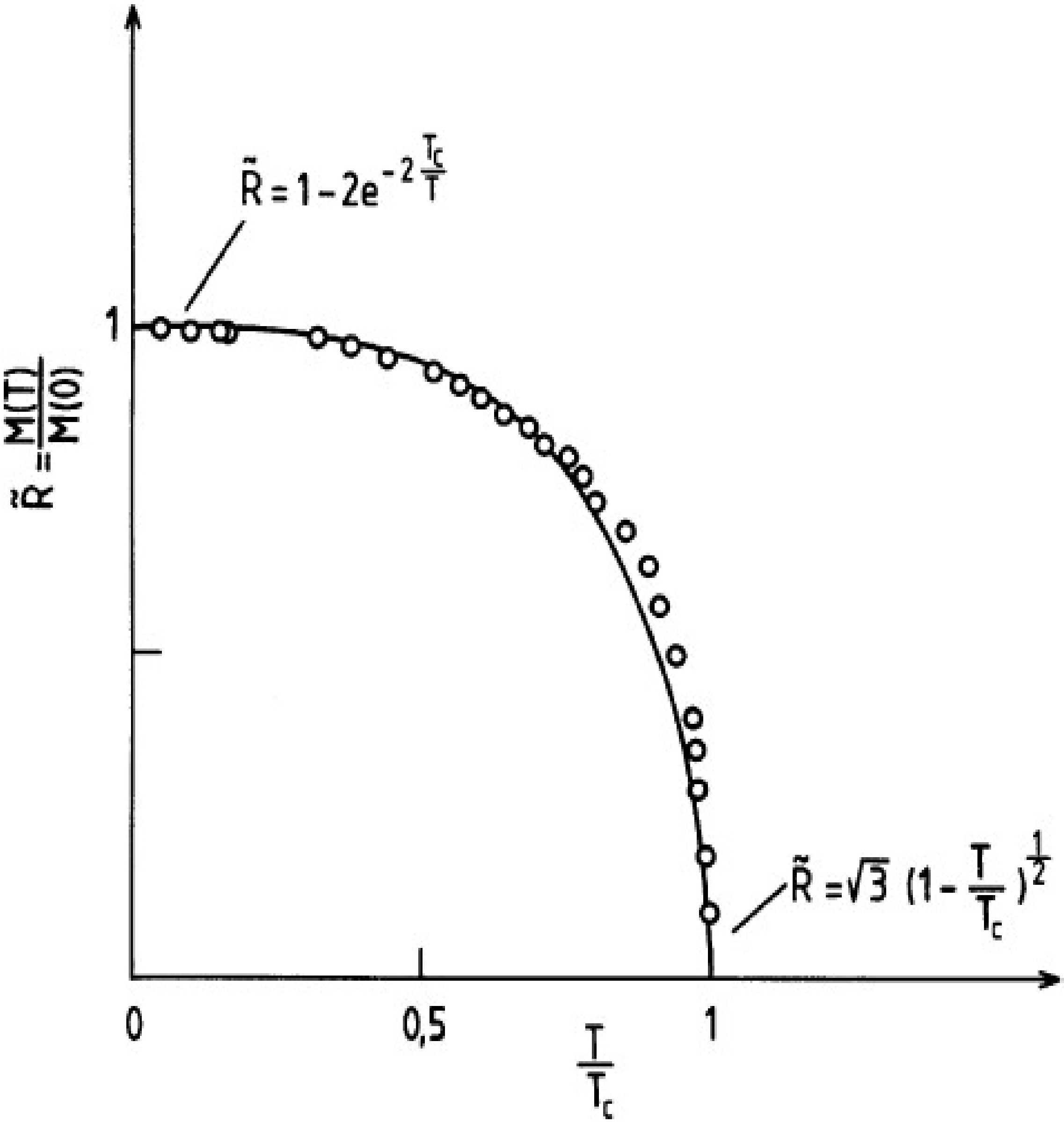

Fig. 8.7. Magnetization of a ferromagnet below the Curie temperature T_c. Experimental values for nickel from [8.4, 8.5]

Above the Curie temperature, (8.50) yields a magnetization only when the field B_0 is non-zero. We can expand the Fermi function for small R and B_0 to give

$$\tilde{R} = \frac{\mu_B}{\ell T} B_0 + \frac{T_c}{T} \tilde{R} \quad \text{or} \tag{8.54}$$

$$\tilde{R} = \frac{\mu_B}{\ell} \frac{1}{T - T_c} B_0 \, . \tag{8.55}$$

As T approaches T_c from above the paramagnetic susceptibility should thus diverge according to the law

$$\chi = \frac{C}{T - T_c} \, .$$

Lei de Curie-Weiss

Magnetismo Localizado (Modelo de Heisenberg)

$$\mathscr{H} = -\sum_i \sum_\delta J_{i\delta}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_{i\delta} - g\mu_{\mathrm{B}} \boldsymbol{B}_0 \sum_i \boldsymbol{S}_i \, .$$

Acoplamento dipolar com campo externo

Interação de Troca

Hamiltoniano não linear → difícil diagonalização

Aproximação de campo médio:

$$\mathscr{H}_{\mathrm{MF}} = -\sum_i \boldsymbol{S}_i \cdot \left(\sum_\delta J_{i\delta} \langle \boldsymbol{S}_{i\delta} \rangle + g\mu_{\mathrm{B}} \boldsymbol{B}_0 \right) .$$

$$\boldsymbol{B}_{\mathrm{MF}} = \frac{1}{g\mu_{\mathrm{B}}} \sum_\delta J_{i\delta} \langle \boldsymbol{S}_{i\delta} \rangle \, .$$

$$B_{\mathrm{MF}} = \frac{1}{g\mu_{\mathrm{B}}} \sum_{\delta} J_{i\delta} \langle \boldsymbol{S}_{i\delta} \rangle \ .$$

Para um material ferromagnético, todos os spins têm valores médios idênticos:

$$\langle \boldsymbol{S}_{i\delta} \rangle = \langle \boldsymbol{S} \rangle$$

Além disso:

$$\boldsymbol{M} = g\mu_{\mathrm{B}} \frac{N}{V} \langle \boldsymbol{S} \rangle$$

$$\Downarrow$$

$$\boldsymbol{B}_{\mathrm{MF}} = \frac{V}{Ng^2\mu_{\mathrm{B}}^2} \nu \boldsymbol{J} \boldsymbol{M}$$

where the exchange interaction is restricted to the ν nearest neighbors. The Hamiltonian in the mean field approximation (8.58) is now mathematically identical to the Hamiltonian of N independent spins in an effective magnetic field $B_{\text{eff}} = B_{\text{MF}} + B_0$. Its eigenvalues are

$$E = \pm \tfrac{1}{2} g \mu_{\text{B}} B_{\text{eff}} \tag{8.62}$$

for each electron spin. We denote the number of electrons in states with spin parallel and antiparallel to the B-field by $N_\uparrow$ and $N_\downarrow$.

In thermal equilibrium one has

$$\frac{N\downarrow}{N\uparrow} = \mathrm{e}^{-g\mu_{\text{B}} B_{\text{eff}}/\not{k}T} \tag{8.63}$$

and the magnetization is thus

$$M = \frac{1}{2} g \mu_{\text{B}} \frac{N\uparrow - N\downarrow}{V} = \frac{1}{2} g \mu_{\text{B}} \frac{N}{V} \tanh\left(\frac{1}{2} g \mu_{\text{B}} B_{\text{eff}}/\not{k}T\right) .$$

and the magnetization is thus

$$M = \frac{1}{2} g \mu_{\rm B} \frac{N\!\uparrow - N\!\downarrow}{V} = \frac{1}{2} g \mu_{\rm B} \frac{N}{V} \tanh\left(\frac{1}{2} g \mu_{\rm B} B_{\rm eff} / k T \right) .$$

This equation together with (8.61) has non-zero solutions for the magnetization (even without an external magnetic field) provided $J > 0$, i.e., whenever there is ferromagnetic coupling of the spins. With the abbreviations

$$M_{\rm s} = \frac{N}{V} \frac{1}{2} g \mu_{\rm B} \quad \text{and} \tag{8.65}$$

$$T_{\rm c} = \tfrac{1}{4} \nu J / k \tag{8.66}$$

we obtain from (8.61, 8.64), and with no external magnetic field B_0

$$M(T)/M_{\rm s} = \tanh\left(\frac{T_{\rm c}}{T} \frac{M}{M_{\rm s}} \right) . \tag{8.67}$$

Solução é equivalente ao caso de magnetismo metálico !!

For temperatures above T_c, we can once again derive the Curie-Weiss law for the susceptibility. With an external field B_0, and using the series expansion (8.68), we obtain from (8.64)

$$M(T) = \frac{g^2 \mu_B^2 N}{4 V k} \frac{1}{T - T_c} B_0 \,. \tag{8.70}$$

Lei de Curie-Weiss (de novo !)

Antiferromagnetismo

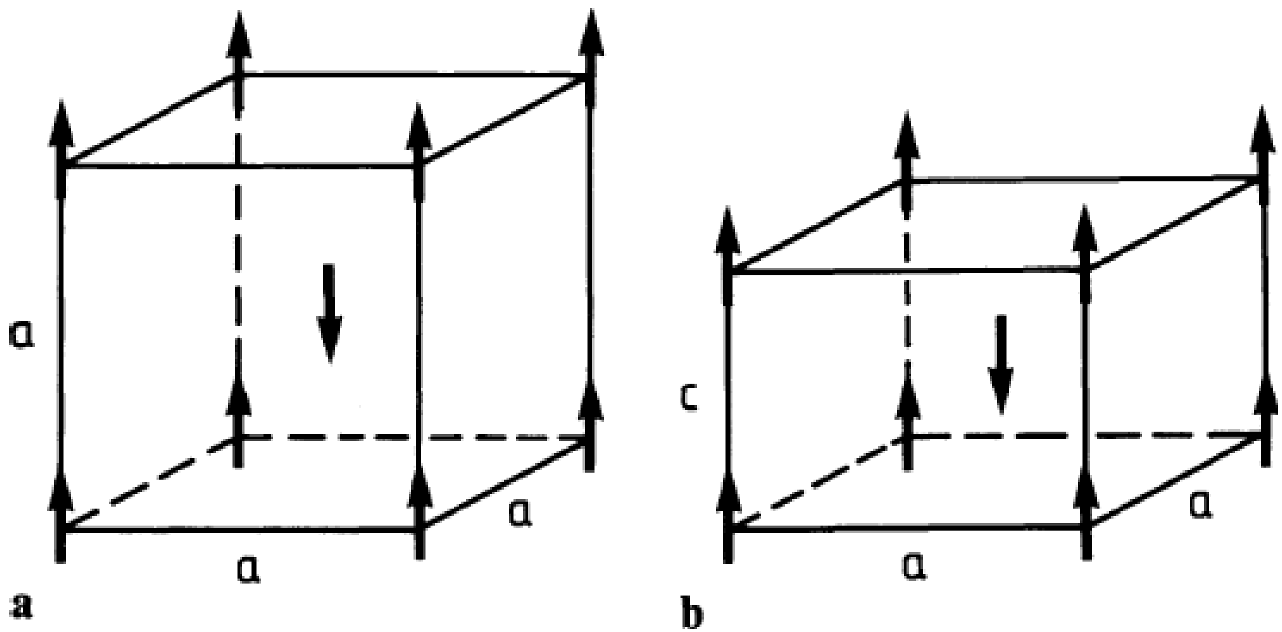

Fig. 8.9. (**a**) A model crystal with antiferromagnetic orientation of the nearest neighbor spins. (**b**) An equally simple spin structure, but with a tetragonal lattice, is observed for the compounds MnF_2, FeF_2 and CoF_2. In this case the atoms along the c axis are the nearest neighbors. If the transition metal ions form a face-centered cubic lattice, it is topologically impossible to have only antiferromagnetic orientation between nearest neighbors. The magnetic superstructures become correspondingly more complex

Através de um tratamento similar ao caso ferromagnético:

$$M^+ = \frac{1}{2} g \mu_B \frac{N^+}{V} \tanh\left(\frac{V}{2 k T N^- g \mu_B} \nu J M^- \right), \tag{8.71}$$

$$M^- = \frac{1}{2} g \mu_B \frac{N^-}{V} \tanh\left(\frac{V}{2 k T N^+ g \mu_B} \nu J M^+ \right), \tag{8.72}$$

$N^+ = N^-$ is the number of metal ions in each of the sub-lattices. In the anti-ferromagnetic state $M^+ = -M^-$ and we obtain, in analogy with (8.67),

$$M^+ = \frac{1}{2} g \mu_B \frac{N^+}{V} \tanh\left(-\frac{V}{2 k T N^+ g \mu_B} \nu J M^+ \right) \tag{8.73}$$

M+ → 0 para

$$T_N = -\frac{1}{4} \frac{\nu J}{k} .$$

Para T > TN:

$$\chi(T) = \mu_0 \frac{g^2 \mu_B^2 N}{4 V k} \frac{1}{T + T_N} .$$

Lei de Curie-Weiss (de novo !)

Néel temperature itself, the susceptibility remains finite. For temperatures far enough below the Néel temperature $M^+(T) = M_s^+$ and we obtain

$$\chi_{\parallel}(T) \approx \mu_0 \frac{g^2 \mu_B^2 N}{4 V k} \frac{1}{T \cosh^2(T_N/T) + T_N} , \tag{8.81}$$

which for low temperatures can further be approximated by

$$\chi_{\parallel}(T) \approx \mu_0 \frac{g^2 \mu_B^2 N}{V k T} e^{-2T_N/T} \quad T \ll T_N . \tag{8.82}$$

This expression for the susceptibility and the equations (8.75, 8.76) are valid only for an external field oriented parallel to the polarization of the spin sub-lattice. For the direction perpendicular to the spin orientation, the Hamiltonian (8.58) should be interpreted as a classical energy equation. In an external field, each spin sub-lattice rotates its magnetic moment by an angle α in the direction of the field B_0. The energy of an elementary magnet in the field B_0 is then

$$E_r = -\tfrac{1}{2} g \mu_{\mathrm{B}} B_0 \sin\alpha + \tfrac{1}{2} \nu J \cos\alpha \; . \tag{8.83}$$

The magnitude of the second term can be derived by considering that the energy needed to reverse an elementary magnet is νJ (8.27). The equilibrium condition

$$\partial E_r / \partial \alpha = 0 \tag{8.84}$$

leads, for small angles α, to

$$\alpha = -\frac{g \mu_{\mathrm{B}} B_0}{\nu J} \; . \tag{8.85}$$

With the magnetization

$$M = M^{+} + M^{-} = \tfrac{1}{2} g \mu_{\mathrm{B}} \alpha N / V \tag{8.86}$$

This expression for the susceptibility and the equations (8.75, 8.76) are valid only for an external field oriented parallel to the polarization of the spin sub-lattice. For the direction perpendicular to the spin orientation, the Hamiltonian (8.58) should be interpreted as a classical energy equation. In an external field, each spin sub-lattice rotates its magnetic moment by an angle α in the direction of the field B_0. The energy of an elementary magnet in the field B_0 is then

$$E_r = -\tfrac{1}{2} g \mu_B B_0 \sin\alpha + \tfrac{1}{2} \nu J \cos\alpha \,. \tag{8.83}$$

The magnitude of the second term can be derived by considering that the energy needed to reverse an elementary magnet is νJ (8.27). The equilibrium condition

$$\partial E_r / \partial\alpha = 0 \tag{8.84}$$

leads, for small angles α, to

$$\alpha = -\frac{g \mu_B B_0}{\nu J} \,. \tag{8.85}$$

With the magnetization

$$M = M^+ + M^- = \tfrac{1}{2} g \mu_B \alpha N / V \tag{8.86}$$

one obtains for the susceptibility below T_N the (approximately) temperature-independent value

$$\chi_\perp = -\frac{g^2\mu_B^2 N}{2\nu J V} = \frac{g^2\mu_B^2 N}{2\nu |J| V}, \tag{8.87}$$

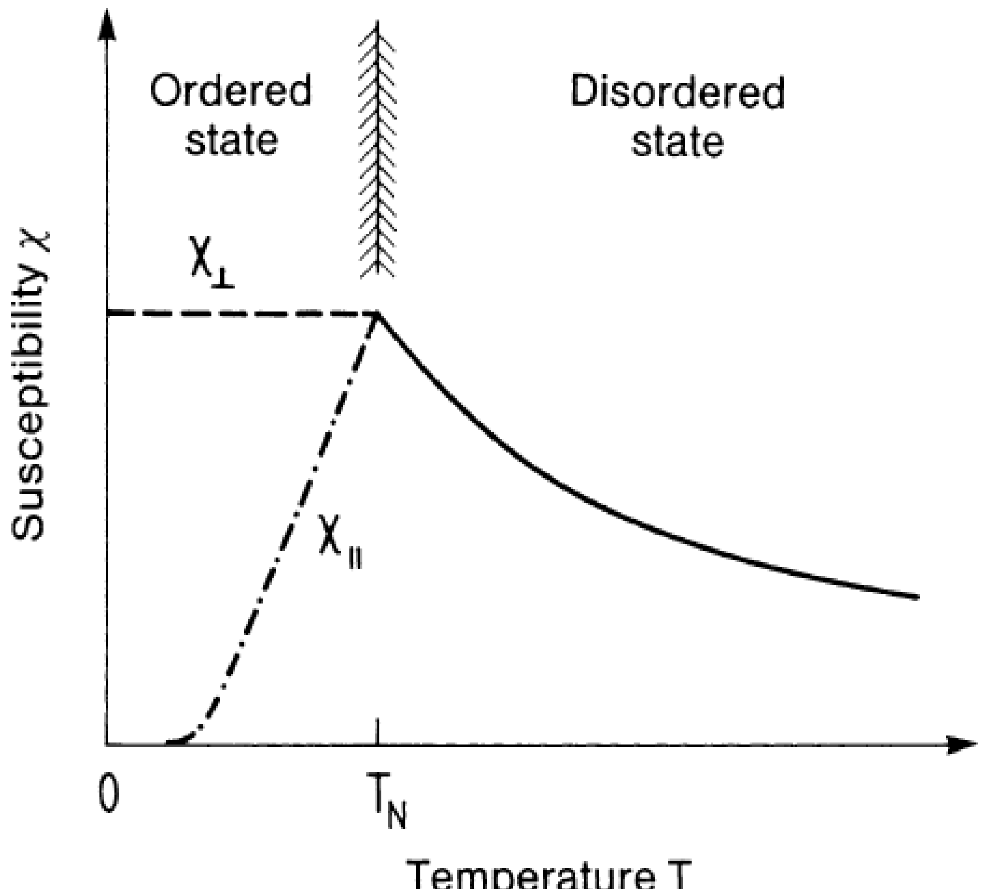

Fig. 8.10. Schematic representation of the magnetic susceptibility of an antiferromagnet. Below the Néel temperature T_N (i.e., in the antiferromagnetically ordered state) the susceptibility differs for parallel and perpendicular orientation of the magnetic field relative to the spin axis

Ondas de Spin

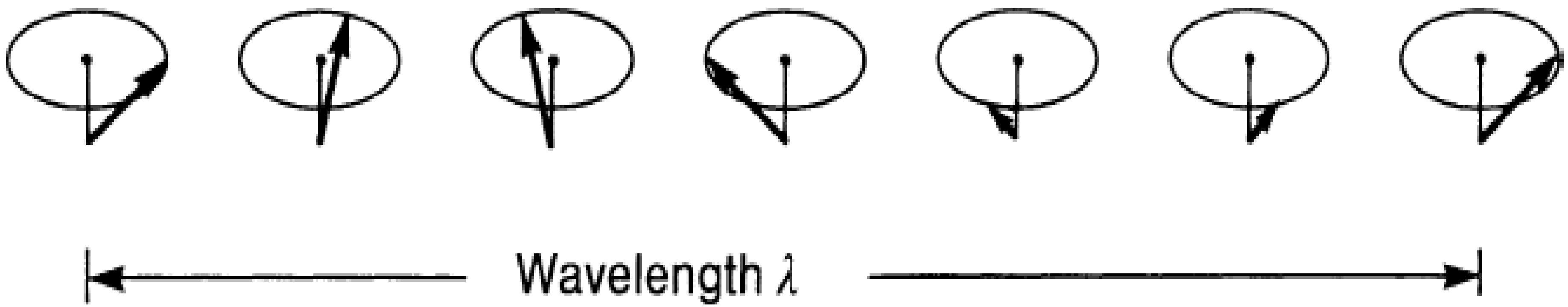

Fig. 8.11. Schematic representation of a spin wave

Magnetização de uma amostra ferromagnética

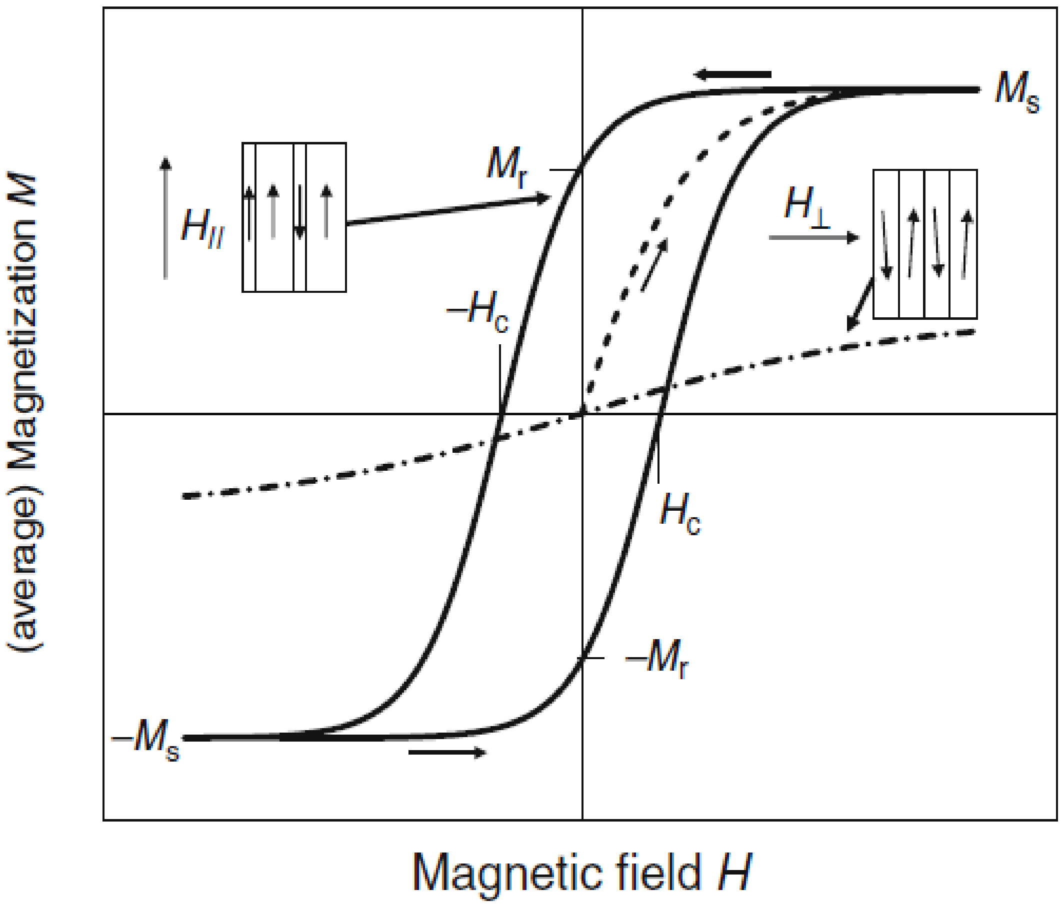

Fig. 8.14. Schematic plot of the magnetization M of a ferromagnet with a single easy axis versus the magnetic field H. *Dashed line:* initial magnetization starting from zero, H parallel to easy axis. *Solid lines:* magnetization hysteresis, H parallel to easy axis. *Dash-dotted line:* H perpendicular to easy axis