# Fundamental properties

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As we know, electron states in atoms are characterized by 4 quantum numbers:

n (=0, 1, ..), l (=0, 1, .., n-1), $m_l$ (=-l ,-l+1, .., l) and $m_s$ (=-1/2, +1/2).

The latter three determine the magnetic response to an applied magnetic field. In isolated atoms, the individual magnetic moments within one shell add up, according to Hund's rules, to the total magnetic moment of the shell, characterized by the quantum number J. For the 4f-shell this yields a reasonable description of the observed moments, even in the metallic state (local model).

In the absence of interaction the magnetization M of a material is given by the field derivative of Helmholtz free energy A.

$$M = -\left(\frac{\partial A}{\partial H}\right)_T = Ng\mu_B J\, \mathrm{B}_\mathrm{J}(x) \qquad (1)$$

where $x = g\mu_B JH/(kT)$, $g$ is known as Lande's-factor, $\mu_B$ is the Bohr magneton, $k$ is the Boltzmann constant, $H$ is the magnetic field, $T$ is the absolute temperature, and $N$ is the numbers of the magnetic moments and

$$\mathrm{B}_\mathrm{J}(x) = \frac{2J+1}{2J}\coth(\frac{2J+1}{2J}x) - \frac{1}{2J}\coth(\frac{1}{2J}x)$$

is the Brillouin function that varies between 0 and 1 for $x = 0$ and x = ∞, respectively. When $x \ll 1$, Eq. (1) becomes the Curie law (Buschow et al. 2003),

$$M = \frac{CH}{T}, \qquad (2)$$

where $C = Ng^2 u_B^2 J(J+1)/3k$ is the Curie constant. This equation gives the well known inverse proportionality of the magnetic susceptibility χ = M/H.

When the argument of the Brillouin function is very large, thus either at low temperatures and or high magnetic field, the magnetization will saturate to the maximal value $M_S$

$$M_S = Ng\mu_B J \tag{3}$$

When the distance between magnetic moments is small, the Pauli exclusion principle, which states that two identical fermions may not have the same quantum states, results in interaction between magnetic moments. Heisenberg introduced a model to describe this exchange interaction on microscopic scale. The Heisenberg exchange Hamiltonian may be written in the form

$$H_{exch} = -\sum_{i<j} 2J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{4}$$

where the summation extends over all magnetic moment pairs in the crystal lattice. For positive values of the exchange constant $J_{ij}$ one finds parallel alignment else antiparallel. Ferromagnetism is observed for positive exchange interactions below a critical temperature.

The exchange interaction can be described as effective field acting on the moments. This field is produced by the surrounding magnetic moments and called the molecular field. As the size of the surrounding moments is proportional to the magnetization, the molecular field $H_m$ is written as

$$H_m = N_W M \tag{5}$$

with $N_W$ the Weiss-field constant. This constant was already introduced in the early 20th century long before the development of quantum physics. The total magnetic field experienced by a magnetic material is thus the sum of the externally applied field $H_0$ and the internal field

$$H = H_0 + H_m \tag{6}$$

and equation 2 needs to be rewritten as

$$M = \frac{C}{T}(H_0 + N_W M).$$

<div align="right">(7)</div>

Thus, in the presence of ferromagnetic interaction much lower fields are sufficient to saturate the magnetization. The magnetic susceptibility is given by

$$\chi = \frac{C}{T - N_W C} = \frac{C}{T - T_C}.$$

<div align="right">(8)</div>

This is the Curie-Weiss law, where $T_C$ is the Curie temperature. Below the Curie temperature spontaneous magnetization is observed. For most materials, the phase transition from the paramagnetic state to the ferromagnetic state is found to be of second order. This means that the temperature dependence of the first derivative of the free energy (S, M, V) is continuous and only the second derivative of the free energy (specific heat $C_H$, $\chi$, thermal expansion $\alpha$) is discontinuous.

In 3d-metals the adjacent atoms break the symmetry to an extent that the orbital quantum number is no longer a good quantum number. Moreover, hybridization leads to energy bands in which the spin quantum number S is best describing the properties (itinerant model). In this model, the value of S is no longer necessarily a whole number. In itinerant systems equations 1, 2, 3 and 8 also hold when we substitute J by S. Magnetism in 3d metals is well described by the Stoner band model, that distinguishes spin up and spin down bands:

$$E_\uparrow(k) = E(k) - \frac{I_S n_\uparrow}{N}$$

$$E_\downarrow(k) = E(k) - \frac{I_S n_\downarrow}{N}$$

<div align="right">(9)</div>

with $I_S$ the Stoner parameter that describes the energy change due to electron spin correlations. Ferromagnetism occurs when the density of states at the Fermi level $D(E_F)$ is exceeding some critical value which is expressed by the Stoner condition

$$\widetilde{D}(E_F)I_s > 1$$

(10)

where $\widetilde{D}(E_F)$ is the normalized density per spin and volume.

N.B. Exchange energy in 3d metals $\approx 30$meV

1. Buschow, K. H. J. and F. R. de Boer (2003). "Physics of Magnetism and Magnetic Materials." New York, Kluwer Academic / Plenum Publishers