

Magnetization of Rare Earth Materials

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Abstract

The formal procedure is demonstrated for calculating the magnetization of a rare earth material, in the mean field approximation, at arbitrary fields and temperatures when account is taken of crystal-field splittings, interionic exchange interactions and conduction electron polarization effects.

The main influences which determine the magnetization of a rare earth compound are (i) crystal fields, (ii) RKKY interionic exchange interactions and (iii) the effects of conduction electron polarization. The procedure for calculating the magnetization while taking account of (i) and (ii) has been known for some time (Bleaney 1963; Trammell 1963). However, there are some materials in which conduction electron polarization effects are very large (Wohleben 1968), so it is desirable to include these also. This has been done previously to obtain the paramagnetic susceptibility (Stewart 1972*a*, 1972*b*) and the zero temperature ferromagnetic moment (Stewart 1972*c*), in some rather limited circumstances. In the present note the procedure for finding the magnetization at any arbitrary field and temperature is demonstrated.

The starting point is the effective mean field Hamiltonian \mathcal{H} for the ions (Yosida 1957; Stewart 1972*a*):

$$\mathcal{H} = V_c + g\mu_B J^z [H\{1 + 2J(0)\rho(g-1)/g\} + \lambda m^i] + \frac{1}{2}\lambda(m^i)^2, \quad (1)$$

where V_c is the crystal field Hamiltonian, g is the Landé factor, μ_B is the magnitude of the electronic Bohr magneton, J^z is the operator for the z component of the ionic angular momentum, H is the applied magnetic field, $J(0)$ is the s - f coupling constant associated with the interaction $-2J(q)\mathbf{S}\cdot\mathbf{s}$ between the spin \mathbf{S} of a rare earth and the spin \mathbf{s} of a conduction electron, ρ is the conduction electron density of states per atom for one spin direction (or, more generally, is proportional to the uniform Pauli susceptibility), m^i is the expectation value of the ionic magnetization and

$$\lambda = 2(g-1)^2 \sum_j' A_{ij}/g^2\mu_B^2$$

is the molecular field parameter, where the RKKY interactions between the ions are of the form

$$-\sum_{i,j}' A_{ij} \mathbf{S}_i \cdot \mathbf{S}_j.$$

The second relevant equation, which relates the induced conduction electron magnetization m^e to the ionic magnetization (Yosida 1957; Stewart 1972a), is

$$m^e = m^i 2J(0) \rho(g-1)/g. \quad (2)$$

We want to calculate the sum of the two magnetizations

$$m = m^i + m^e = m^i \{1 + 2J(0) \rho(g-1)/g\}. \quad (3)$$

Equations (1)–(3) are valid for the situation in which all the moments are parallel, but they may be generalized to other forms of ordering.

The eigenvalues and eigenvectors of the sub-Hamiltonian $V_c + \mu_B g J^z H$ are found by the usual methods (Stevens 1952; Williams and Hirst 1969) and from them m^i is calculated as a function \mathcal{L} of the temperature T and field H ,

$$m^i = \mathcal{L}(T, H). \quad (4)$$

This implies that the interactions are accounted for by finding the solution with lowest free energy to the equation

$$m^i = \mathcal{L}(T, [H\{1 + 2J(0) \rho(g-1)/g\} + \lambda m^i]), \quad (5)$$

or, more conveniently, the expression obtained by substituting m for m^i using equation (3).

When crystal-field splittings are negligible, \mathcal{L} may be replaced by the Brillouin function B_J to give

$$\frac{m}{m_0} = B_J \left(\frac{m_0}{kT} \left(H + \frac{\lambda m}{\{1 + 2J(0) \rho(g-1)/g\}^2} \right) \right), \quad (6)$$

where

$$m_0 = \mu_B g J \{1 + 2J(0) \rho(g-1)/g\}.$$

For the case in which $\lambda = 0$, $J = \frac{1}{2}$ and $g = 2$, equation (6) agrees with the result of Giovannini *et al.* (1966) to order $J(0) \rho$. To order $\{J(0) \rho\}^2$, terms associated with the Kondo effect, which we do not take account of, appear in their equations. Another expression for the magnetization has been proposed by Loram *et al.* (1970) for the case $\lambda = 0$ and $g = 2$, and to order $J(0) \rho$ this is also in agreement with equation (6).

From equation (5) it may be noted that conduction electron polarization effects (i.e. the effects obtained if $J(0) \rho$ is imagined to vary while λ remains constant) do not alter the ordering temperature or the shape of the curve of spontaneous magnetization against temperature.

The above procedure may be applied in a parallel manner to samarium materials, in which conduction electron polarization effects are sometimes particularly large (Stewart 1972a), if account is taken of the admixture of the $J = 7/2$ level into the $J = 5/2$ ground state by the applied fields.

Arguments which have been put forward previously (Stewart and Grüner 1973) suggest that the magnetization m given by the Hartree–Fock solution of Anderson's (1961) magnetic impurity model in the magnetic and high temperature ($T \gg T_K$, the Kondo temperature) regime is

$$m = n_0 \mu_B \tanh\{n_0 \mu_B (H + \lambda' m)/kT\}, \quad (7)$$

where $n_0 = (n_b - n_a)$, n_a and n_b being the number of electrons in the virtual states respectively above and below the Fermi level, and where λ' is associated with Caroli's (1967) interaction mechanism. A condition for this equation to be valid is that the effective fields should not be great enough to alter n_a and n_b . In the magnetic limit, $(n_b - n_a) \rightarrow (1 + \hat{J}\rho)$ (Stewart and Grüner 1973), where \hat{J} is the Schrieffer-Wolff (1966) exchange parameter, and Caroli's mechanism tends to the RKKY interaction which incorporates \hat{J} as the coupling constant (Blandin 1968). Consequently equation (7) tends to equation (6) with $J = \frac{1}{2}$ and $g = 2$. There is therefore a complete correspondence between the magnetization given by the s-d (s-f) model and that given by the Hartree-Fock solution of Anderson's model in the magnetic limit.

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