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MAGNETIC RESPONSE OF LOCALIZED SPINS COUPLED TO ITINERANT ELECTRONS IN AN INHOMOGENEOUS CRYSTAL FIELD+

by

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ABSTRACT

The magnetic behavior at T = 0 K of a system consisting of conduction electrons coupled to localized electrons (e.g. 4f electrons), the latter submitted to an inhomogeneous crystal field distribution, is studied. We consider a simple crystal field distribution and define an average ionic magnetic moment using the results of the homogeneous case. We obtain a condition for the onset of spontaneous magnetic order and study the magnetic behavior in the paramagnetic and ferromagnetic regions of the phase diagram. The study implies that the inhomogeneity of the crystal field attenuates the quenching effects. The model is interesting to the study of disordered rare-earth intermetallic compounds.

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Key-words: Magnetism; Crystal field distribution; Conduction band; Rare earth intermetallic compounds.

1. Introduction

The crystal field interactions are important in the study of magnetic and thermal properties of rare-earth intermetallic compounds, particularly in systems containing light rare-earths[1]. In the case of amorphous systems, crystal field effects have been discussed[2] in the framework of the Harris-Plischke-Zuckermann model[3].

In the present work we will discuss the magnetic behavior of a system formed of conduction electrons interacting with localized electrons from rare earth ions (4f electrons). The localized electrons are exposed to an axial crystal field that varies from ion to ion (effect of disorder in the crystal lattice). This study may be of interest in the case of disordered alloys, where there is a distribution of crystal field parameters. In an earlier publication[4] we have examined the problem of a constant crystal field parameter.

The present paper is organized as follows: in Section 2 the model hamiltonian is detailed, the quantities of interest defined, an ionic magnetic state equation is derived at T = 0 K, and a magnetic phase diagram is presented; in Sections 3 and 4 the paramagnetic and ferromagnetic behaviors are discussed.

2. Model Hamiltonian and Equation of State at T = 0 K

The total hamiltonian for conduction electrons and localized ions is

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_{ion} \tag{1}$$

Where the hamiltonians for the electron and ion are given by

$$\mathcal{H}_e = \mathcal{H}_{kin} + \mathcal{H}^e_{mag} \tag{2-a}$$

$$\mathcal{H}_{ion} = \mathcal{H}_{cf} + \mathcal{H}^i_{mag} \tag{2-b}$$

$\mathcal{H}_{kin}$ describes the dynamics of the conduction electrons. These are characterized by a density of states, assumed of rectangular shape in the present work. $\mathcal{H}_{cf} = \sum_i D^i(J^i_z)^2$ describes the crystal field, where J_z is the z component of the ionic angular momentum. The terms describing the Zeeman interaction of electrons and ions are:

$$\mathcal{H}^e_{mag} = -2\,\mu_B h_e \sum_j s^j_x \tag{3-a}$$

$$\mathcal{H}^i_{mag} = -g\,\mu_B h_i \sum_j J^j_x \tag{3-b}$$

where s_x is the x component of the electronic spin. g is Landé's factor and h_i and h_e are the effective magnetic fields acting on the sub-systems (ions and electrons). These effective magnetic fields satisfy

$$\alpha = g\,\mu_B h_i = g\,\mu_B h_o + J_o(g-1)\,\langle s_x\rangle \tag{4-a}$$

$$2\,\mu_B h_e = 2\,\mu_B h_o + J_o(g-1)\langle 0|J_x|0\rangle \tag{4-b}$$

where h_o is an external magnetic field, applied in the x direction. The terms containing J_o in Eqs. 4 describe the exchange fields acting on electrons and on ions.

From (2-b) one may obtain the magnetic moment per ion, for the ground state*

$$\langle 0|J_x|0\rangle = \frac{2\alpha}{(D^2 + 4\bar{\alpha}^2)^{1/2}} \qquad (5\text{-a})$$

and from (2-a) the electronic magnetization*:

$$8\varepsilon_0 \gamma \langle s_x \rangle = 2\,\mu_B h_e \qquad (5\text{-b})$$

where γ is the occupied fraction of the band.

The main purpose of this work is the computation of the average ground state ionic magnetization $\overline{\langle 0|J_x|0\rangle}$, defined as

$$\overline{\langle 0|J_x|0\rangle} = \int dD\, f(D)\, \langle 0|J_x|0\rangle / \int dD\, f(D) \qquad (6)$$

We have adopted a rectangular function f(D) for the distribution of crystal field parameters, centered in D_e and having a width 2Δ

$$f(D) = \begin{cases} 1/2\,\Delta & \text{if} \quad D_e - \Delta \le D \le D_e + \Delta \\ 0 & \text{otherwise} \end{cases} \qquad (7)$$

Within this approximation, one obtains

$$\overline{\langle 0|J_x|0\rangle} = \frac{\bar{\alpha}/2\varepsilon_0}{\Delta/2\varepsilon_0}$$

$$\times \ln \frac{\dfrac{D_e}{2\varepsilon_0} + \dfrac{\Delta}{2\varepsilon_0} + \left[\left(\dfrac{D_e}{2\varepsilon_0} + \dfrac{\Delta}{2\varepsilon_0}\right)^2 + 4\left(\dfrac{\bar{\alpha}}{2\varepsilon_0}\right)^2\right]^{1/2}}{\dfrac{D_e}{2\varepsilon_0} - \dfrac{\Delta}{2\varepsilon_0} + \left[\left(\dfrac{D_e}{2\varepsilon_0} - \dfrac{\Delta}{2\varepsilon_0}\right)^2 + 4\left(\dfrac{\bar{\alpha}}{2\varepsilon_0}\right)^2\right]^{1/2}}$$

(8-a)

$$\frac{g\mu_B h_o}{2\varepsilon_o} = \frac{1}{1 + \frac{1}{2\gamma g} \frac{J_o(g-1)}{2\varepsilon_o}} \left\{ \frac{\bar{\alpha}}{2\varepsilon_o} - \frac{1}{4\gamma}\left(\frac{J_o(g-1)}{2\varepsilon_o}\right)^2 \overline{\langle 0|J_x|0\rangle} \right\}$$

(8-b)

Equation (8-b) relates $\bar{\alpha}$ to $\overline{\langle 0|J_x|0\rangle}$.

With $h_o = 0$, in the limit $\overline{\langle 0|J_x|0\rangle} = 0$, one obtains

$$\frac{\Delta}{2\varepsilon_o} = \frac{1}{4\gamma}\left(\frac{J_o(g-1)}{2\varepsilon_o}\right)^2 \ln \left[\left(\frac{D_s}{2\varepsilon_o} + \frac{\Delta}{2\varepsilon_o} \right) / \left(\frac{D_s}{2\varepsilon_o} - \frac{\Delta}{2\varepsilon_o} \right) \right]$$

(9)

The above equation, in the space $J_o(g-1)/2\varepsilon_o$ versus $\Delta/2\varepsilon_o$ (fixed γ and $D_s/2\varepsilon_o$) describes the frontier between the paramagnetic and ferromagnetic regions.

3. Paramagnetic Region

Curves of $\overline{\langle 0|J_x|0\rangle}$ versus $g\,\mu_B h_o/2\varepsilon_o$ obtained from Eq. 8 are shown in Fig. 1 for two sets of parameters. It can be seen that for larger values of $\Delta/2\varepsilon_o$ (larger inhomogeneity) the magnetic response saturates more gradually.

4. Ferromagnetic Region

Curves of $\overline{\langle 0|J_x|0\rangle}$ versus $J_o(g-1)/2\varepsilon_o$, with h_o = 0, are shown in Fig. 2, for several sets of parameters. It should be noted that the effect of the inhomogeneity (of width 2Δ) is to attenuate the quenching due to the crystal field. For a given crystal field parameter of mean value D_e, the larger the value of $\Delta/2\varepsilon_o$, the smaller the exchange parameter required to establish spontaneous magnetic order; also the value of $\overline{\langle 0|J_x|0\rangle}$, given a value of $J_o(g-1)/2\varepsilon_o$, is larger for larger values of $\Delta/2\varepsilon_o$.

5. Comments

The simplicity of the model (we have considered a distribution of the crystal field parameter D, but a single J_o, whereas a distribution of values of would be also important) and the approximations used (e.g. rectangular energy density shape and distribution of D) allowed us to obtain an analytic magnetic state equation t T=0 K (Eq. 8-a and 8-b). From it we derived a magnetic phase diagram and performed a parametric study in the para- and ferromagnetic regions.

The extreme simplicity of the model and of its approximations, particularly the use of a single J_o does not allow a numerical comparison of our results with the data for real systems. However, a qualitative description of the role of the crystal field inhomogeneity and of the other parameters in the magnetic behavior may be of interest in the case of disordered systems - disordered pseudo-binary compounds and amorphous alloys. In amorphous systems, the quadratic contribution to the crystal field (involving the O_z^0 and O_z^2 Stevens' operators) exceeds by one order of magnitude the effect of higher order terms[6]; this justifies our use of a simple quadratic crystal field term. In the present study we have not considered the distribution of directions of the crystal field axis, as in the HPZ (Harris-Plischke-Zuckerman) model[9]; our derivation would be more appropriate to an amorphous film in which the directions of the crystal field axes are perpendicular to the plane of the film.

FIGURE CAPTIONS

Fig. 1. Average ionic magnetization (in units of $g\mu_B$) versus applied magnetic field. We have taken γ = 0.5, g = 2 and $D_s/2\varepsilon_o=10^{-3}$. Curves 1 and 2 are for $(J_o(g-1)/2\varepsilon_o,\ \Delta/2\varepsilon_o)$ equal to (0.0314, 0.0002) and (0.0270, 0.0008), respectively. Both sets of parameters satisfy Eq. 9.

Fig. 2. Average ionic magnetization (in units of $g\mu_B$) versus $J_o(g-1)/2\varepsilon_o$. The quantity $D_s/2\varepsilon_o$ equals 10^{-3}. For curves 1, 2, 3 and 4, $\Delta/2\varepsilon_o$ equals 0.2×10^{-3}, 0.4×10^{-3}, 0.6×10^{-3} and 0.8×10^{-3}, respectively. Here again γ = 0.5.

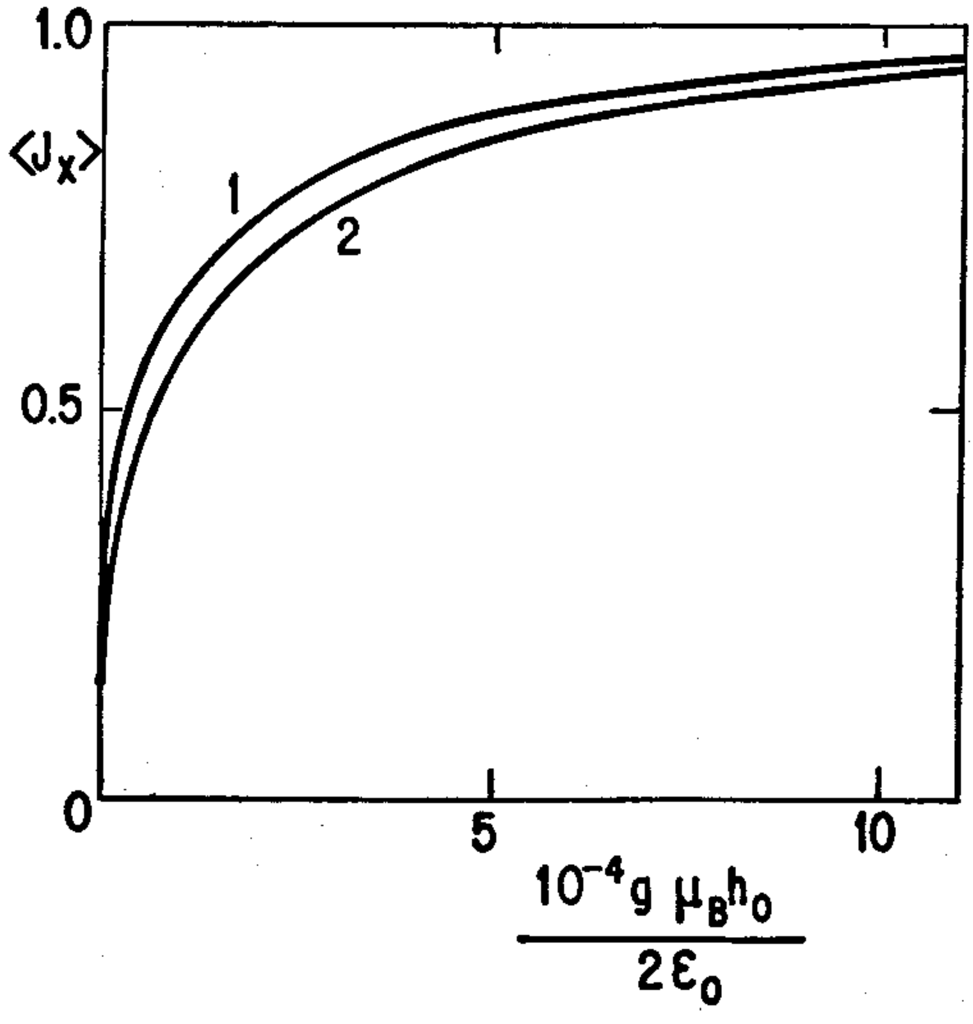

Fig. 1

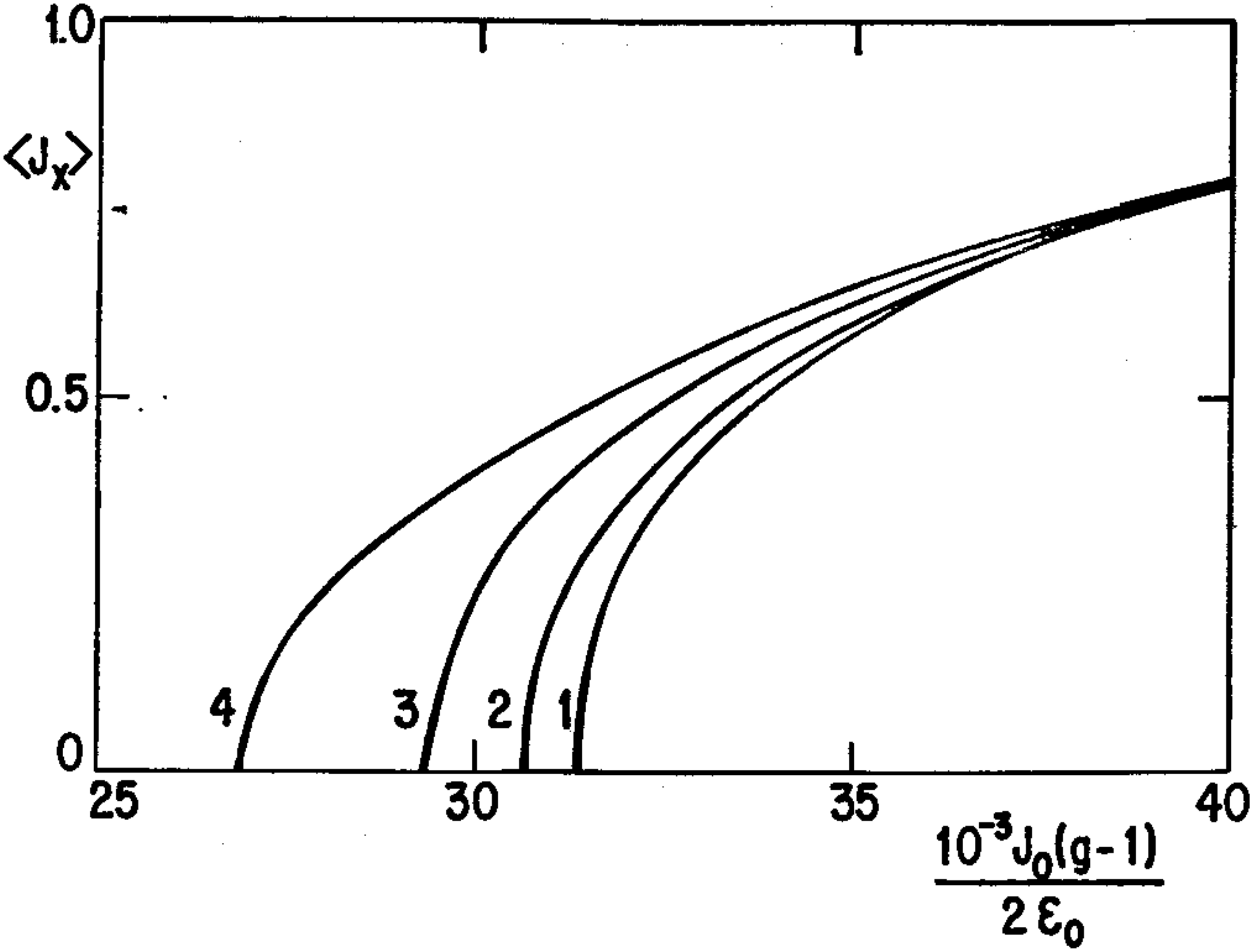
1.0
0.5
0
$\langle J_x \rangle$
4
3
2
1
25
30
35
40
$\frac{10^{-3} J_0 (g-1)}{2 \varepsilon_0}$

Fig. 2

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