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# EFFECT OF A DISTRIBUTION OF EXCHANGE PARAMETERS WITHIN A SIMPLE LOCALIZED-ITINERANT MODEL*

by

L. IANNARELLA[1], A.P. GUIMARÃES and X.A. da SILVA

Centro Brasileiro de Pesquisas Físicas - CNPq/CBPF
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ - Brasil

[1]Departamento de Física
Universidade Federal do Rio de Janeiro - UFRJ
23851 - Rio de Janeiro, RJ - Brasil

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## ABSTRACT

The magnetic behavior at T = 0 K of a system consisting of conduction electrons coupled to localized electrons submitted to an axial crystal field is studied in the molecular field approximation. We assume that the exchange parameter J varies spatially, with a gaussian probability distribution. We define an average ionic magnetic moment and obtain the condition for spontaneous magnetic order, involving the crystal field parameter, the width and the mean value of the exchange parameter distribution. We also obtain graphs of the magnetic moment versus mean value of the exchange parameter distribution, for different distributions showing that the distribution of J's reduces the rate of increase of magnetization versus the mean J.

Key-words: Disordered magnetic films; Rare-earth intermetallics; Crystal field anisotropy; Gaussian exchange distribution; Magnetic behaviour.

# 1 INTRODUCTION

Metallic magnetic systems containing rare-earth metals exhibit features both of localized and of itinerant magnetism; these features are associated to the properties of the 4f and conduction electrons. The disorder (structural, topological or chemical) affects the magnetic properties of such systems. The interest in their novel physical properties has led to a rapid growth of the literature on this subject, generally focusing on disordered alloys or intermetallic compounds in the form of thin films.

Models used to describe such localized-itinerant systems, introduce the disorder in a simple way either through i)a modified density of electronic states, ii)a distribution in the magnitude and in the direction of the magnetic exchange field, and/or iii)a distribution of the strength and direction of the axis of the crystal electric field (as discussed in the HPZ model[2]). In a recent work [3]we examined the magnetic phase diagram and the behavior of the magnetization at T = 0 K for a magnetic system where the localized electrons are subject to a distribution of values of the crystal field parameter. One consequence of this distribution on the magnetization is an effect equivalent to that of a decrease in the crystal field parameter D.

In the present work we shall discuss the consequences of the distribution of the exchange parameter J on the magnetism of the localized-itinerant system. Using simple assumptions like the hypothesis of a rectangular density of electronic states and an axial crystal field of fixed direction, and considering an external field parallel to the direction of easy magnetization, one can find an analytic expression for the magnetic phase equation. The study performed here may be of interest to understand the magnetic behavior of films in which the easy magnetic direction is in the plane of the film, the axial crystal field in the perpendicular direction.

The present paper is organized as follows: in Section 2 the model hamiltonian is introduced, the quantities of interest defined, an ionic magnetic state equation is derived at T = 0 K, and a magnetic phase diagram is obtained; in Sections 3 and 4 we discuss the magnetic behavior implicit in the magnetic state equation, in the paramagnetic and ferromagnetic regions.

## 2 MODEL HAMILTONIAN AND EQUATION OF STATE AT T = 0 K

The total hamiltonian for the system of localized ions and conduction electrons is

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

where the individual hamiltonians for the electron and ion are given by

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

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

The term $\mathcal{H}_{cf} = D \sum_j (J^j_z)^2$ describes the interaction of the localized electrons (the ion) with an axially symmetric crystal field, where $J^j_z$ is the z component of the angular momentum of the ion j and D is the energy splitting. $\mathcal{H}_{kin}$ describes the dynamics of the conduction electrons characterized by an energy density of states, in the present study assumed of rectangular shape.

As the easy direction of magnetization is along the x axis, the magnetic interáction between ions and electrons is given by

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

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

where g is Landé's factor and $h_i$ and $h_e$ are the effective magnetic fields acting on the sub-systems (ions and electrons) that include an external field $h_0$ also in the x direction. These effective magnetic fields are

$$\alpha = g\ \mu_B h_i = g\ \mu_B h_0 + J_0(g-1)\ \langle s_x \rangle \tag{4-a}$$

$$2\ \mu_B h_e = 2\ \mu_B h_0 + J_0(g-1)\langle J_x \rangle \tag{4-b}$$

where $\langle s_x \rangle$ and $\langle J_x \rangle$ are the thermal averages of the x component of the electronic spin and of the ionic angular momentum. The terms containing $J_0$

in Eqs. 4 describe the exchange fields (in the molecular field approximation) acting on electrons and on ions.

From (2-a) one may obtain the magnetic moment per ion, for the ground state[4]

$$<0|J_x|0> = \frac{2g\mu_B h_1}{[D^2+4(g\mu_B h_1)^2]^{1/2}} \tag{5-a}$$

and from (2-b) the electronic magnetization[5] (in $\mu_B$ units) at T = 0 K:

$$8\varepsilon_0\gamma<0|s_x|0> = 2\ \mu_B h_e \tag{5-b}$$

where $\gamma$ is the occupied fraction of the band, of width $2\varepsilon_0$.

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

$$\overline{<0|J_x|0>} = \int dJ_0\ f(J_0)\ <0|J_x|0>/ \int dJ_0\ f(J_0) \tag{6}$$

One should note that in averaging $<0|J_x|0>$, taken from Eq. (5-a), we assume that each ion sees a different effective magnetic field (different $J_0$'s), but in using equations 4 and 5 $\overline{<0|J_x|0>}$ and $\overline{<0|s_x|0>}$ substitute $<0|J_x|0>$ and $<0|s_x|0>$, respectively.

We have adopted for $f(J_0)$, the distribution of exchange parameters centered in $J_c$ , the expression

$$f(J_0) = \sum_i c_i\delta(J_0 - J_i) \tag{7}$$

where $c_i$ are normalized coefficients computed from a Gaussian distribution of half width $\sigma\sqrt{2}$, centered in $J_c$.

With Eq. 7 one obtains, from Eq. 6

$$\overline{\langle 0|J_x|0\rangle} = \sum_i c_i \frac{2\bar{\alpha}_i/2\varepsilon_0}{[(D/2\varepsilon_0)^2 + 4(\bar{\alpha}_i/2\varepsilon_0)^2]^{1/2}} \tag{8-a}$$

where

$$\frac{\bar{\alpha}_i}{2\varepsilon_0} = \frac{g\mu_B h_0}{2\varepsilon_0} + J_i\frac{(g-1)}{2\varepsilon_0}\,\frac{1}{2\gamma}\,\frac{g\mu_B h_0}{2\varepsilon_0} + \left(J_i\frac{(g-1)}{2\varepsilon_0}\right)^2\frac{1}{4\gamma}\,\overline{\langle 0|J_x|0\rangle} \tag{8-b}$$

With $h_0 = 0$, in the limit $\overline{\langle 0|J_x|0\rangle} = 0$, one obtains

$$2\gamma D/2\varepsilon_0 = \sum_i c_i \left(J_i\frac{(g-1)}{2\varepsilon_0}\right)^2 \tag{9}$$

The above equation, in the parameter space $J_c/2\varepsilon_0$ (the center of the exchange distribution) versus $D/2\varepsilon_0$ (fixed $\gamma$ and $\sigma\sqrt{2}/2\varepsilon_0$) describes the frontier between the paramagnetic and ferromagnetic regions.

## 3 PARAMAGNETIC REGION

Curves of $\overline{\langle 0|J_x|0\rangle}$ versus $\mu_B h_0/2\varepsilon_0$ obtained using Eq. 8 are shown in Fig. 1 . The parameter $J_c/2\varepsilon_0$ (the center of the distribution of exchange parameters), the half-width of this distribution $\sigma\sqrt{2}/\varepsilon_0$, and $D/2\varepsilon_0$ (the crystal field parameter) were chosen in order to satisfy Eq. 9, so that we are on the threshold of the paramagnetic-ferromagnetic transition. It can be seen that for larger values of $J_c$, the magnetic response $\overline{\langle 0|J_x|0\rangle}$ saturates more gradually. This also occurs for larger values of $\sigma\sqrt{2}/\varepsilon_0$ (larger inhomogeneity) for a given value of $J_c/2\varepsilon_0$; this effect is less important for lárger values of $J_c$.

## 4 FERROMAGNETIC REGION

Increasing $J_c/2\varepsilon_0$, for the crystal field parameters used in Fig. 1, we enter the region of spontaneous magnetization ($h_0 = 0$). Curves of $\overline{\langle 0|J_x|0\rangle}$ versus $J_c/2\varepsilon_0$, with $h_0 = 0$, are shown in Fig. 2, for several values of the parameters. The values of $J_c$ where the curves cross the abscissae axis are the same used in drawing Fig. 1; the widths of the distributions are also taken from Fig. 1. It can be seen that for a given value of $J_c$, the effect of increasing the width of the distribution is to make the average magnetization $\overline{\langle 0|J_x|0\rangle}$ saturate more slowly; this effect is less important for larger values of $J_c$.

## 5 CONCLUSIONS

The simplicity of the model and the approximations used allowed us to obtain an analytical state equation for the average magnetization with an exchange parameter distribution and fixed values of the crystal field and band parameters at T=0 K (Eq. 8-a and Eq. 8-b). From it we derived a magnetic phase diagram in the parametric space ($J_c/2\varepsilon_0$, $\sigma\sqrt{2}/2\varepsilon_0$, $D/2\varepsilon_0$). We also made a parametric study in the para- and ferromagnetic regions, showing the effects of varying the center and width of the exchange distribution on the magnetic behavior of the system.

This study may be of interest is discussing magnetic properties of some amorphous metallic films. In amorphous systems the quadratic contribution to the crystal field (involving the $O_2^0$ Stevens operator) exceeds by one order of magnitude the effect of higher order terms[6], and this justifies our use of a simple quadratic term. This work is restricted to amorphous films in which the directions of the crystal field axes are perpendicular to the plane of the film.

FIGURE CAPTIONS

Fig. 1. Magnetic response versus applied magnetic field. The groups of curves a, b and c have values of $J_c/2\varepsilon_0$ = 0.0, 0.04 and 0.06. For each group, 1, 2 and 3 are obtained for different values of $\sigma\sqrt{2}/2\varepsilon_0$ :0.02, 0.03 and 0.04. In each curve $D/2\varepsilon_0$ is chosen in such way to assure that we are always in the frontier of the para- to ferromagnetic transition.

Fig. 2. Curves of average magnetization versus the center value of the exchange distribution. Groups of curves a, b and c cross the abscissae axis for the same values of $J_c/2\varepsilon_0$ used previously. Also, curves 1, 2 and 3 are obtained for the same values of $\sigma\sqrt{2}/2\varepsilon_0$ of the paramagnetic study.

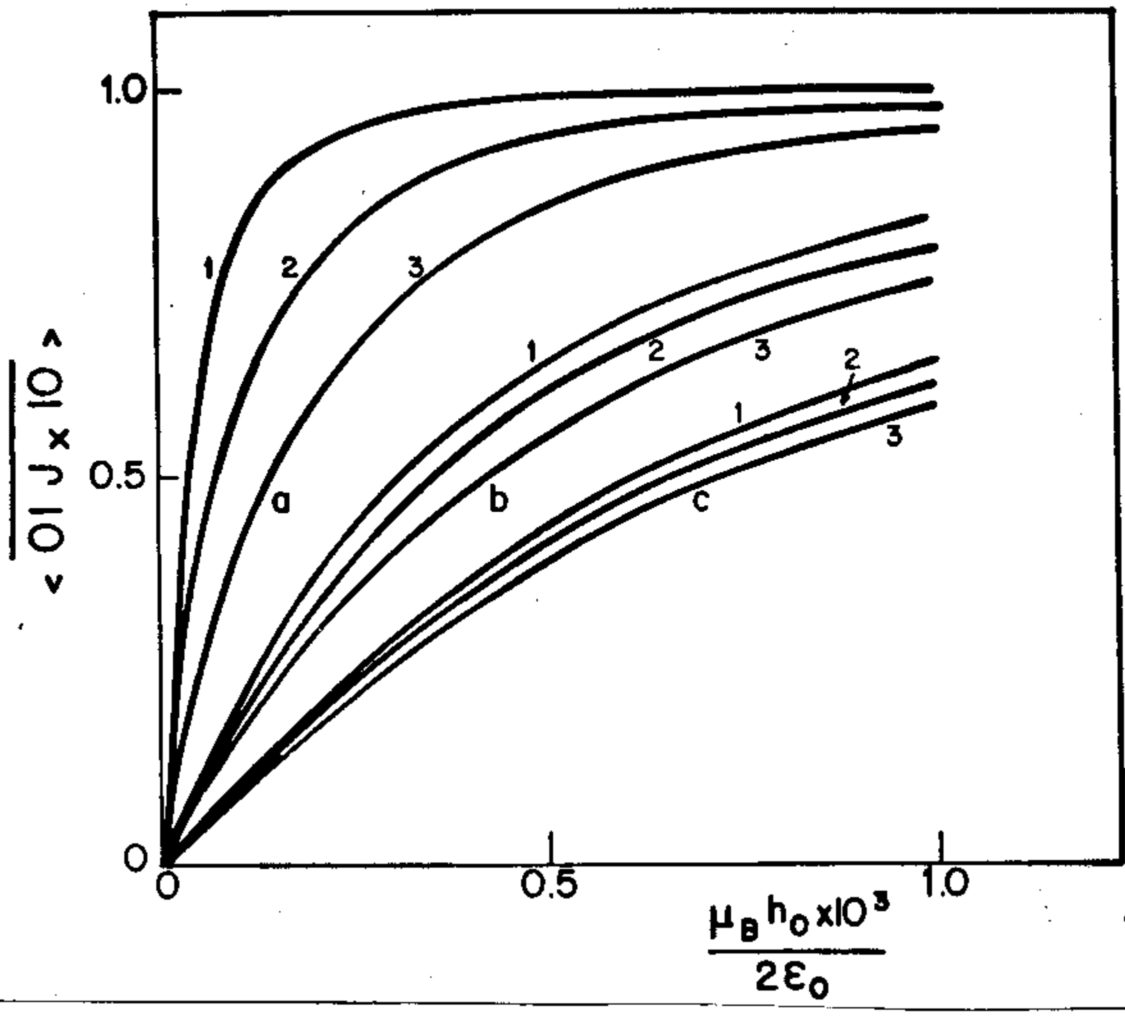
1.0
0.5
0
0
0.5
1.0
1
2
3
a
1
2
3
b
2
1
3
c
$<0|J\times 10>$
$\frac{\mu_B h_0 \times 10^3}{2\varepsilon_0}$

FIG. 1

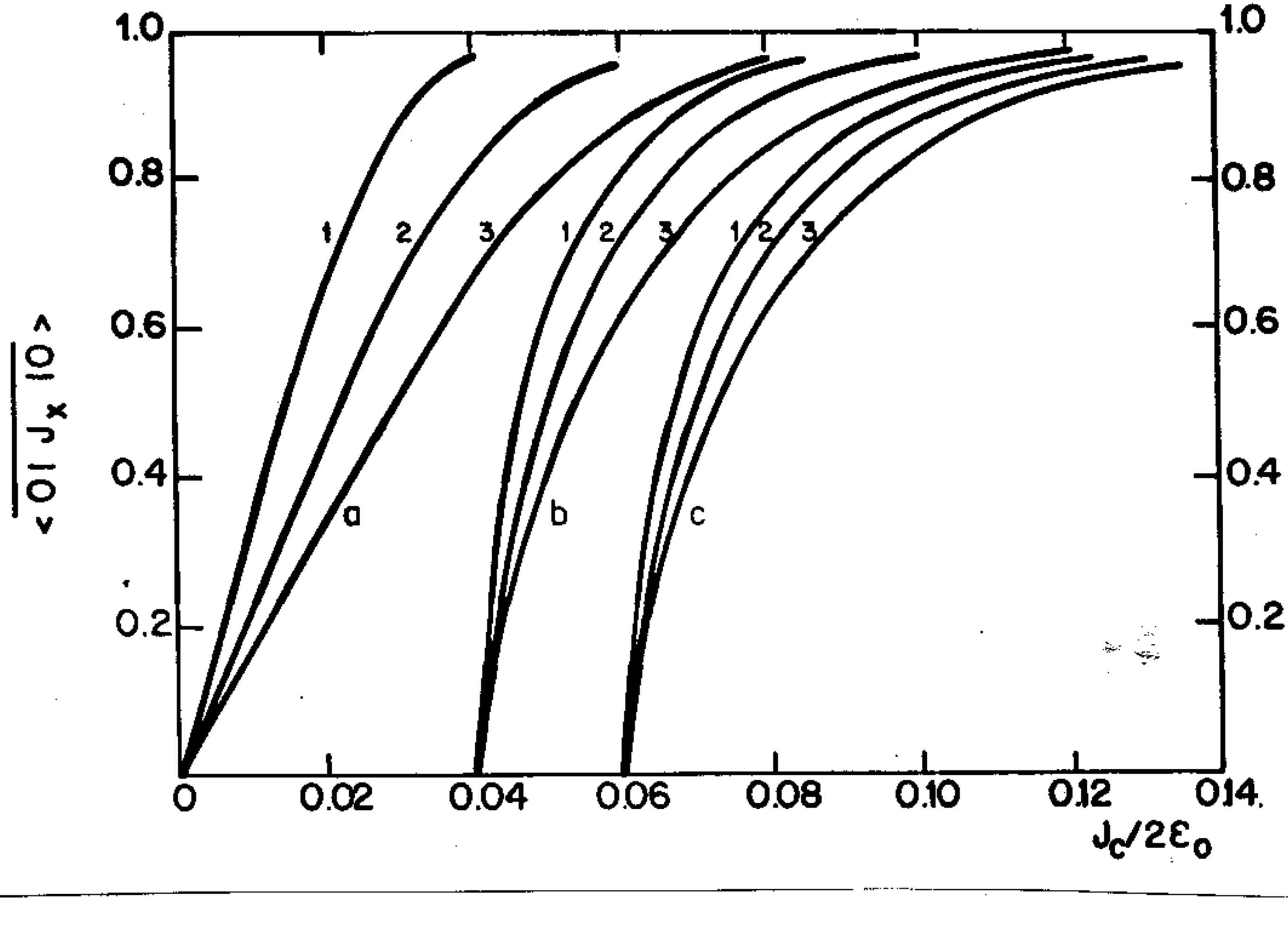
1.0
0.8
0.6
0.4
0.2
$\overline{<0 | J_x | 0>}$
1
2
3
1
2
3
1
2
3
a
b
c
0
0.02
0.04
0.06
0.08
0.10
0.12
0.14
$J_c/2\varepsilon_0$

FIG. 2

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