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The magnetic properties of disordered Fe–Al alloy system

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ABSTRACT

Using the effective field theory with a probability distribution technique that accounts for the self-spin correlation functions, the magnetic properties of disordered Fe–Al alloys on the basis of a site-diluted quantum Heisenberg spin model are examined. We calculated the critical temperature and the hysteresis loops for this system. We find a number of characteristic phenomena. In particular, the effect of concentration c of magnetic atoms and the reduced exchange anisotropic parameter η on both the critical temperature and magnetization profiles are clarified.

1. Introduction

Magnetic systems have always been of great practical interest, mainly due to their possible usage in information technology, as well as novel materials for a variety of applications. In the former case, the giant magnetoresistance is a special example for technological information storage [1,2]. These materials have also been the subject of intense theoretical investigation in both, pure and disordered versions [3]. Among the family of magnetic alloys, the Fe–Al system has been one of the most interesting because of the several magnetic phases that can be present in this system, such as ferromagnetism, paramagnetism, and even the spin-glass phase [4,5]. The region of the magnetic phase diagram in which these phases exist are strongly dependent upon how the constituent atoms are distributed in the crystalline lattice. The $Fe_{1-q}Al_q$ system in the bcc structure shows an interesting magnetic behavior since its critical temperature decreases with $q = 1 - c$ but shows a kind of plateau for low Al concentrations. Theoretical studies [5,6], using mean field renormalization group [7] and Bogoliubov inequality [8] approaches have been used to explain this behavior by taking a simple Ising Hamiltonian. Sato and Arrot [9] obtained the magnetization by assuming a ferromagnetic exchange between nearest-neighbor Fe atoms and an antiferromagnetic superexchange between two Fe atoms separated by an Al atom. This model, however, predicts an antiferromagnetic phase at low temperatures which was not revealed by neutron scattering experiments [10]. Shukla and Wortis [11] and Grest [12] did their estimates assuming a spin-glass state near the critical Al concentration. In this case, a rather good agreement with experimental data has been achieved. More recently, an experimental study of Fe–Al alloys in the disordered phase has been reported for Al concentrations $q = 1 - c$ with c is the concentration of Fe atoms, in the range $0 \leq q \leq 0.5$ [13]. It has been shown that this system, at room temperature, undergoes a ferro- to paramagnetic phase transition at a critical Al concentration $q_c = 0.475$ [13]. It has also been noted that the critical temperature of the ferro- to paramagnetic transition decreases as the Al concentration increases. Moreover, these alloys

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are all ferromagnetic and do not show the anomalous behavior of the ordered ones. Moreno and Montenegro [14] reported an investigation of the ferromagnetic disordered $Fe_{1-q}Al_q$ alloys by magnetization measurements. For a special value of concentration q, they obtained the critical temperature and critical exponents for different alloys. Our aim in this paper is to extend the results reported in Ref. [15] for studying the phase transition and the site-diluted quantum Heisenberg spin model applied to the magnetic properties of Fe–Al disordered alloys, in the framework of the effective field theory with a probability distribution technique [16]. The model studied is the same as that analyzed in Ref. [15]. In particular, an anisotropic Heisenberg model with site dilution is investigated in mean-field approximation. To simplify the consideration further a two-site cluster approximation is already used which is based on a two-site cluster theory introduced by Bobak and Jascur [17] in which attention is focused on a cluster comprising just two selected Heisenberg spins. The magnetic properties such as the hysteresis loops and coercive field as functions of the temperature and concentration respectively are discussed. We discuss on simple cubic symmetric with nearest-neighbor exchange interactions in which the strength is assumed to be different from the bulk value in the surface. In Section 2, we outline the formalism and derive the equations that determine the phase diagrams, the hysteresis loops and critical temperature. The phase diagram of the system as functions of the parameters R, η and c are discussed in Section 3. The conclusion is given in Section 4.

2. Formalism

In order to obtain the critical properties of the Fe–Al disordered alloys we assume a quenched site-diluted quantum Heisenberg model with only the nearest-neighbor interactions. The model is defined on a simple cubic lattice and the Hamiltonian of the system is given by

$$H = -\sum_{\langle ij\rangle} J_{ij} c_i c_j (\xi S_{i,x} S_{j,x} + \eta S_{i,y} S_{j,y} + \zeta S_{i,z} S_{j,z}) \tag{1}$$

where c_i is a random variable which takes the value 1 or 0 according to whether the site i is occupied by a spin S_i, or not. J_{ij} is the exchange parameter between spins. The parameters ξ, η and ζ control the anisotropy of the exchange interaction J_{ij}. For some special values of ξ, η and ζ one recovers the well-known models, namely, the Ising model [I] ($\xi = \eta = 0$), the isotropic Heisenberg model [H] ($\xi = \eta = \zeta$) and the X–Y model [XY] ($\xi = \eta,\ \zeta = 0$).

In this paper we report results for the two-site cluster approximation. The following notation will be adopted throughout. The two nearest-neighboring sites forming the pair cluster are denoted by 1 and 2. λ_i ($i = 1$ to N_1) denote the nearest-neighboring sites of 1 (excluding 2), while α_i ($i = 1$ to N_2) those of 2 (excluding 1). Some lattices have sites common to both the sets $\{\lambda_i\}$ and $\{\alpha_i\}$. These are denoted by $\varphi_i (i = 1 \text{ to } N)$. $\{\lambda_i'\}$ and $\{\alpha_i'\}$ denote the sets $\{\lambda_i\}$ and $\{\alpha_i\}$ when the sets $\{\varphi_i\}$ have been removed. $S_{i,z}$, $S_{i,x}$ and $S_{i,y}$ denote the Pauli matrices which are the components of the quantum spin $\overrightarrow{S_i}$ of magnitude $S = 1/2$ at site i, and the summation runs over all pairs of nearest neighbors.

The starting point for the two-site cluster approximation is to split the Hamiltonian into the following terms

$$H = H_{12} + H_1 + H_2 + H' = H_0 + H' \tag{2}$$

with

$$H_{12} = -c_1 c_2 J \left(\xi S_{1,x} S_{2,x} + \eta S_{1,y} S_{2,y} + \zeta S_{1,z} S_{2,z}\right) \tag{3}$$

and $H_1(H_2)$ is the Hamiltonian type, namely

$$H_1 = -J c_1 \left(\xi S_{1,x} \sum_{i=1}^{N_1} c_{\lambda_i} S_{\lambda_i,x} + \eta S_{1,y} \sum_{i=1}^{N_1} c_{\lambda_i} S_{\lambda_i,y} + \zeta S_{1,z} \sum_{i=1}^{N_1} c_{\lambda_i} S_{\lambda_i,z}\right) \tag{4}$$

$$H_2 = -J c_2 \left(\xi S_{2,x} \sum_{i=1}^{N_2} c_{\alpha_i} S_{\alpha_i,x} + \eta S_{2,y} \sum_{i=1}^{N_2} c_{\alpha_i} S_{\alpha_i,y} + \zeta S_{2,z} \sum_{i=1}^{N_2} c_{\alpha_i} S_{\alpha_i,z}\right). \tag{5}$$

Allowing for the fact that H_0 and H' do not commute, the thermal average of $S_{1,z}$, for example, can be written as

$$\langle S_z\rangle = \left\langle \frac{B}{A} \right\rangle - \left\langle \left(\frac{B}{A} - S_{1,z}\right) \Delta \right\rangle, \tag{6}$$

where

$$A = Tr^0 \exp(-\beta H_0), \qquad B = Tr^0 [S_{1,z} \exp(-\beta H_0)], \tag{7}$$

$$\Delta = 1 - \exp(-\beta H_0) \exp(-\beta H') \exp(\beta H_0). \tag{8}$$

In the above, Tr^0 means the partial trace with respect to the states of the cluster spins S_1 and S_2. Eq. (6) is an exact relation, but is difficult to the presence of the second thermal on the right-hand side. Following Ref. [18], we avoid this difficulty by