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Phase diagram of the mixed spin-2 and spin-5/2 Ising system with two different single-ion anisotropies

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HIGHLIGHTS

- Phase diagrams and compensation temperatures are examined for the mixed spin-2 and spin-5/2 Ising system with two single-ion anisotropies.
- The mean-field theory based on the Bogoliubov inequality for the Gibbs free energy is examined for the system.
- The Landau expansion of the free energy in the order parameter is obtained to describe the phase diagrams.
- The tricritical behavior is examined.

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ABSTRACT

We study the effect of two different single-ion anisotropies in the phase diagram and in the compensation temperature of mixed spin-2 and spin-5/2 Ising ferrimagnetic system. We employed the mean-field theory based on the Bogoliubov inequality for Gibbs free energy. We use the Landau expansion of free energy in the order parameter to describe the phase diagram. In the temperature versus single-ion anisotropy plane the phase diagram displays tricritical behavior. The critical and compensation temperatures increase with increasing values of the single-ion anisotropies.

1. Introduction

In the last five decades, the Ising model has been one of the most largely used models to describe critical behavior of several systems in nature. It is important to stress that in condensed matter theory it is relevant to describe the critical behavior and thermodynamic properties of a variety of physical systems (including disordered systems, spins glass, random field Ising systems, etc.). Recently, several extensions have been made in the spin-1/2 Ising model to describe a wide variety of systems. For example, the models consisting of mixed spins with different magnitudes are interesting extensions, forming the so-called mixed-spin Ising class.

Indeed, the discovery of molecular-based (MB) magnetic materials [1] has been one of the advances in modern magnetism. Many MB magnetic materials have two types of magnetic atoms regularly alternating which exhibit ferrimagnetism. In this context, a good description of their physical properties is given by means of mixed-spin configurations. Additionally, the interest in studying magnetic properties of molecular-based ferrimagnetic magnetic materials is due to their reduced translational symmetry rather than to their single-spin counterparts, since they consist of two interpenetrating sublattices. In this sense, Kaneyoshi et al. [2,3] have studied the magnetic properties as well as the influence of a single ion anisotropy in the compensation temperature (T) of bipartite molecular-based ferrimagnet. They considered two problems, the first is that of a two-dimensional ferromagnetic Ising system composed of ferrimagnetically

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ordered chains with alternating atoms of spin-1/2 and spin-$S(S > 1/2)$ by using Ising spin identities and the differential operator technique. In the second case a diluted spin-2 and spin-5/2 ferrimagnetic Ising system was investigated on the basis of the effective-field theory with correlations. On other hand, Drillon et al. [4] analyze the thermodynamic behavior of an exchange-coupled linear system with two alternating spin sublattices, showing that a bimetallic complex chain like MnNi(EDTA)$6H_2O$ is a good example of an experimental realization of the mixed-spin system. Thus, ferrimagnetic materials are of great interest due to their possible technological applications and from a fundamental point of view. As discussed above, these materials are modeled by mixed-spin Ising model that can be built up by infinite combinations of different spins, where the pairs constituted by spins with values small are the simplest ((spin-1/2, spin-1), (spin-1/2, spin-3/2), (spin-1, spin-3/2), (spin-2, spin-3/2), (spin-2, spin-5/2), and so on).

Noteworthy, there are many studies on mixed-spin Ising systems aiming to explain the physical properties of disordered systems. This interesting topic has been a great challenge in statistical mechanics. In this regard, in the last years there has been great interest in the study of magnetic properties of systems formed by two sublattices with different spins and crystal field interactions [5]. One of the earliest and simplest type of these models was the mixed-spin Ising system consisting of spin-1/2 and spin-S ($S > 1/2$) in an uniaxial crystal field [6,7]. However, from a pure theoretical point of view, such systems have been widely studied by a variety of approaches, e.g., effective-field theory [8–17], mean-field approximation [18–20], renormalization-group technique [21], numerical simulation based on Monte-Carlo [22–32] and, finally, exact solutions for the mixed spin-1 and spin-S Ising model in an uniaxial crystal field [33–38]. More recent interest is to extend such investigations into a more general mixed-spin Ising model with one constituent spin-1 and, in the simplest case, the other constituent spin-3/2. In this context, Abubrig et al. [39] presented a mean-field theory study to elucidate crystal field effects in the phase diagram of mixed spin-1 and spin-3/2 Ising configurations. Interestingly, they have found some outstanding new features in the T-dependence of both total and sublattice magnetizations.

In this paper, we study the effect of two different single-ion anisotropies in the phase diagram as well as in the compensation temperature of the mixed spin-2 and spin-5/2 Ising ferrimagnetic system. This case (the mixed spin-2 and spin-5/2 Ising ferrimagnetic system with two crystal-field interactions) primarily was studied on the Bethe lattice by using the exact recursion equations [40,41]. On the other hand, we employed the mean-field theory based on the Bogoliubov inequality for Gibbs free energy to describe the phase diagram. Thus, even knowing the limitation of the mean field theory, it is still an adequate starting point, and produces a very simple way to understand the possible critical behavior of physical systems. The paper is organized as follows: In Section 2, the model is introduced and analytical expressions for free-energy and equations of state are obtained. In addition, we derive the Landau expansion of free energy in the order parameter. In Section 3, we describe our theoretical results and discuss the phase diagram and the compensation temperature dependence. Finally, in Section 4 we present our conclusions.

2. The model and calculation

The mixed-spin ferrimagnetic Ising system consists of two interpenetrating square sublattices (A and B) with spin $S^A = 0, \pm 1, \pm 2$ and spin $S^B = \pm 1/2, \pm 3/2, \pm 5/2$. In each site of the lattice there is a single-ion anisotropy (D_A in the sublattice A and D_B in the sublattice B) acting on the spins $S = 2$ and spins $S = 5/2$ at the lattice sites. The system is described by the following model Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i^A S_j^B - D_A \sum_{i \in A} (S_i^A)^2 - D_B \sum_{j \in B} (S_j^B)^2, \tag{1}$$

where the first term represents the interaction between the nearest neighbor spins at sites i, j located on sublattices A, B, respectively. J is the magnitude of the spin–spin interaction, and the sum is over all nearest neighbor pairs of spins. The second and third terms represent the single-ion anisotropies at all points of the sublattices A and B. The sums are performed over $N/2$ spins of each sublattice.

In order to derive analytical expressions for free energy and equations of state, we employ the variational method based on the Bogoliubov inequality for Gibbs free energy [42], which reads

$$G(\mathcal{H}) \le G_0(\mathcal{H}_0) + \langle \mathcal{H} - \mathcal{H}_0(\eta) \rangle_0 = \Phi(\eta). \tag{2}$$

Here, $G(\mathcal{H})$ is the free energy of $\mathcal{H}$, and $G_0(\mathcal{H}_0)$ is the free energy of a trial Hamiltonian $\mathcal{H}_0(\eta)$ depending on variational parameters. $\langle \cdots \rangle_0$ denotes a thermal average over the ensemble defined by $\mathcal{H}_0(\eta)$. To facilitate the calculations, we choose the simplest trial Hamiltonian, which is given by

$$\mathcal{H}_0 = -\sum_{i \in A} \left[D_A (S_i^A)^2 + \eta_A S_i^A \right] - \sum_{j \in B} \left[D_B (S_j^B)^2 + \eta_B S_j^B \right], \tag{3}$$

where η_A and η_B are variational parameters related to two different spins configurations. Within this approach we obtain the free energy and the equations of state (i.e., sublattice magnetization per site m_A and m_B):

$$g = -\frac{1}{2\beta} \ln \left[2 \exp(4\beta D_A) \cosh(2\beta \eta_A) + 2 \exp(\beta D_A) \cosh(\beta \eta_A) + 1 \right]$$