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Magnetic properties of an Ising ferromagnetic model on a square lattice with next-nearest-neighbor and crystal field interactions

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ABSTRACT

We studied an Ising ferromagnet on a bipartite square lattice with nearest-neighbor ferromagnetic exchange couplings between spin values $S_i^A = 2$ and $\sigma_j^B = 5/2$, next-nearest-neighbor exchange couplings between spins, $S_i^A = 2$ and an average term of single-ion anisotropy for each lattice site. We carried out Monte Carlo simulations on the planes (D', k_BT') and (J_2', k_BT') to investigate the influence of exchange parameters J_2' and anisotropy of D' lattice on the critical temperature of the system. The thermal behaviors of the sublattice magnetizations, total magnetization and specific heat were investigated. We found that the critical behavior system depends linearly on the next-nearest-neighbor interaction J_2' and for antiferromagnetic exchange interactions the system undergoes reentrant phenomena.

1. Introduction

Within the wide range of molecular magnetic materials the ferromagnetic materials were found which can be characterized theoretically by appropriate models of mixed spins. These complex structures have important physical properties that contribute to technological development. For example, the ferromagnetism discovered in some diluted magnetic semiconductors and ferromagnetic thin films has served for a variety of important applications in high technology devices [1–5]. Similarly, some ferromagnetic materials based on graphene (graphene-based, materials) have been useful in the operation of various spintronic devices [6–9]. Ferromagnetic and ferrimagnetic systems are computationally modeled through mixed Ising systems, because they are good "laboratories" for the magnetic analysis of these materials, since they can exhibit many phenomena related with various applications in the field of thermomagnetic recordings, which are not observed in simple spin Ising systems [10].

The importance of ferromagnetic systems highlights the previous research of a variety of theoretical approaches and experimental works, which modeled such structures. Liu et al. studied the magnetic properties of a mixed spin-3/2 and spin-1 Ising ferromagnetic system on an expanded FCC lattice in Fe_4N [11], and Ekiz and Keskin analyzed the magnetic properties of a mixed spin-1/2 and spin-1 Ising ferromagnetic system with a crystal field interaction in the absence and presence of an external magnetic field [12]. Using the mean-field approximation with correlated clusters, Yamamoto analyzed magnetically ferromagnetic systems [13] and by the theory effective correlated mean-field was studied by the spin-1/2 Ising ferromagnetic model with nearest-neighbor interactions on a square lattice [14]. Also the magnetic properties of the Ising ferromagnetic/antiferromagnetic superlattice were characterized, which is composed of a spin-1/2 ferromagnetic monolayer and a spin-1 antiferromagnetic monolayer [15]. Žukovič and Bobák analyzed the critical properties of an Ising bilayer spin system and mixed spin-1/2 and spin-1 Ising ferromagnets, in triangular lattices antiferromagnetic and ferromagnetic coupled to ferromagnetic exchange interaction [16,17]. Also these are noteworthy studies of the ferromagnetic–paramagnetic phase transition in the ferromagnetic classical and quantum thin films [18] and the magnetic properties of an antiferromagnetic surface coupled ferromagnetically to a ferromagnetic material [19]. For some layered mixed spin Ising systems, the structural and magnetic properties of the magnetic thin films have been studied experimentally, such as surface magnetoelastic coupling and surface magnetic anisotropy [20–23]. Likewise, for Ising ferromagnetic thin film systems the dynamic phase transition properties by means of detailed Monte Carlo simulations and effective-field theory with correlations [24–26] have been analyzed, showing interesting behavior which includes triple point and isolated

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critical point, tricritical points and first- and second-order phase transitions [27]. No less interesting is the study of the short-range ferromagnetic order in perovskite manganite $La_{0.62}Er_{0.05}Ba_{0.33}Mn_{0.95}Fe_{0.05}O_3$, using *dc* magnetometry in the vicinity of paramagnetic to ferromagnetic second order phase transition [28].

Ferromagnetic and ferrimagnetic nanostructures have also been the subject of research through the use of mixed spin configurations and the interest in its study is due to many peculiar physical properties compared with those in bulk materials and potential technological applications in information storage devices [29,30], permanent magnets [31], environmental remediation [32] and biomedical applications [33]. For example, by using the double-time Green's function method, Mi et al. investigated the effect of magnetic spin correlation on the thermodynamic properties of Heisenberg ferromagnetic single-walled nanotubes [34] and experimentally it has been possible to synthesize some nanomaterials and analyze their magnetic properties, as in the case of magnetic nanowires Co–Cu [35], $Ga_{1-x}Cu_xN$ [36] and Fe_3O_4 [37]. Previous works on the analysis of ferro- and ferrimagnetic Ising systems include the use of spin configurations in square lattices with next-nearest and next-nearest-neighbor interactions and crystal and external fields [38–42].

In this theoretical work, we analyzed a Ising ferromagnet structured on a square lattice with spins $S_i^A = 2$ and $\sigma_j^B = 5/2$, considering ferromagnetic couplings next-nearest-neighbor between spins type S and crystal field interactions. This model has been used as the prototype of certain molecular-based magnetic materials. For example, the model properly represents the compound $AFe^{II}Fe^{III}(C_2O_4)_3$, $A{=}N(n\text{-}C_nH_{2n+1})_4$, $n{=}3$–5, where $Fe^{II}{=}2$ and $Fe^{III}{=}5/2$ [43]. Through Monte Carlo simulations and mean field approximations of the Hamiltonian, this model has served for the understanding of a rich variety of thermomagnetic phenomena, such as critical and compensation temperatures obtained with different single-ion anisotropies [44], magnetic hysteresis cycles on a Bethe lattice for different values of exchange interactions, crystal field and sizes [45], thermal total magnetization and sublattice magnetizations with different exchange interactions, external magnetic fields and temperatures on a Bethe lattice [46], first and second order phase transition, tricritical points and compensation points on a honeycomb lattice in a longitudinal magnetic field [47], first order phase transitions due to the effects of two single ion anisotropies on a honeycomb lattice when the temperature increases [48], compensation phenomenon by the effect of a single-ion anisotropy and an interlayer interaction on a layered honeycomb lattice [49], and the existence and location of compensation points due to the anisotropy of the mixture of spins (2, 5/2) [50].

As interesting as the previous investigations on spins model (2, 5/2) are those made on its dynamic magnetic properties. By using dynamic mean-field calculations Ertaş extended the study of dynamic phase transition temperatures, the dynamic compensation points and the dynamic phase diagrams of the model, adding the dynamic hysteresis behaviors on a hexagonal lattice in an oscillating magnetic field [51]. Similarly, in the analysis of the nonequilibrium magnetic properties in the presence of a time-varying magnetic field, within the effective-field theory, Ertaş et al found the dynamic tricritical and reentrant behaviors, the thermal behavior of the dynamic magnetizations, the hysteresis loop area and dynamic correlation of the model [52]. Additionally, for a bilayer square lattice spins 2 and 5/2 in the presence of a time-dependent oscillating external magnetic field, the time variations of average magnetizations and the temperature dependence of the dynamic magnetizations [53], as well as the effects of the antiferromagnetic/antiferromagnetic (AFM/AFM) interactions on the critical behavior of the system [54], were investigated, Also is noteworthy the use of repulsive biquadratic coupling and Glauber dynamic approach in the calculations multicritical dynamic phase diagrams and dynamic hysteresis loops of the model [55].

The outline of this work is as follows. In Section 2 we define the model and present the Monte Carlo method. The effects of exchange interaction next-nearest-neighbors and single-ion anisotropy on the phase diagrams are discussed in Section 3. Finally, Section 4 is devoted to brief conclusions.

2. Model and Monte Carlo simulation

The model studied is a mixed Ising ferromagnet with spins 2 and 5/2, alternating on a square lattice of side $L{=}80$. The interaction Hamiltonian of the system is defined as:

$$H = -J_1 \sum_{i,j\in\langle nn\rangle} S_i^A \sigma_j^B - J_2 \sum_{i,k\in\langle nnn\rangle} S_i^A S_k^A - D\sum_{i\in A} (S_i^A)^2 - D\sum_{j\in B} (\sigma_j^B)^2 \tag{1}$$

where $S_i^A{=}\pm 2, \pm 1, 0$ and $\sigma_j^B{=}\pm 5/2, \pm 3/2, \pm 1/2$ are the spins on the sites of the sublattices A and B, respectively. J_1 is the exchange interaction between pairs of spins to nearest neighbors, J_2 is the exchange parameter between pairs of spins next nearest neighbors of the sublattice A, and D is the crystal field, which cause anisotropy of the system. The first sum is performed over all pairs of spins with nearest neighbor interaction, i.e., between sites with spins $S_i^A = 2$ and $\sigma_j^B = 5/2$, the second sum runs over all pairs of spins with next nearest neighbors interaction of spins S_i^A, and sums $\sum_i$ and $\sum_j$ are performed on all sites of spins of the sublattices A and B, respectively. We choose a ferromagnetic coupling to nearest neighbors, $J_1 > 0$, and we take periodic boundary conditions. All variables in the Hamiltonian are in units of energy.

The simulation of the model is carried out by the Monte Carlo method, generating states randomly by a heatbath algorithm, described below. We choose a spin at random, and calculate the energy difference ΔE_{ij} and the transition probability $\exp(-\beta\Delta E_{ij})$ associated with each possible change. Then, whether the spin changes its value is considered, generating a random number θ in the interval $(0, \sum P_i)$, where $\sum P_i$ represents the sum of transition probabilities. The data are generated with 5×10^4 Monte Carlo steps per site after discarding the first 10^4 steps per site to reach equilibrium of the system. Error calculation is estimated using the method of blocks, where the sample L-size is divided into n_b blocks of length $L_b = L/n_b$. Thus, the errors are calculated taking the averages of the blocks instead of the original measurements. Error bars are calculated by grouping all the mensurations in 10 blocks and taking the standard deviation [56].

The magnetization per site of the sublattices (M_A, M_B), and the total magnetization per spin, M_T, is defined as:

$$M_A = \frac{2}{L^2}\left\langle \sum_{i\epsilon A} S_i^A \right\rangle \tag{2}$$

$$M_B = \frac{2}{L^2}\left\langle \sum_{j\epsilon B} \sigma_j^B \right\rangle \tag{3}$$

$$M_T = \frac{M_A + M_B}{2} \tag{4}$$

Defining $\beta = 1/k_B T$, we calculate the specific heat per site (C), by the expression: