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Current Perspectives

Spin-1 and -2 bilayer Bethe lattice: A Monte Carlo study

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ABSTRACT

The magnetic behaviors of bilayer with spin-1 and 2 Ising model on the Bethe lattice are investigated using the Monte Carlo simulations. The thermal magnetizations, the magnetic susceptibilities and the transition temperature of the bilayer spin-1 and 2 on the Bethe lattice are studied for different values of crystal field and intralayer coupling constants of the two layers and interlayer coupling constant between the layers. The thermal and magnetic hysteresis cycles are given for different values of the crystal field, for different temperatures and for different exchange interactions.

1. Introduction

The study of magnetic thin films consisting of various magnetic layered structures or superlattices has received intense attention in the recent years for both theoretical and experimental point of views [1]. Since these materials are made up with multiple layers of different magnetic substances, there is a high potential for technological advances in information storage and retrieval and in synthesis of new magnets for a variety of applications [2]. The magnetic phase diagram of a thin film is determined at $T=0$ by including the exchange coupling, the magnetic dipole coupling, as well as second- and fourth-order lattice anisotropies [3], the complete global phase diagram for a spin-1 bilayer Blume–Emery–Griffiths (BEG) model is studied by the use of cluster variational theory in the pair approximation [4]. Some of the Bethe lattice considerations of spin-3/2 Ising model are: the bifurcation sets for the paramagnetic unstable fixed points for some values of co-ordination numbers were presented [5] based on the Katsura–Takizawa method [6], the Blume–Capel [7,8] and the Blume–Emery–Griffiths [9] models were studied on the Bethe lattice by using the exact recursion equations [10] and the exact expressions for the magnetization or the dipole moment, the quadrupole moment and the Curie or the second-order phase transition temperatures are presented. A Bethe lattice is an infinitely Cayley or regular tree, i.e. a connected graph without circuits, and historically gets its name from the fact that its partition function is exactly that of an Ising model in the Bethe approximation [11]. The magnetic properties of the bond and crystal field dilution in the presence of magnetic field were investigated on a simple cubic lattice by using effective-field theory [12]. The crystal field plays an important role for materials consisting of spins with $S>1/2$ [13]. The dynamic behavior of a mixed spin-1 and spin-2 Ising system with a crystal-field interaction in the presence of a time-dependent oscillating external magnetic field on a hexagonal lattice is studied by using the Glauber-type stochastic dynamics [14]. On the other hand, to date, few people have ever touched upon a mixed Ising model with both spin integer ions, namely the mixed spin-1 and spin-2 Ising system. An early attempt to study the equilibrium phase diagrams of the spin-1 and spin-2 mixed system was made by Ref. [15], who used the pair approximation with discretized path-integral representation. Iwashita et al. studied the temperature dependence of magnetization of the spin-1 and spin-2 mixed system by using the four spin model approximation [16]. The magnetic properties of the spin-1 and spin-2 mixed system on a layered honeycomb lattice by effective field theory and Monte Carlo (MC) simulations are studied by Zhang et al. [17]. The critical behavior of the mixed spin-1 and spin- 2 Ising ferromagnetic system by using exact recursion equations on the Bethe lattice are investigated by Albayrak et al. [18]. The magnetic properties of the mixed spin-1

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and spin-2 Ising ferromagnetic system with different anisotropies calculations are studied using mean field approximation and MC simulation by Wie et al. [19]. Mixed-spin Ising model on a decorated square lattice with two different decorating spins of integer magnitudes have been studied by Canova et al. [20]. The critical phenomena in a mixed spin-1 and spin-2 Ising model on honeycomb and square lattices have been studied using effective-field theory by Deviren et al. [21]. The mixed spin-1 and spin-2 Ising ferromagnetic model may represent a real system constituted of two layers; the first one contains chromium atoms of spin 2 and the second layer contains nickel atoms of spin1.

In this work, the ground state phase diagram of two-layer Bethe lattice is given. The thermal total magnetization, thermal magnetization and magnetic susceptibilities of each layer on Bethe lattice are obtained. The total magnetization versus the exchange interactions between two layers is established for different values of crystal field. The total magnetization versus the crystal field, Δ, for different values of exchange interactions and different values of external magnetic field. The magnetic hysteresis cycle of the two layers and of each layer with different exchange interactions, with different temperatures and different crystal field have been obtained.

2. Model and formulation

We consider a bilayer Bethe lattice, one-layer version consists of a central spin which may be called as the first generation spin. This central spin has n nearest-neighbors (NN), i.e., coordination number, which forms the second-generation spins. Each spin in the second-generation is joined to $(1-n)$ NNs. Therefore, in total this generation has $n(n-1)$ NNs which form the third-generation and so on to infinity. We consider two identical layer of Bethe lattices G_1 and G_2 which are placed parallel to each other forming the bilayer Bethe lattice as shown in Fig. 1. In each layer, every spin interacts with its NN and the corresponding adjacent spins in the other layer whose sites are labeled by k and l, respectively.

The Hamiltonian of the bilayer with spin-1 and 2 Ising model on the Bethe lattice including nearest neighbors interactions, external magnetic field and the crystal field is given by:

$$H = -J_1 \sum_{<i,j>} \sigma_i\sigma_j - J_2 \sum_{<k,l>} S_k S_l - J_3 \sum_{<i,k>} S_i\sigma_k - \Delta\left(\sum_i \sigma_i^2 + \sum_k S_k^2\right) - h\left(\sum_i \sigma_i + \sum_k S_k\right) \quad (1)$$

where $\langle i, j\rangle$, $\langle k, l\rangle$ and $\langle i, k\rangle$ stand for the first nearest neighbor sites (i and j), (k and l) and (i and k), Δ represents the crystal field and h is the external magnetic field. The J_1, J_2 and J_3 are the exchange interactions parameters between the first exchange interactions in layer with spin-σ, in layer with spin-S and between spin σ and S, respectively (see Fig. 1). The spin moments of spins σ and S are: $\sigma = \pm 1$, 0 and $S = \pm 2$, ± 1, 0. In full text $J_1 = 1$.

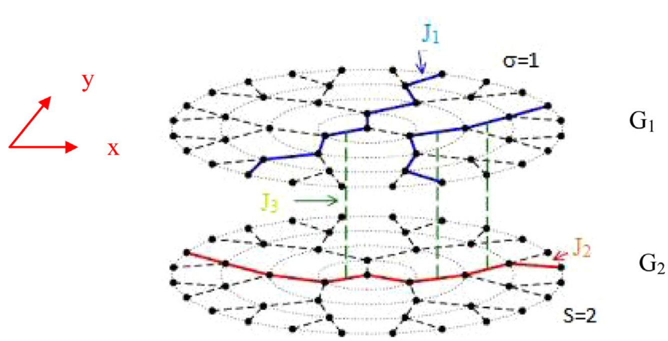

Fig. 1. The two-layer Bethe lattice of coordination number $n=3$. G_1 and G_2 refer to the upper and lower layer containing the spins labeled as $\sigma=1$ and $S=2$, respectively. While J_1 and J_2 are the bilinear interactions of spins in G_1 and G_2, J_3 is the one for the adjacent spins of two identical atomic layer G_1 and G_2.

3. Monte Carlo simulation

The bilayer with spin-1 and 2 Ising model on the Bethe lattice are assumed to reside in the unit cells and the system consists of the total number of spins $N=N_S+N_\sigma$, with $N_S=N_\sigma=46$ sites. We apply a standard sampling method to simulate the Hamiltonian given by Eq. (1). Cyclic boundary conditions in the x–y direction on the lattice were imposed and the configurations were generated by sequentially traversing the lattice and making single-spin flip attempts. The flips are accepted or rejected according to a heat-bath algorithm under the Metropolis approximation. The different initial conditions are chosen randomly following the spins states $\sigma = \pm 1$, 0 and $S = \pm 2$, ± 1, 0.

Our data were generated with 10^5 Monte Carlo steps per spin, discarding the first 10^4 Monte Carlo simulations. Starting from different initial conditions, we performed the average of each parameter and estimate the Monte Carlo simulations, averaging over many initial conditions. Our program calculates the following parameters, namely:

The magnetizations of core and shell are:

$$M_\sigma = \left\langle \frac{1}{N_\sigma} \sum_i \sigma_i \right\rangle \quad (2)$$

$$M_S = \left\langle \frac{1}{N_S} \sum_j S_j \right\rangle \quad (3)$$

where $N = N_\sigma + N_S$

The total magnetization is given by:

$$M_{tot} = \frac{M_\sigma + M_S}{2} \quad (4)$$

The internal energy per site:

$$E = \frac{1}{N}\langle H\rangle \quad (5)$$

$$E = \frac{1}{N}\left\langle -J_1 \sum_{<i,j>} \sigma_i\sigma_j - J_2 \sum_{<k,l>} S_k S_l - J_3 \sum_{<i,k>} S_i\sigma_k - \Delta\left(\sum_i \sigma_i^2 + \sum_k S_k^2\right) - h\left(\sum_i \sigma_i + \sum_k S_k\right)\right\rangle \quad (6)$$

The magnetic susceptibilities are given by:

$$\chi_\sigma = \beta\left(\left\langle M_\sigma^2\right\rangle - \langle M_\sigma\rangle^2\right) \quad (7)$$

$$\chi_s = \beta\left(\left\langle M_S^2\right\rangle - \langle M_S\rangle^2\right) \quad (8)$$

Total magnetic susceptibility is:

$$\chi_{tot} = \frac{\chi_\sigma + \chi_S}{2} \quad (9)$$

where $\beta = \frac{1}{k_B T}$, T denotes the absolute temperature and k_B is the Boltzmann's constant.