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Mixed spin-1 and spin-3/2 Blume-Emery-Griffiths model with external field on a honeycomb lattice

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ABSTRACT

In the present work, we use Monte Carlo simulations (MCS) to study the ferrimagnetic of the mixed spin-1 and 3/2 Blume-Emery-Griffiths (BEG) model on a honeycomb lattice. The ground state phase diagram has been obtained for T = 0 whereas at non vanishing, total and partial magnetizations have been calculated. Moroever, we have presented the results of phase diagrams depending on different parameters: exchange coupling paramaters (r_1 and r_2), crystal field (d_1 and d_2), biquadratic coupling interaction (k) and external magnetic field (h). On the other hand, the compensation temperature and hysterisis cycle have been established.

1. Introduction

For many years ago, one of the most studied mixed spin systems with BEG model consisting of two sublattices one is occupied by a spin and the other by other magnitude of spin like (1/2; 3/2), (1; 3/2), (2; 5/2) and so on …. These mixed spin systems present an interesting properties whose: the compenstation temperature in which the magnetic moments compensate each other and the total magnetization is zero and give richer phase diagrams consisting of ferromagnetic, antiferromagnetic (ferrimgnetic) and mixed spin states, the compensation temperature has a lot of technological applications such as achieving high speed magnetization in reversal magnetic materials [1] and in thermomagnetic recording media [2] We can also say that these systems are considererd as a possible models for some types of molecular-based materials, not only for theoretical physical description.

Therefore, the physical properties of magnetic honeycomb lattice has been investigated by different theoretical point of view, it's can also be described by a simple [3] and mixed BEG models [4,5], this model has been introduced first by Blume emergy grifits to simulates the thermodynamic behavior of He^3-He^4 mixture [6] and latter has been elaborated to outline another multi-component physical systems, such as liquid crystal mixtures, methamagnets, semiconductor alloys, etc.

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Moroever in the mixed spin systems already mentioned the compensation points appears. For, thus theoretical studies has been conducted by a various of methods in equilibrium statistical physics such as Monte-Carlo (MC) simulations [7], mean-field approximation (MFA) [8,9] renormalization group (RG) calculation [10], high and low temperature series expansions studied for mixed spin-1/2 and spin-1 Ising model with the effect of the crystal field [11], the transfer matrix method [12,13] numerical transfer matrix techniques supplemented by Monte Carlo simulations (MCS) [14,15] and by transfer matrix Green function methods [16] and finally by the cluster method in pair-approximation [17]. As we all know, the Monte Carlo simulation (MCS) is the most using method for understanding the physical properties of the magnetic materials, also it has a major importance to explore the physical properties of magnetic systems specifically for these mixed spin systems. Recently, M. Žukovič and A. Bobak presented results for the frustrated mixed with spin 1 and 1/2 ferrimagnets on a triangular lattice [18], also the phase boundaries of a spin-3/2 Blume−Emery−Griffiths model on a honeycomb lattice has been calculated, they compare the results obtained for order-disorder critical frontier with EFT for a specific parameter α and they found that the EFT doesn't reproduce these results exactly as obtained by MCS, thus the EFT approximation deemed for an artifact [19]. Deviren et al. [20] used the effective field theory to study the magnetic properties of the ferrimagnetic mixed spin −2 and spin-3/2 with equal crystal -field in a longitudinal magnetic field on the honeycomb and a square lattice and got interesting results.

Indeed, the Monte carlo simulation are not only specified for theoretical calculations, it can be also used for molecular based materials, the Monte Carlo simulation has been applied to discuss the step effect on a zigzag graphene nanoribbon structure in a longitudinal magnetic field, authors have been examined the effects of single-ion anisotropies and external magnetic fields on the magnetization, the susceptibility, the internal energy and the blocking temperature on graphene [21] Moroever, understanding ferromagnetism in C-doped CdS: has been extensively investigated by MCS for a potential use in spintronic devices [22], Qi. Yan and Du. An investigated the magnetoelectric properties in a rotating magnetic field and perform the Monte Carlo simulation on a two-dimensional lattice of $LiCu_2O_2$ compound with ground state of ellipsoidal helical structure [23].

However in the last work we have studied the mixed spin (1/2, 1) by using Mont Carlo simulation in the framework of BEG model on the Bethe lattice [24]. Recently the mixed spins on different geometrical structure have attracted many recherches for instance [25-30].

In this work we use also MCS to simulate the mixed spins system with a higher degree of spins states: the mixed (3/2, 1), we are studying the variation of magnetization as a function of exchange coupling, crystal field, biquadratic exchange interaction and external magnetic field parameters.

This study is composed in two steps; First, at zero temperature (T = 0), we present the ground state phase diagrams. Second, for temperature T≠0, where the stable phase diagrams has been found and can be affected by the Hamiltonian parameters.

This paper is organized as follows: In section 2, we present the Monte Carlo analysis and the theoretical model. In section 3, we first present, the ground-state phase diagrams. Then, we discuss the thermal behavior of the system magnetization; we show the compensation point appears at high coordination number and weak values of the crystal field, we also Investigate the influence of both the crystal field and the biquadratic exchange interaction on critical behaviors. We present the hysteresis loops and deduce the coercive magnetic field value which depends on biquadratic exchange interaction. Section 4, is devoted to the conclusion.

2. Simulated model

According to the crystal structure of the system, the model could host three exchange interactions. The first one is an A′-B interaction resulting from the coupling between σ = 1in A′-sites and s = 3/2 in B-sites, the second is an A′-A′ interaction resulting from the coupling σin A′-sites and S in B-sites, the third is a B-B'.

The model could also include the energy resulting from the crystal field of each magnetic spin and the energy resulting from the interaction with an external magnetic field. Therefore, the Hamiltonian of the system could be given by:

$$\mathcal{H} = -J_1 \sum_{<\mathrm{i,j}>} S_i S_j - J_2 \sum_{<\mathrm{i,j}>} \sigma_i \sigma_j - J_3 \sum_{<\mathrm{i,j}>} \sigma_i s_j - K \sum_{\mathrm{j,i}} S_i^2 \sigma_j^2 - \Delta_s \sum_{\mathrm{i}} S_i^2 - \Delta_\sigma \sum_{\mathrm{i}} \sigma_i^2 - H \sum_{\mathrm{i}} (\sigma_i + S_i) \quad (1)$$

where $\sigma,\ and\ s$ stand for the spins of A, and B "$A(\sigma = \pm 1 \text{and } 0),\ B(s = \pm 3/2,\ \pm 1/2)$" , respectively. $J_{\sigma S}$ denotes the exchange coupling between A and B. J_2 denotes the exchange coupling between A ions them selves ($J_{\sigma-\sigma}$). J_1 denotes the exchange coupling between B ions them selves; $\Delta_\sigma,\ and\ \Delta_s$ stand for crystal fields of A, and B, respectively. H designates an external magnetic field, and the k is the biquadratic coupling interaction.

3. Simulation method

To simulate the magnetic behavior of this complex system a MCS has been performed and combined with a Metropolis algorithm. The system has been conceived in the simulation program as a cubic bulk $L_B = 75$, which remains larger than the thermodynamic limit determined at $L_{ThL} = 30$ for this class of materials [38, 42]. A standard sampling method has been employed to dealt with the Hamiltonian in eq. (1). Initial configuration has been randomly generated in a way A-spins

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