Superlattices and Microstructures 104 (2017) 46–53

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Monte Carlo study of the mixed Blume-Capel model with four-spin interactions

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ARTICLE INFO

Article history:
Received 4 November 2016
Received in revised form 28 January 2017
Accepted 30 January 2017

Keywords:
Monte Carlo simulations
Blume-Capel model
Ferri-magnetic system
Four-spin interactions
Hysteresis loops

ABSTRACT

Using Monte Carlo simulations, we study the magnetic properties of a ferri-magnetic mixed spins (3/2,2) in a three-dimensional lattice with four-spin interactions. In one hand, we elaborated analytically the ground state phase diagrams in different planes. We found that the all $4 \times 5 = 20$ configurations are found to be stable. On the other hand, for non null temperature values, the magnetic properties and phase diagrams are deduced. The total and partial magnetizations/susceptibilities are also presented and discussed for different values of the reduced exchange interactions. The critical temperature is displaced towardslower temperatures. To complete this study, we examined the corresponding hysteresis loop behaviors, of the studied system, for different values of the physical parameters.

1. Introduction

Nowadays, growing interest is continuously directed towards the study of the magnetic properties of two-sub-lattice mixed-spin ferri-magnetic Ising systems. Researches published are based on theoretical and experimental methods. The theoretical methods are Monte Carlo simulations [1,2], effective field theory [3–8], cluster variation method [9,10], renormalization-group techniques [11–14], series expansions [15,16] and exact calculations [17]. The experimental ones are, the models with multi-spin interactions which can be applied to various interesting physical systems such as classical fluids [18], solid ^3He [19], lipid bi-layer [20], metamagnets [21] and rare gases [22].

There have been also applied to describe the thermodynamic properties of hydrogen-bonded ferroelectrics $PbHPO_4$ and $PbDPO_4$ [23], copolymers [24], and optical conductivity [25] observed in the cuprate ladder $La_xCa_{14-x}Cu_{24}O_{41}$. The model with four-spin interactions adopted in our work, have been used to study and to explain the existence of first-order phase transition in a square acid crystal $H_2C_2O_4$ [26]. It is worthy to note here that the four-spin interaction plays an important role in the two-dimensional anti-ferromagnet La_2CuO_4 [27], the parent material of high-T_c superconductors.

In recent years, much attention has been paid to the study of the mixed-spin nano-particles. The phase diagrams of a ferri-magnetic cubic nano-particle with spin-3/2 and spin-1 structure have been investigated in Refs. [28,29]. It was observed that the occupation of the sites of the particle core by the spin-3/2 plays an important role on the shape of the phase diagrams. Other work studied by using Monte Carlo simulation [30], the dynamic phase transition properties of a single spherical

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http://dx.doi.org/10.1016/j.spmi.2017.01.047
0749-6036/

ferromagnetic core–shell nano-particle. It has been found that the dynamic phase boundaries depend strongly on the Hamiltonian parameters such as the high amplitude and the period of the external field.

In this work, we are studying the magnetic properties of a ferri-magnetic mixed-spin-3/2 and spin-2 in a three-dimensional lattice, using Monte Carlo simulations with four-spin interactions. The considered Hamiltonian includes both the first nearest-neighbor and the four-spin interactions. An external and crystal magnetic field, are applied on the two sub-lattices.

The outline of the paper is organized as follows: in section 2, we briefly present our model and the related formalism. Results and discussions are presented in section 3, and finally section 4 is devoted to our conclusions.

2. Model and Monte Carlo simulations

We consider here is a three-dimensional lattice mixed-spin σ = 3/2 and S = 2 Ising model, governed by the following Hamiltonian:

$$H = -J_1 \sum \sigma_i S_j - J_P \sum_{<i,l>} \sigma_i S_l - J_4 \sum_{<i,j,l,k>} \sigma_i S_j \sigma_k S_l - \Delta \left(\sum_i \sigma_i^2 + \sum_j S_j^2 \right) - h \left(\sum_i \sigma_i + \sum_j S_j \right) \quad (1)$$

where $\sum_{<i,j>}$ indicates summations over all the first nearest-neighbors, while $\sum_{<i,j,k,l>}$ indicates summations over the four sites in every squares, see Fig. 1. J_1 is the ferri-magnetic coupling constant between spins **σ** and S belonging to the same plane. J_p stands for the coupling exchange interaction between spins belonging to the adjacent planes. J_4 is the four-spin interaction, see Ref. [31]; h is the external magnetic field and Δ is the crystal magnetic field applied on all the sites of the system. For simplicity, we will normalize the all system parameters by the constant J_P. So that, $R_1 = J_1/J_P$, $R_4 = J_4/J_P$, $d = \Delta/J_P$ and $t = T/J_P$, stand for the reduced parameters, see for example Ref. [31].

The Monte Carlo Metropolis method has been used to obtain the equilibrium properties of the physical system in contact with a heat bath of temperature **T** in order to simulate the Hamiltonian given by Eq. (1). Periodic conditions are taken into account. The method makes changes in the configuration by sweeping the system spins. The algorithm accepts or rejects the new configuration according to some probability based on the Boltzmann statistics. Each iteration of this algorithm is called a Monte Carlo step (MCS). The Metropolis Monte Carlo simulations generate new configurations according to the Boltzmann distribution. We start from different initial conditions and perform 10^6 Monte Carlo steps (MCS) for each spin configuration, discarding the first 10^5 generated ones. We start from different initial configurations, averaging over different initial conditions. We tried several system sizes and checked that the magnetic properties and found beyond a specific system size, the studied parameters are independent on the system sizes. For this reason we give in this work, numerical values for the specific system size LxLxL = 8 × 8 × 8. Our program calculates the following parameters, namely:

The internal energy per site:

$$E_T = \frac{1}{LxLxL} < H > \quad (2)$$

The magnetizations per site:

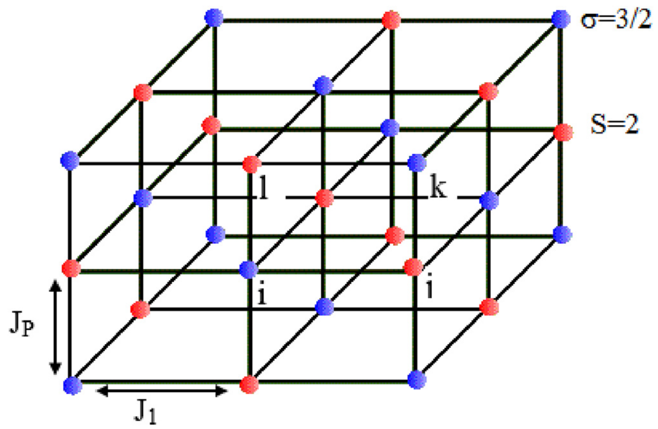

Fig. 1. A sketch of the geometry of the studied system formed with mixed spins with the exchange interacting J_1 and J_P between the spins σ and S respectively in the same plane and different planes.