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Monte Carlo studies of the first order phase transitions on a mixed spin-2 and spin-5/2 system

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ABSTRACT

The first order phase transition of mixed spin-2 and spin-5/2 Ising system in honeycomb lattice with two single ion anisotropies is studied by Monte Carlo (MC) simulation. We have investigated in detail the regime of anisotropies where first order phase transition can occur as the temperature increases. The results show that only when the single ion anisotropies are located around the critical line separating the order and disorder ground states will the first order phase transition arise, which contests the previous studies obtained by mean-field theory (MFT). In addition, interesting magnetic changes around the two critical points of anisotropies are found and all the results are related to the magnetic behavior of a molecular based magnet.

1. Introduction

The enthusiasm and intensive interest to molecular based magnetic endured during the last decade due to its extraordinary properties. For example, its low density, electrical insulation, and low temperature fabrication make it a good candidature to the material manufacturing; the existence of one or several compensation temperature is very useful in electronic, computer technologies, and thermomagnetic recording [1,2]; and a series of novel magnetic properties such as enhanced surface magnetic moment [3], surface magnetic anisotropy [4], and giant magnetoresistance [5] have been found in such materials. Specifically, the celebrated ferrimagnetic material $AM^{II}Fe^{III}(C_2O_4)_3$ ($A=N(n-C_3H_7)_4$, M=Mn, Fe) has attracted intensive attention since first synthesized [6] due to its great properties. As a result, the various aspects regarding mixed spin-2 and spin-5/2 Ising model with single ion anisotropies, which can describe $AM^{II}Fe^{III}(C_2O_4)_3$ effectively, have been intensively studied [7–15] within various theoretical methods.

As far as we know, researchers usually pay more attention to the common second-order phase transition in magnetic material and Ising model, while studies focusing on the first order phase transition are still lacking. In fact, first order phase transition is also important during which many interesting phenomena occur such as the discontinuity in the order parameter, the jump in dynamic and magnetic quantities, and the existence of latent heat. Thus the potential application of first-order magnetic transition in molecular based magnets should be great. Even though first order transition exists in a variety of systems [16,17], the detailed conditions for it to occur have not been clarified.

Moreover, the widely used methods associated with Ising first-order transition are limited to MFT [17] and effective-field theory (EFT) [16], which is not necessarily reliable due to the coarse approximation. Although the MFT and EFT can generally predict the valid magnetic behavior of Ising model (except that the approximation will lead to higher second order phase transition point), we noticed that, in some special case, the EFT or MFT can lead to qualitatively wrong results. For example, in the study of monolayer mixed spin-2 and spin-5/2 honeycomb system with one anisotropy, there is no compensation temperature to be found by MC simulation [10]; however, it was found in large parameter range using the EFT method [11]. In addition, even when the parameter is in the region where the ground state (zero temperature) is paramagnetic, the MFT and EFT can lead to the existence of first order transition. Therefore, MC simulation should be employed to clarify the real situation.

In this paper, we carry out Monte Carlo simulation on a mixed spin-2 and spin-5/2 honeycomb lattice to study the possible first order phase transition in molecular based magnet $AM^{II}Fe^{III}(C_2O_4)_3$. As an orientation and starting point, the mean-field results are also presented for comparison. We start at the ground state diagram and find that first order transition would occur only at a small region above the boundary of ferrimagnetic and paramagnetic phase. Around the critical points at the ground state diagram,

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the magnetization will decrease from ground state to a state that is the mixture of all the states around the points at very low temperature. At the region where the ground state is paramagnetic phase, no phase transition would occur even though the MC simulation will lead to a seemingly reentrant due to finite size effect. The comparison with MFT shows that MFT results are not necessarily reliable and should be re-examined.

This paper is arranged as follows: in Section 2, the model and MC simulations method are described in detail; in Section 3, the first-order phase transitions and some discussion are presented; finally, the conclusions are summarized in Section 4.

2. The honeycomb lattice and Monte Carlo simulation

We consider a mixed spin-5/2 and spin-2 system on a honeycomb lattice. The Hamiltonian reads,

$$H = -J\sum_{i,j} S_i\sigma_j - D_1\sum_i S_i^2 - D_2\sum_j \sigma_j^2 \tag{1}$$

where S and σ stand for the 5/2 spins and the 2 spins, respectively, occupying alternative lattice sites ($S = \pm 5/2, \pm 3/2, \pm 1/2$, $\sigma = \pm 2, \pm 1, 0$). J denotes the exchange interaction between the nearest neighbor spins. D_1 and D_2 are the single ion anisotropy of spin S and spin σ, respectively. According to the structure of $AM^{II}Fe^{III}(C_2O_4)_3$ compound, all the nearest-neighbors of σ (S) are $S(\sigma)$ and the coordination number is $z = 3$ for two dimensional honeycomb lattice.

We employ the standard single-spin-flip Monte Carlo method to simulate the Hamiltonian described by Eq. (1) with $2N^2$ sites, and apply periodic boundary conditions in both of the two directions. Configurations are generated by sweeping through the lattice and making single spin flip attempt. The accept ratio of flip is determined by the metropolis algorithm [18]

$$p = \exp(-\beta\Delta H), \tag{2}$$

where $\beta = 1/k_BT$ and ΔH is the energy variation due to the flip of the spin. Data are collected by using 10,000 Monte Carlo steps after discarding the first 5000 steps during which the system reaches equilibration.

The internal energy per site is calculated according to

$$E = \frac{\langle H\rangle}{2N^2} \tag{3}$$

The sublattice magnetizations m_A and m_B per site are calculated as

$$m_A = \frac{1}{N^2}\left\langle \sum_i S_i \right\rangle, \quad m_B = \frac{1}{N^2}\left\langle \sum_j \sigma_j \right\rangle, \tag{4}$$

The total magnetization per site is then

$$M = \frac{1}{2}(m_A + m_B) \tag{5}$$

and the specific heat is computed by

$$\frac{C}{k_B} = \frac{\beta^2}{2N^2}(\langle H^2\rangle - \langle H\rangle^2) \tag{6}$$

The first-order phase transition in MC will be determined by the maximum of specific heat.

In addition, the MFT method will also be used for the test, with the Gibbs free energy being the criterion for the first order transition [17].

3. Results and discussion

3.1. Ground state phase diagram

Before the MC simulation, we first investigate the ground state phase diagram, where the spin states at zero temperature in the system are determined by minimizing the Hamiltonian. Because the first-order phase transition generally occurs near the critical lines separating different ground states, the ground state phase diagram can provide a basis for our ensuing study.

Due to the competition of the exchange interaction J and the single-ion anisotropy constants D_1 and D_2, the ground state may be the one among $[S,\sigma] = [5/2,-2]$, $[5/2,-1]$, $[5/2,0]$, $[3/2,-2]$, $[3/2,-1]$, $[3/2,0]$, $[1/2,-2]$, $[1/2,-1]$, $[1/2,0]$, where Hamiltonian takes the smallest value. The phase diagram is shown in $D_1/|J|, D_2/|J|$ plane in Fig. 1, where different sections denote different spin configurations. In sections I–VI, the spin S and spin σ are antiparallel with different values, which represent ferrimagnetic phases; in section VII, all σ spins are zero and S spins can be either 5/2 or $-5/2$, representing a paramagnetic phase; section VIII also denotes a paramagnetic phase with spin σ being zero and spin S being $S = \pm 1/2$. The boundary between ferrimagnetic and paramagnetic phases is plotted in the red line shown in Fig. 1. It should be noted here that the first order phase transition can only occur when the parameters $D_1/|J|, D_2/|J|$ are taken near this boundary, which stands for our main finding.

Moreover, there are two special critical points away from the boundary of ferrimagnetic and paramagnetic phases. One point is $(D_1/|J|, D_2/|J|) = (-3, -0.5)$, separating the states $[S,\sigma] = [3/2,-2]$, $[1/2,-2]$ and $[1/2,-1]$. Another point is $(-0.75,-2.5)$, surrounded by states $[5/2,-2]$, $[5/2,-1]$ and $[3/2,-1]$. Because there are three states around the two points, the competing effect may be more intensive. As a result, the statistical behavior near the two specific points will be investigated. As will be seen later, in contrast with all the previous MFT results, MC simulation excludes the first order phase transition near this sort of points.

3.2. Phase transition near the boundary between ferrimagnetic and paramagnetic phases

Now we turn to study the first order phase transition in detail. Since all the previous MFT results show that the first order phase transition occurs when the anisotropies are near the critical points

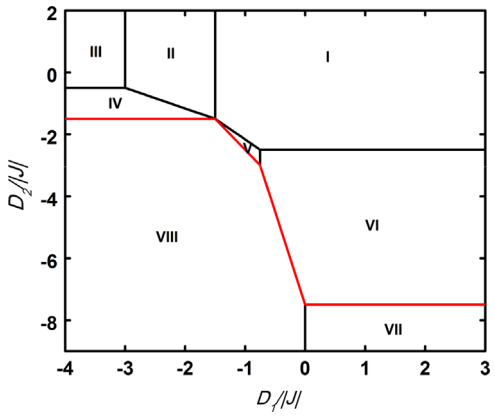

Fig. 1. The ground state phase diagram in the $D_1/|J|, D_2/|J|$ plane, where section I to section VIII stand for states $[5/2,-2]$, $[3/5,-2]$, $[1/2,-2]$, $[1/2,-1]$, $[3/2,-1]$, $[5/2,-1]$, $[\pm 5/2,0]$, $[\pm 1/2,0]$ respectively. Sections I–VI are ferrimagnetic phases, and sections VII and VIII are paramagnetic phases, respectively. The red line is the boundary separating the ferrimagnetic and paramagnetic phases. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)