Effective-field and Monte Carlo studies of mixed spin-2 and spin-1/2 Ising diamond chain*

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The magnetic properties of a mixed spin-2 and spin-1/2 ferromagnetic diamond chain are studied by effective-field theory and Monte Carlo (MC) simulation based on the Ising model. The temperature dependences of magnetization, magnetic susceptibility, internal energy, and specific heat are studied, respectively. The exchange interaction dependences of magnetization and the critical temperature are calculated by MC simulation. The changes of magnetization depending on the field increasing and then the field decreasing under steady-static conditions are also given.

Keywords: Ising diamond chain, effective-field theory, Monte Carlo simulation, magnetic property

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1. Introduction

Ising models are important spin models in statistical physics, and during the past several decades much effort has been devoted to investigating the critical and other statistical properties of various Ising systems,[1–4] which would enable one to understand order–disorder phenomena in statistical physics in depth. The one-dimensional (1D) and two-dimensional (2D) Ising models as well as the high-dimensional Ising models have been well studied.

With the development of the molecule-based magnets, various purely organic molecule-based ferrimagnets have been synthesized.[5] Properties of the diamond-chain have been investigated both theoretically[6–17] and experimentally.[18–23] It is worth mentioning that Rajca *et al.*[24] have designed a polymer with a large density of cross-links and an alternating connectivity of radical modules with unequal spin quantum numbers (S), macrocyclic $S = 2$, and cross-linking $S = 1/2$ modules, which permits large net S values for either ferromagnetic or antiferromagnetic exchange coupling between the modules. The corresponding theoretical problems are less investigated. So in this work, the magnetic properties of an organic diamond chain polymer is studied from a theoretical point of view.

As is well known the effective-field theory (EFT) with correlations allows the complete study of all thermodynamic properties in a uniform and relatively simple way. The method takes into consideration the fluctuation of the effective field and correctly accounts for the correlations at the same site, so it can well reflect the physical essence of the system.[25–27] So, when applied to a one-dimensional diamond-chain, the EFT results will be expected to be comparable to those of the Monte Carlo (MC) simulation method. Thus, in spite of its limitations, the EFT is an adequate starting point for studying this kind of spin system. For explicitness, we use the MC method to validate the magnetization behavior obtained in the EFT. It should be noted that although the results of the MC method are rather reliable, it is always constrained by the speed of the computer.

The remainder of this paper is organized as follows. In Section 2 we present the model and two kinds of theoretical methods of the system, EFT and MC. In the framework of the EFT, the expressions of magnetization, magnetic susceptibility, internal energy, and specific heat of the system are derived. In the MC part, we give out the expressions used during the simulation. The main result and discussion are arranged in Section 3, where the magnetic behavior and phase transition properties are given. Also, the comparisons between the results obtained by these two methods are made in this section. Finally, a brief conclusion is presented in Section 4.

2. Model and methods

The model used in this paper is a mixed spin-2 and spin-1/2 diamond-chain model, which is shown in Fig. 1. The Hamiltonian in the presence of an external field of this system can be described by

$$H = -\sum_{i=1}^{N}\sum_{j=1}^{2}\left(J_1 S_i^A S_{ij}^B + J_1 S_i^A S_{i+1,j}^B\right) - \sum_{i=1}^{N}\left(J_2 S_{i1}^B S_{i2}^B + S_{i1}^B h + S_{i2}^B h + S_i^A h\right), \quad (1)$$

where i represents the site number; the unit cell is composed of three subcells A, B_1, and B_2; J_1 denotes the exchange interaction between A and B; J_2 refers to the exchange interaction

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between B_1 and B_2; S_i^A denotes the z-component spin value of A at site i, which takes the values of ± 2, ± 1, and 0; S_{ij}^B denote the z-component spin value of B, which takes the values of $\pm 1/2$; h is the external field along z axes; the summation is carried out only over the nearest-neighbor pairs. The model under discussion is the Ising model.

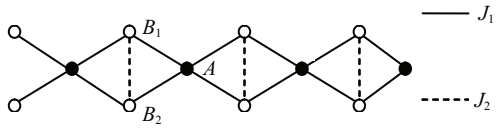


Fig. 1. Spin-2 and spin-1/2 diamond-chain model. Solid dot represents atom A and the hollow one represents atom B. J_1 denotes the exchange interaction between atoms A and B, while J_2 refers to the exchange interaction between atoms B_1 and B_2.

2.1. Effective field analysis

The magnetization is defined as

$$m_A = \langle S_i^A \rangle, \quad m_B = \langle S_i^B \rangle, \tag{2}$$

where the bracket refers to the thermal average. For obtaining the thermal average, the scheme of the EFT proposed by Kaneyoshi[28] and Kaneyoshi *et al.*[29] is used. According to the EFT, for a fixed configuration of neighboring spins, the thermal average of the spin and the square of the spin are given by

$$\langle S_i^A \rangle = \langle f_1(E_i^A + h) \rangle, \tag{3}$$
$$\langle S_i^B \rangle = \langle f_2(E_i^B + h) \rangle, \tag{4}$$
$$\langle (S_i^A)^2 \rangle = \langle g(E_i^A + h) \rangle. \tag{5}$$

The functions $f_1(x)$, $f_2(x)$, and $g(x)$ are expressed as

$$f_1(x) = \frac{2e^{2\beta x} + e^{\beta x} - e^{-\beta x} - 2e^{-2\beta x}}{e^{2\beta x} + e^{\beta x} + e^{-\beta x} + e^{-2\beta x} + 1}, \tag{6}$$
$$f_2(x) = \frac{1}{2}\tanh\left(\frac{1}{2}\beta x\right), \tag{7}$$
$$g(x) = \frac{4e^{2\beta x} + e^{\beta x} + e^{-\beta x} + 4e^{-2\beta x}}{e^{2\beta x} + e^{\beta x} + e^{-\beta x} + e^{-2\beta x} + 1}. \tag{8}$$

Then the average of magnetization could be written as

$$m_A = \left[\cosh\left(\frac{1}{2}J_1\nabla\right) + 2m_B \sinh\left(\frac{1}{2}J_1\nabla\right)\right]^4 \times f_1(x)|_{x=h}, \tag{9}$$
$$m_B = \left[\cosh(\eta_A J_1\nabla) + \frac{m_A}{\eta_A}\sinh(\eta_A J_1\nabla)\right]^2 \times \left[\cosh\left(\frac{1}{2}J_2\nabla\right) + 2m_B \sinh\left(\frac{1}{2}J_2\nabla\right)\right] \times f_2(x)|_{x=h}, \tag{10}$$
$$\eta_A^2 = \langle (S_i^A)^2 \rangle = \left[\cosh\left(\frac{1}{2}J_1\nabla\right) + 2m_B \sinh\left(\frac{1}{2}J_1\nabla\right)\right]^4 \times g(x)|_{x=h}, \tag{11}$$

where $\nabla = \partial/\partial x$ is the differential operator, $\beta = 1/(k_B T)$, η_A in Eq. (10) is used to represent the correlation of spin at the same site.

All the information about the magnetic properties, such as temperature dependence of the magnetization, the exchange interaction dependence of the magnetization, and the critical temperature are contained in Eqs. (9)–(11). Up to now, we have not assigned precise values to the parameters J_1, J_2, and h. In this paper, we set $J_1 > 0$, $J_2 > 0$ for the ferromagnetic system.

In order to calculate the internal energy under the EFT, the Hamiltonian can be written as

$$H_i = -S_i^A E_A - S_i^B E_B. \tag{12}$$

So the internal energy per site could be obtained from

$$U_= - \langle S_i^A E_A \rangle - \langle S_i^B E_B \rangle. \tag{13}$$

The magnetic contribution to the specific heat could be determined from

$$C = \frac{\partial U}{\partial T}. \tag{14}$$

The magnetic susceptibility could be obtained from

$$\chi = \frac{\partial M}{\partial h}. \tag{15}$$

2.2. Monte Carlo simulation

We employ a standard importance sampling method to simulate the system described by the Hamiltonian (1) on a one-dimensional diamond-chain and N is taken to be 10^3. The spin configuration is obtained by randomly sweeping through the chain and making single-spin-flip attempts, which are accepted or rejected according to the Metropolis algorithm. Data are generated with 5×10^3 Monte Carlo steps per site after the first 1.5×10^4 steps per site for equilibration have been discarded.

The magnetization per site is calculated from

$$m_A = \frac{1}{N}\left\langle \sum_{i=1}^{N} S_i^A \right\rangle, \quad m_B = \frac{1}{2N}\left\langle \sum_{i=1}^{N} (S_{i1}^B + S_{i2}^B) \right\rangle. \tag{16}$$

The total magnetization per site $M = (m_A + 2m_B)/3$, and the susceptibility could be obtained from

$$\chi = \beta(\langle S_i^2 \rangle - \langle S_i \rangle^2). \tag{17}$$

The internal energy per site is

$$E = \frac{1}{N}\langle H \rangle. \tag{18}$$

The specific heat per site is

$$C = \frac{\beta^2}{N}(\langle H^2\rangle - \langle H\rangle^2), \tag{19}$$

where $N = 10^3$ and $\beta = 1/(k_B T)$.

The critical temperature is the temperature at which the susceptibility reaches its maximum, and it could be obtained from the simulation.

3. Results and discussion

3.1. Magnetic properties obtained from EFT and MC

Now we give the temperature dependences of magnetization, magnetic susceptibility, internal energy, and specific heat obtained from MC and EFT. Here we set $J_1 = 1.0$, $J_2 = 0.8$, and $h = 0.1$.

The temperature dependence of magnetization is shown in Fig. 2. It is clear that the magnetization decreases from saturate value at zero temperature to zero at infinite temperature, indicating that in the model there exists spontaneous magnetization at low temperature. From Fig. 2 we can see that the magnetizations of atoms A and B, i.e., M_A and M_B decrease from their initial values $M = 2.0$ and $M = 0.5$ at $T = 0.0$ with the increase of temperature, respectively. The results obtained by the EFT are well consistent with those of MC at low temperature, approximately at $T < 1.0$. However, when $T > 1.0$, the situation values become different, the magnetization obtained by the EFT is bigger than that of MC. With temperature further increasing, the results obtained by the two methods become consistent with each other. That means the EFT may induce errors near the critical point.

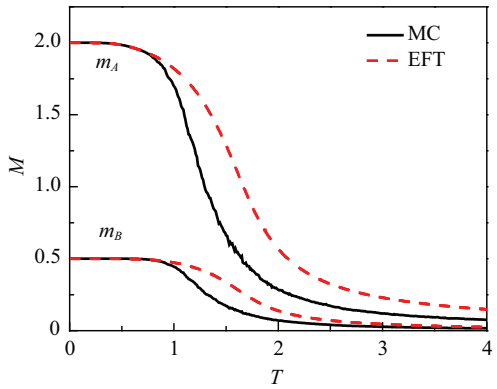


Fig. 2. (color online) Curves of magnetization (M) versus temperature (T) obtained by MC and EFT, respectively. Here we set $J_1 = 1.0$, $J_2 = 0.8$, and $h = 0.1$.

We also calculated the temperature dependence of the magnetic susceptibility. From Fig. 3 we can see that the magnetic susceptibility increases abruptly with the increase of temperature, and reaches its peak at $T = 1.3$ by EFT and $T = 1.9$ by the MC method. With temperature further increasing, the results obtained by EFT are in good agreement with those of MC. It is clear that the maximum of magnetic susceptibility obtained using EFT is smaller than that of MC.

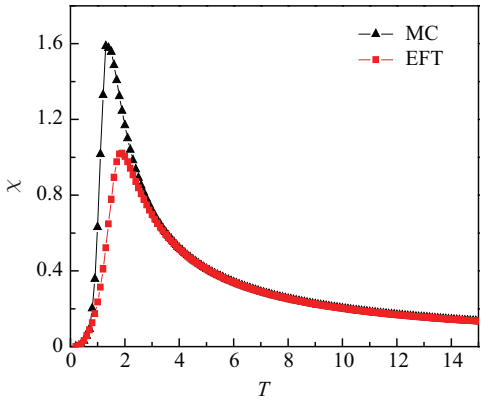


Fig. 3. (color online) Curves of magnetic susceptibility versus temperature obtained by MC and EFT, respectively. Here we set $J_1 = 1.0$, $J_2 = 0.8$, and $h = 0.1$.

The thermodynamic properties are also investigated and given in the following figures. From Fig. 4 we can see that the internal energy keeps its minimum value ($U = -4.5$) at low temperature, and increases abruptly with the increase of temperature when $0.8 < T < 2.1$. With the further increase of temperature, the internal energy increases slowly to its maximum ($U = -0.2$). The result obtained by the EFT is in good agreement with that of MC.

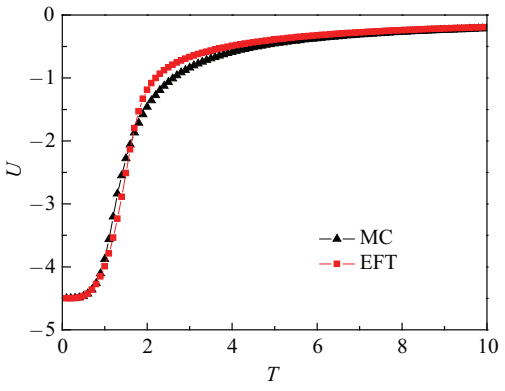


Fig. 4. (color online) Curves of internal energy of the system (U) versus temperature (T) obtained by MC and EFT respectively. Here we set $J_1 = 1.0$, $J_2 = 0.8$, and $h = 0.1$.

The specific heat of the system is also calculated. Figure 5 shows the temperature dependence of the specific heat of the system. We can see that the specific heat increases sharply with the increase of temperature. Two sharp peaks are observed, one is $C = 2.0$ at $T = 1.1$ by MC and the other is $C = 3.5$ at $T = 1.3$ by EFT. The result obtained by EFT is in good agreement with that of MC when $T < 1.1$, but is much bigger than that of MC when $1.1 < T < 2.0$. With the further increase of temperature, the results obtained from the two methods are almost the same.

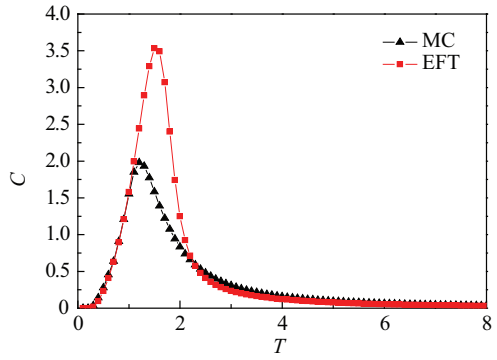


Fig. 5. (color online) Curves of specific heat (C) versus temperature (T) obtained by MC and EFT, respectively. Here we set $J_1 = 1.0$, $J_2 = 0.8$, and $h = 0.1$.

3.2. Effect of exchange interaction on magnetization

Now the exchange interaction dependence of magnetization obtained by MC is given. Here we set $T = 0.5$ and $h = 0.1$. From Fig. 6 we can see that the magnetization increases quickly with interaction J_1 increasing, but increases very slowly with interaction J_2 increasing. It indicates that the interaction between atoms A and B plays an important part in the magnetization of the system, while the effect of the interaction between atoms B_1 and B_2 is inconspicuous. This phenomenon is attributed to the high spin of atom A, which is much bigger than that of atom B. Another reason is that there are two J_1 interactions in one cell in this model.

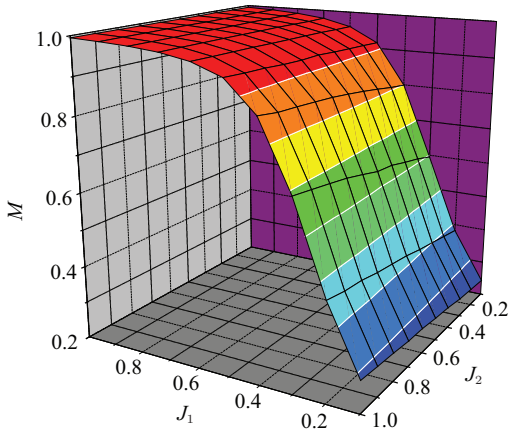


Fig. 6. (color online) Exchange interaction dependence of magnetization obtained by MC. Here $T = 0.5$, $h = 0.1$.

Figure 7 shows the exchange interaction dependence of critical temperature obtained by MC. Here we set $h = 0.1$. From Fig. 7 we can see that the critical temperature almost linearly increases with interaction J_1 increasing, but increases very slowly with interaction J_2 increasing.

3.3. *M*–*h* hysteresis

The magnetic hysteresis of this system is shown in Fig. 8. The measured dependence of magnetization on the field increasing (FI) and then field decreasing (FD) cycle is hysteretic under steady-static conditions. As shown in Fig. 8, no hysteresis is identified at $T = 0.8$ and above. As temperature decreases down to 0.5, a weak hysteresis appears. With T further decreasing the hysteresis becomes more significant and spreads over the whole range. In Fig. 8(a), the exchange interaction between atoms A and B is bigger than that between atoms B_1 and B_2. On the contrary, the exchange interaction between atoms B_1 and B_2 is bigger than that between atoms A and B in Fig. 8(b). It is seen that the evolution of the spin configuration is path-related, the latter state will always keep some characteristics of the earlier state. Different jumping-off points and evolution directions lead to different evolution paths.

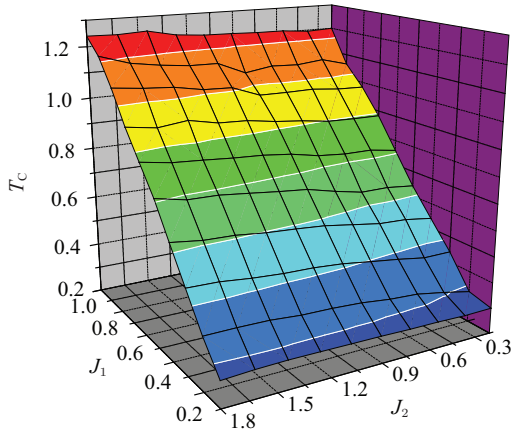


Fig. 7. (color online) Exchange interaction dependence of critical temperature obtained by MC, $h = 0.1$.

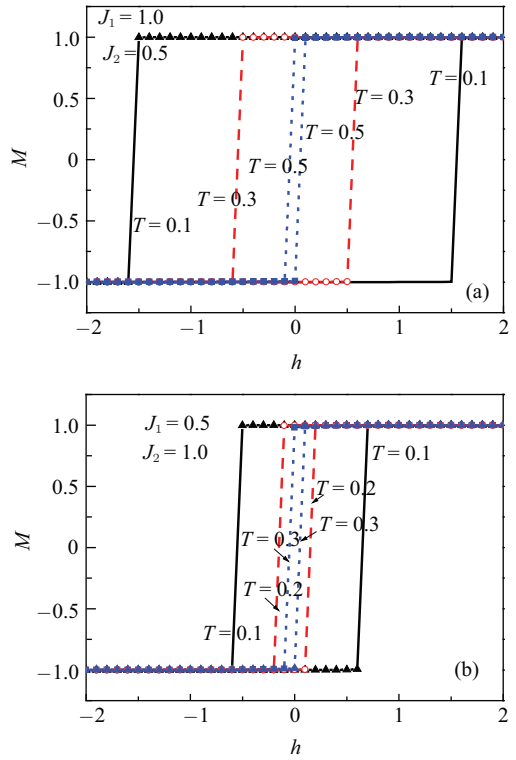


Fig. 8. (color online) The M–h dependence on field increasing (FI) and then field decreasing (FD) cycle under steady-static conditions: (a) the exchange interaction between atoms A and B is bigger than that between atoms B_1 and B_2, (b) the exchange interaction between atoms B_1 and B_2 is bigger than that between atoms A and B.

4. Conclusion

In the framework of the EFT, we studied the magnetic behaviors and phase properties of the mixed spin-2 and spin-1/2 Ising diamond chain. The theoretical expressions of magnetization, internal energy, magnetic susceptibility, and specific heat are obtained. To validate our results, MC simulation is used. From the comparison of the results we find that the two methods are confirmed well in the low temperature and high temperature regions, but have some differences near critical temperature. That means the EFT may induce errors near the critical point.

The interaction between atoms A and B plays an important part in the magnetization of the system, while the effect of the interaction between atoms B_1 and B_2 is inconspicuous. This phenomenon is attributed to the high spin of atom A, which is bigger than that of atom B. Another reason is that there are two J_1 interactions in one cell in this model.

The M–h dependence on the field increasing (FI) and then field decreasing (FD) cycle is observed. No hysteresis is identified at $T = 0.8$ and above. As T decreases down to 0.5, a weak hysteresis appears. With T further decreasing the hysteresis becomes more significant and spreads over the whole range. It is seen that the evolution of the spin configuration is path-related, and the latter state will always keep some characteristics of the earlier state. Different jumping-off points and evolution directions lead to different evolution paths.

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