Monte Carlo Simulations of the Spin-2 Blume-Emery-Griffiths Model

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Abstract. The magnetic properties of the spin $S = 2$ Ising system with the bilinear exchange interaction $J_1 S_i z S_j z$, the biquadratic exchange interaction $J_2 S_i z^2 S_j z^2$ and the single-ion anisotropy $D S_i z^2$ are discussed by making use of the Monte Carlo (MC) simulation for the magnetization $<S_z>$, sublattice magnetizations $<S_z(A)>$ and $<S_z(B)>$, the magnetic specific heat $C_M$ and spin structures. This Ising spin system of $S = 2$ with interactions $J_1$ and $J_2$ and with anisotropy $D$ corresponds to the spin-2 Blume-Emery-Griffiths model. The phase diagram of this Ising spin system on a two-dimensional square lattice has been obtained for exchange parameter $J_2/J_1$ and anisotropy parameter $D/J_1$. The shapes of the temperature dependence of sublattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ are related with abnormal behavior of temperature dependence of $<S_z>$ at low temperatures and affected significantly by the single-ion anisotropy $D$. The staggered quadrupolar (SQ) ordering turns out to be different largely between Ising systems with the single-ion anisotropy ($D \neq 0$) and without the one ($D = 0$).

In Heisenberg and Ising ferromagnets, the existence and the importance of such higher-order exchange interactions as $J_2(S_i \cdot S_j)^2$, $J_3(S_i \cdot S_j)(S_j \cdot S_k)$, $J_4(S_i \cdot S_j)(S_k \cdot S_l)$ are discussed extensively by many investigators [1-3]. Theoretical explanations of the origin of these interactions have been given in the theory of the super exchange interaction, the magnetoelastic effect, the perturbation expansion and the spin-phonon coupling [3].

In solid helium and some other materials showing such phenomena as quadrupolar ordering of molecules (solid hydrogen, liquid crystal) or the cooperative Jahn Teller phase transitions, the higher-order exchange interactions turned out to be the main ones [4]. The Ising system of $S = 1$ with a bilinear interaction $J_1 S_i z S_j z$ and the biquadratic exchange interaction $J_2 S_i z^2 S_j z^2$ and the single-ion anisotropy $DS_i^2$ is quite famous as so-called Blume-Emery-Griffiths (BEG) model [5] and applied for many problems, e.g. super-liquid helium, magnetic material, semiconductor, alloy, lattice gas and so on. This interaction $J_2$ is expected to have significant effects on magnetic properties and spin arrangement in the low-temperature region for the case of $J_2$ not negligible compared to $J_1/S^2$[6].

Therefore, we have developed the Monte Carlo (MC) simulation to the Ising spin system with large spin of $S = 2$, and investigated more precisely the growth of the spin ordering and the ground state (GS) spin structures. In the present study, the effects of the biquadratic interaction $J_2 S_i z^2 S_j z^2$ and the single-ion
anisotropy $D S_z^2$ on the magnetization $<S_z>$, sublattice magnetizations $<S_z(A)>$ and $<S_z(B)>$, the magnetic specific heat $C_M$ of Ising spin system of $S = 2$ on a two-dimensional square lattice are investigated by making use of the MC simulation. The obtained characteristic behaviors of $<S_z>$, $C_M$ are discussed in conjunction with the GS spin structures determined by energy evaluations. The temperature dependences of spin structure are also studied for various values of parameters $J_z/J_1$ and $D/J_1$, and the phase diagram is obtained for these parameters. The spin Hamiltonian for the present Ising spin system with $S = 2$ can be written as follows:

\[ H = -J_1 \sum_{(ij)} S_{ix} S_{jx} - J_2 \sum_{(ij)} S_{iz} S_{jz} - D \sum_i S_{iz}^2 \]

The GS spin structures are determined for the Ising spin system with both interactions $J_1$ and $J_2$ and without anisotropy term ($D = 0$) by comparing the energies of various spin structures with each other (see e.g. [7]). The GS spin structures obtained for the spin system of $S = 2$ with positive interaction $J_1$ and negative interaction $J_2$ are shown in figure 1.

The energies per one spin for the structures $S(a)$ ~ $S(d)$ are given as $E_a = -8J_1 - 32J_2$, $E_b = -4J_1 - 8J_2$, $E_c = -2J_1 - 2J_2$ and $E_d = 0$, respectively. Therefore, by comparing these energies, phase transitions turn out to occur at the conditions of $J_2/J_1 = -1/6$, $-1/3$ and $-1$. Furthermore, the structures $S(a)$ ~ $S(d)$ may be the GS spin structures in the interaction range of $-1/6 < J_2/J_1$, $-1/3 < J_2/J_1 < -1/6$, $-1 < J_2/J_1 < -1/3$, $J_2/J_1 < -1$, respectively.

MC simulations based on the Metropolis method are carried out assuming a periodic boundary condition for a two-dimensional square lattice with linear lattice size $L = 240$. For fixed values of $J_2/J_1$, we start the simulation at high temperatures adopting random initial configurations, and advance gradually this simulation to lower temperature. We use the last spin configuration as an input for the calculation at the next point. Thermal averages of $<S_z>$ are calculated using $2 \times 10^5$ MC steps per spin (MCS/s) after discarding the first $3 \times 10^4$ MCS/s.

The temperature dependences of $<S_z>/S$ and $C_M$ have been calculated for the spin system both with interactions $J_1$ and $J_2$ ($J_1 > 0$ and $J_2 < 0$), and the results of $<S_z>/S$ and $C_M$ for the system of $S = 2$ on the two-dimensional square lattice are shown in figure 2 and (a) in figure 3, respectively. The values of $<S_z>/S$ at $T = 0$ have been turned out to be 1, 0.75, 0.5 and 0 for interaction parameter in the range of —
1/6 < \frac{J_2}{J_1}, \quad -1/3 < \frac{J_2}{J_1} < -1/6, \quad -1 < \frac{J_2}{J_1} < -1/3 \quad \text{and} \quad J_2/J_1 < -1, \quad \text{respectively. These values of} \quad \frac{<S_z>}{S} \quad \text{at} \quad T = 0 \quad \text{are confirmed to correspond to those obtained for the spin structures S(a)~S(d) in figure 1, respectively. Judging from the behaviors at low temperatures, the phase transitions are pointed out to occur at the conditions of} \quad J_2/J_1 = -1/6, \quad -1/3 \quad \text{and} -1. \quad \text{These conditions agree quite well with those obtained by above mentioned energy comparisons. As known from spin structure S(b) in figure 1, the GS spin structure is constructed with two sublattices of} \quad S_z = 2 \quad \text{and} \quad S_z = 1 \quad \text{in the range of} \quad -1/3 < \frac{J_2}{J_1} < -1/6. \quad \text{On the other hand, as seen from (a) in figure 3 the temperature dependence curves of} \quad C_M \quad \text{have two peaks in the same range of} \quad J_2/J_1. \quad \text{These facts may suggest that different abrupt spin orderings occur at two different temperatures. Therefore, let us investigate the temperature dependence of the sublattice magnetization. The calculated results of sublattice magnetizations} \quad <S_z(A)> \quad \text{and} \quad <S_z(B)> \quad (<S_z(A)> \quad \geq \quad <S_z(B)> \quad \text{are shown by (b) in figure 3 for above mentioned interaction range. Here, A and B represent the two interpenetrating sublattices.}

**Figure 3.** The temperature dependence of (a) \( C_M \) and (b) \( \frac{<S_z(A)>}{S} \) and \( \frac{<S_z(B)>}{S} \) of spin system with \( S = 2 \) for both interactions of fixed positive \( J_1 \) and various negative values of \( J_2 \) in the range of \( -1/3 < \frac{J_2}{J_1} < -1/6. \)

The different temperature dependences of \( <S_z(A)> \) and \( <S_z(B)> \) at low temperatures may explain the abnormal behavior of \( \frac{<S_z>}{S} \quad \text{(=} \quad \frac{<S_z(A)> + <S_z(B)>}{2}) \). Next, we investigate the temperature dependences of \( <S_z(A)> \) and \( <S_z(B)> \) of the Ising spin system with anisotropy term \( D \). The results for the Ising systems with \( D/J_1 = 1 \) and 1.5 are shown by (a) and (b) in figure 4. It is worth noting that the temperature at which \( <S_z(A)> \) and \( <S_z(B)> \) begin taking different values becomes higher and close to the Curie

**Figure 4.** The sublattice magnetizations \( \frac{<S_z(A)>}{S} \) and \( \frac{<S_z(B)>}{S} \) of spin system with \( S = 2 \) for (a) \( D/J_1 = 1 \) and (b) \( D/J_1 = 1.5 \).
temperature $T_c$ with increasing anisotropy term $D$. The shapes of the temperature dependence of $<S_z(A)>$ and $<S_z(B)>$ also change largely with increasing anisotropy term $D$. Let us define $T_s$ as the critical temperature at which two sublattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ begin taking different values with decreasing temperature. The ranges of the existence of $T_s$ depend on an anisotropy term $D$ and turn out to be $T_s \leq T_c/4$, $T_s \leq T_c/2$, $T_s \leq T_c$ for $D/J_1 = 0, 1, 1.5$, respectively. Especially, critical temperatures $T_s$ and $T_c$ are confirmed to become the same value under the condition of $-0.60 < J_2/J_1 < -0.55$ and $D/J_1 = 1.5$. Therefore, under this condition, two sublattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ take different values at the whole temperature range of $T \leq T_s$. The characteristic temperature dependences of $<S_z(A)>$ and $<S_z(B)>$ just below $T_s$ have been confirmed to be caused by the movement of each spin ($S_z=\pm 2, \pm 1, 0$) between two sublattices as the number of each spin is almost constant just below and above $T_s$. The sublattice B for large anisotropy $D$ consists of only spins of $S_z = 1$ and 0 just below $T_s$. Therefore, $<S_z(B)> = S$ increases gradually with decreasing temperature until $<S_z(B)> = S$ becomes 0.5 at $T = 0$.

Furthermore, we have investigated the phase diagram of the Ising system of $S = 2$. The phase diagram obtained from the MC simulation is shown in figure 5 for parameters $J_2/J_1 (< 0)$ and $D/J_1 (> 0)$. As can be seen from this figure, the structure S(c) as a GS structure varnishes for the anisotropy term $D$ in the range of $D/J_1 > 0.9$. On the other hand, the ranges of structures S(a), S(b) and S(d) as GS spin structures expand with increasing the anisotropy term $D$.

In the magnetic phase with structure S(d) as a GS spin structure, non-zero magnetization can not appears ($<S_z> = 0$), the values of $<S_z^2(A)>$ and $<S_z^2(B)>$ are, however, pointed out to take non-zero value at low temperature. This spin arrangement is called as staggered quadrupolar (SQ) ordering[5]. It has been confirmed that at sufficiently low temperature, the spin structure for Ising system with anisotropy ($D \neq 0$) can take the SQ state with $<S_z^2(A)> = 1$ and $<S_z^2(B)> = 0$, the one without anisotropy ($D = 0$) can, however, take the SQ state with $0 < <S_z^2(A)> < 1$ and $0 < <S_z^2(B)> < 1$ with decreasing temperature.

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