東海大学紀要産業工学部３（2010年）1頁～10頁
Bull. School of Industrial Engineering Tokai Univ., 3 (2010) pp.1 -10

Monte Carlo Simulation of the Blume-Emery-Griffiths Model with Fractional Large Spin

by
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(Received: October 2010, Accepted: February 2011)

Abstract

The magnetic properties of the spin S = 3/2 and 5/2 Ising systems with the bilinear exchange interaction $J_1S_{iz}S_{jz}$, the biquadratic exchange interaction $J_2S_{iz}^2S_{jz}^2$ and the single-ion anisotropy DS_{iz}^2 are discussed by making use of the Monte Carlo (MC) simulation for the magnetization $<S_z>$, sub-lattice magnetizations $<S_z(\mathrm{A})>$ and $<S_z(\mathrm{B})>$, the magnetic specific heat C_M and spin structures. These Ising spin systems of S = 3/2 and 5/2 with interactions J_1 and J_2 and with anisotropy D may correspond to the Blume-Emery-Griffiths model [1] with fractional large spin. The phase diagram of these Ising spin systems on two-dimensional square lattice have been obtained for exchange parameter J_2/J_1 and anisotropy parameter D/J_1. The temperature dependence of sub-lattice magnetizations $<S_z(\mathrm{A})>$ and $<S_z(\mathrm{B})>$ are investigated for various values of the anisotropy D. The relations between the Curie temperature T_c and the critical temperature T_s which sub-lattice magnetizations begin taking different values are also studied.

Keywords: Ising model; Blume-Emery-Griffiths model; Monte Carlo simulation

1. Introduction

In Heisenberg and Ising ferromagnets, the existence and the importance of such higher-order exchange interactions as the biquadratic exchange interaction $J_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2$, the three-site four-spin interaction $J_3(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)(\boldsymbol{S}_j \cdot \boldsymbol{S}_k)$, the four-site four-spin interaction $J_4(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)$ have been discussed extensively by many investigators [1-4]. 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 [4].

It was pointed out that the higher-order exchange interactions are smaller than the bilinear ones for the *3d* group ions [4], and comparable with the bilinear ones in the rare-earth compounds [5,6]. On the other hand, 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 [7]. Furthermore, the four-site four-spin interaction has been pointed out to be important to explain the magnetic properties of the solid helium [8,9] and the magnetic materials such as NiS_2 and C_6Eu [10].

The Ising system of S=1 with the bilinear exchange interaction $J_1S_{iz}S_{jz}$ and the biquadratic exchange interaction $J_2S_{iz}^2S_{jz}^2$ and the single-ion anisotropy DS_{iz}^2 is quite famous as so-called Blume-Emery-Griffiths (BEG) model [1] 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 arrangements in the low-temperature region for the case of J_2 not negligible compared to J_1/S^2[11]. Recently present authors investigated the effects of the three-site and the four-site four-spin interactions on magnetic properties and the GS spin structure of the Ising ferromagnet [12,13] with S=1 by making use of the Monte Carlo (MC) -simulation. Furthermore, we have applied this MC simulation to the Ising spin

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system of large spin S = 2 with interaction J_2, and investigated more precisely the growth of spin ordering and the ground state (GS) spin structures [14].

In the present study, we have developed this Monte Carlo (MC) simulation to the Ising spin systems with fractional large spin such as S = 3/2 and 5/2, and investigated more precisely the growth of spin ordering and the ground state (GS) spin structures. The effects of the biquadratic interaction $J_2S_{iz}^2S_{jz}^2$ and the single-ion anisotropy DS_{iz}^2 on the magnetization $<S_z>$, sub-lattice magnetizations $<S_z(A)>$ and $<S_z(B)>$, the magnetic specific heat C_M of Ising spin systems of S = 3/2 and 5/2 on two-dimensional square lattice are investigated by making use of the MC simulation. Here, A and B represent two interpenetrating sub-lattices. 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 sub-lattice magnetizations $<S_z(A)>$, $<S_z(B)>$ and spin structure are also studied for various values of parameters J_2/J_1 and D/J_1, and the phase diagram is obtained for these parameters.

In Section 2, the spin Hamiltonian is given for present Ising system with S=3/2 and 5/2. The method of the MC simulation is explained briefly. Furthermore, the conditions of phase transition of the Ising spin system with interactions J_1, J_2 and without anisotropy D are obtained for T=0 from the comparison of energies per one spin. In Section 3, the magnetic properties such as $<S_z>$, $<S_z(A)>$ and $<S_z(B)>$, C_M are investigated for the Ising spin system with S=5/2. In the latter part of this section, the interaction J_2 dependence of the Curie temperature T_c and the critical temperature T_s which the sub-lattice magnetizations begin taking different values are studied for various values of D. The phase diagram is obtained for exchange parameter J_2/J_1 and anisotropy parameter D/J_1. In the section 4, this calculation of the MC simulation is applied to the Ising system with S=3/2, and the interaction J_2 dependence of T_c and T_s and the phase diagram are determined. In the last Section 5, new interesting results obtained here are summarized.

2. Spin Hamiltonian, Methods of Simulation and Energy of Spin System

The spin Hamiltonian for the present Ising spin systems with S = 3/2 and 5/2 on two-dimensional square lattice can be written as follows:

$$H = -J_1 \sum_{<ij>} S_{iz} S_{jz} - J_2 \sum_{<ij>} S^2{}_{iz} S^2{}_{jz} - D \sum_{i} S^2{}_{iz} \tag{1}$$

Here, $<ij>$ denotes the sum on the nearest neighboring spin pairs of two-dimensional square lattice. Furthermore, S_z in above expression represents S_z = ±3/2, ±1/2 for S=3/2 and S_z = ±5/2, ±3/2, ±1/2 for S=5/2. From a consideration of the Hamiltonian (1), magnetic properties and spin arrangements of the Ising spin systems of S=3/2 and 5/2 on two-dimensional square lattice are calculated by the MC simulation.

The MC simulations based on the Metropolis method are carried out assuming periodic boundary condition for two-dimensional square lattice with linear lattice size up to L=240. For fixed values of various parameters J_1, J_2 and D, we start the simulation at high temperatures adopting a random, a ferromagnetic, and an antiferromagnetic initial configurations, respectively, and gradually advance this simulation to lower temperature. We use the last spin configuration as an input for the calculation at the next point. The magnetization $<S_z>$, the sub-lattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ and the magnetic specific heat C_M estimated from the energy fluctuation are calculated using 2×10^5 MC steps per spin (MCS/s) after discarding first 3×10^5 MCS/s. In order to check the reliability of these obtained average values, the thermal averages are also calculated separately for each interval of 0.5×10^5 MCS/s in the above mentioned total interval of 2×10^5 MCS/s. In the following section, results in the largest system of L=240 are given without showing error bars which were found to be negligibly small in our calculation at all temperature range.

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. [15]). The GS spin structures with low energy obtained for the spin systems of S = 5/2 and 3/2 with positive interaction J_1 and negative interaction J_2 are shown in Fig. 1.

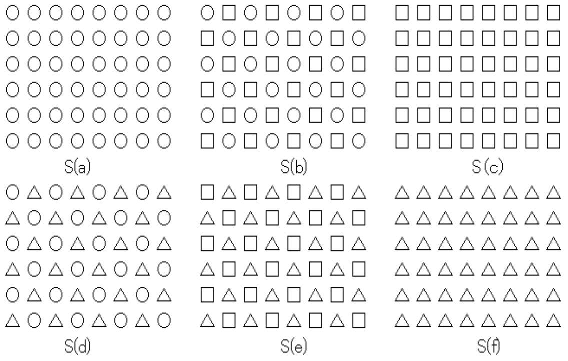


Fig. 1 The GS spin structures S(a), S(b), S(c), S(d), S(e) and S(f) of the Ising spin systems with S=5/2 and S=3/2 (D= 0). Circle, square and triangle denote S_Z =5/2, S_Z =3/2 and S_Z =1/2, respectively.

Let us define the parameter x as J_2/J_1. The energies per one spin for the spin structures S(a)～S(f) of the Ising spin system with S=5/2 are given as $E_a(5/2)=-25/2-625x/8$, $E_b(5/2)=-15/2-225x/8$, $E_c(5/2)=-9/2-81x/8$, $E_d(5/2)=-5/2-25x/8$, $E_e(5/2)=-3/2-9x/8$ and $E_f(5/2)=-1/2-x/8$, respectively. On the other hand, the energies per one spin for the spin structures S(c), S(e), S(f) of the Ising spin system with S=3/2 are given as $E_c(3/2)=-9/2-81x/8$, $E_e(3/2)=-3/2-9x/8$ and $E_f(3/2)=-1/2-x/8$, respectively.

Therefore, by comparing these energies as $E_a(5/2)$ and $E_b(5/2)$, $E_b(5/2)$ and $E_c(5/2)$, $E_c(5/2)$ and $E_d(5/2)$, $E_d(5/2)$ and $E_e(5/2)$, $E_e(5/2)$ and $E_f(5/2)$, phase transitions for the Ising spin system with S=5/2 turn out to occur at the conditions of x (J_2/J_1) = -1/10, -1/6,-2/7,-1/2 and -1. Furthermore, by comparing these energies as $E_c(3/2)$ and $E_e(3/2)$, $E_e(3/2)$ and $E_f(3/2)$, phase transitions for the Ising spin system with S=3/2 turn out to occur at the conditions of $x(J_2/J_1)$ =-1/3 and -1. Therefore, the structures S(a)～S(f) may be the GS spin structures for S=5/2 in the interaction range of $-1/10 < J_2/J_1$, $-1/6 < J_2/J_1 < -1/10$, $-2/7 < J_2/J_1 < -1/6$, $-1/2 < J_2/J_1 < -2/7$, $-1 < J_2/J_1 < -1/2$, $J_2/J_1 < -1$, respectively. The structures S(c), S(e), S(f) may be the GS spin structures for S=3/2 in the interaction range of $-1/3 < J_2/J_1$, $-1 < J_2/J_1 < -1/3$, $J_2/J_1 < -1$, respectively.

3. Results of Simulation and Discussion for Ising Spin System with S=5/2

3.1 Magnetic Properties such as $\langle S_z\rangle$, C_M, $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$

The temperature dependences of the magnetization $\langle S_z\rangle$ and the specific heat C_M have been calculated for the spin system with both interactions J_1 and J_2 (J_1>0 and J_2<0) by the MC simulation, and the results of $\langle S_z\rangle/S$ and C_M for the system of S= 5/2 on two-dimensional square lattice without anisotropy D (D=0) are shown in Fig.2 and in Fig.3, respectively. The values of $\langle S_z\rangle/S$ at T = 0 have been turned out to be 1, 0.8, 0.6, 0.4 and 0.2 for interaction parameter in the range of $-1/10 < J_2/J_1$, $-1/6 < J_2/J_1 < -1/10$, $-1/2 < J_2/J_1 < -1/6$, $-1 < J_2/J_1 < -1/2$, and $J_2/J_1 < -1$, respectively. These values of $\langle S_z\rangle/S$ at T = 0 are confirmed to correspond to those obtained for the spin structures S(a)～S(f) in Fig.1, respectively. At T = 0, the value of $\langle S_z\rangle/S$ for S(c) is 0.6 and equals to the one for S(d). From further calculations for the spin structure by the MC simulation, however, the spin structure at T = 0 is also confirmed to change from S(c) to S(d) at the condition of J_2/J_1 = -2/7. Judging from these facts, the phase transitions are pointed out to occur at the conditions of J_2/J_1 = -1/10, -1/6, -2/7, -1/2 and -1. These conditions agree quite well with those obtained by above mentioned energy comparisons.

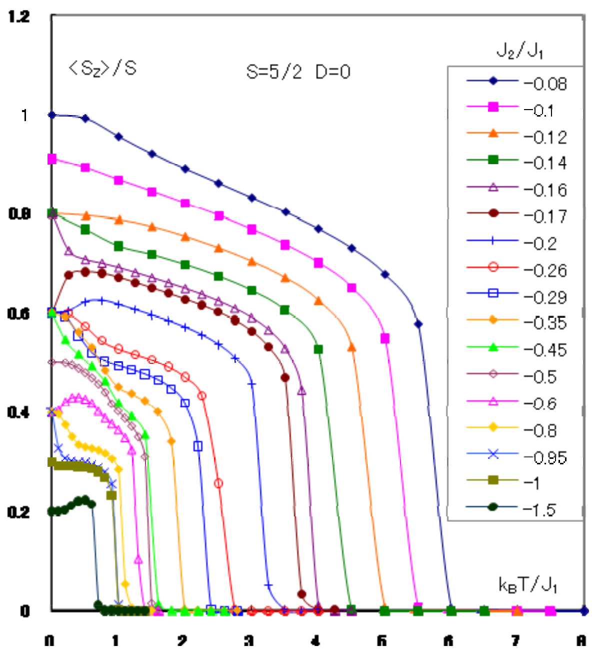


Fig.2 The temperature dependence of the magnetization $\langle S_z\rangle/S$ of Ising spin system with S=5/2 for various negative values of interaction J_2 (D=0).

As known from Fig.1, the GS spin structure S(b), S(d) and S(e) are constructed with two sub-lattices of S_z =5/2 and 3/2, S_z =5/2 and 1/2, S_z

=3/2 and 1/2, respectively. On the other hand, as can seen from Fig.3, the temperature dependence curves of C_M have two peaks in the range of J_2/J_1 in which structures S(b), S(d) and S(e) exist as the GS spin structure.

These facts may suggest that different abrupt spin orderings occur at two different temperatures. Therefore, let us investigate the temperature dependence of the sub-lattice magnetizations. The calculated results of sub-lattice magnetizations $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$ for Ising system without anisotropy term D (D=0) are shown by (a) in Fig.4. Here, (A) and (B) represent two interpenetrating sub-lattices, and $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$ are defined as $\langle S_z(A)\rangle \geqq \langle S_z(B)\rangle$.

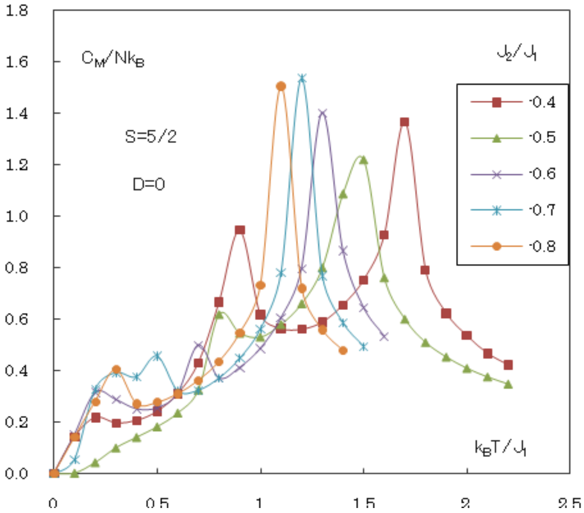
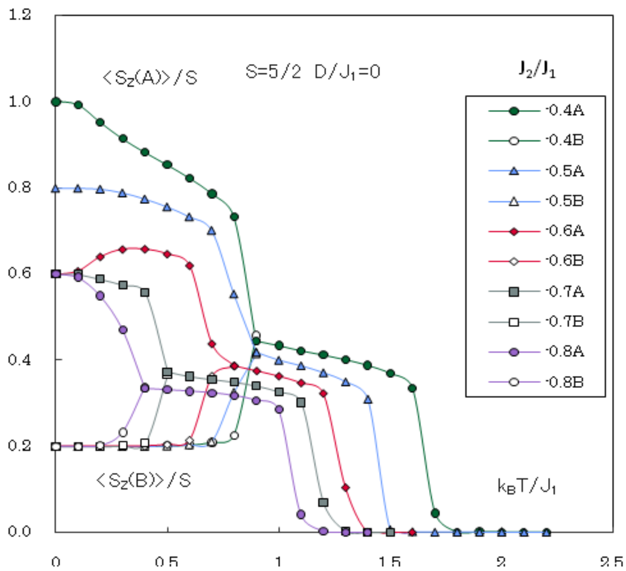


Fig. 3 The temperature dependence of magnetic specific heat C_M of Ising spin system with S=5/2 for various negative values of interaction J_2 (D=0).

As can be seen from (a) in Fig.4, the different temperature dependences of $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$ at low temperatures may explain the abnormal behavior of total magnetization $\langle S_z\rangle$ (= ($\langle S_z(A)\rangle$ + $\langle S_z(B)\rangle$) /2). It is remarkable that the sub-lattice magnetization $\langle S_z(A)\rangle$ for J_2/J_1 = -0.6 shows interesting behavior of inverse temperature dependence at low temperatures with decreasing temperature. This behavior may cause by the disappearance of spin S_z =5/2 which is mixed at high temperatures in the range of $T<T_s$ with decreasing temperature. The temperature dependence of the spin structure mixed with S_z =5/2 on the sub-lattice (A) is shown in Fig.5 for the Ising spin system with J_2/J_1=-0.6 (D=0) at various temperatures of T=1.4J_1/k_B, T=0.9J_1/k_B, T= 0.5J_1/k_B and T= 0.1J_1/k_B.

Next, we investigate the temperature dependences of $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$ of the Ising spin system with anisotropy term D. The results for the Ising systems with D/J_1 = 0.5 and 1 are shown by (b) and (c) in Fig.4, respectively. Let us define T_s as the critical temperature at which two sub-lattice magnetizations $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$ begin taking different values with decreasing temperature. It is worth noting that the critical temperature T_s becomes higher and close to the Curie temperature T_c with increasing anisotropy term D. The shapes of the temperature dependence curves of $\langle S_z(A)\rangle$ and $\langle S_z(B)\rangle$ also change largely with increasing anisotropy term D.

It should be noted from (b) and (c) in Fig.4 that at the condition of J_2/J_1 =-0.6 and D/J_1 =0.5, and at the condition of J_2/J_1 =-0.8 and D/J_1 =1, the sub-lattice magnetization $\langle S_z(A)\rangle$ takes different value from $\langle S_z(B)\rangle$ in whole temperature range of $T< T_c$. Therefore, in these conditions of J_2 and D, T_s turns out to be equal to T_c. Furthermore, the temperature dependence of $\langle S_z(B)\rangle$ for system with J_2/J_1 = -0.2 and D/J_1 =1, and $\langle S_z(A)\rangle$ for system with J_2/J_1 = -1.6 and D/J_1 =1 show interesting behaviors at the low temperatures of $T< T_s$. These behaviors of $\langle S_z(B)\rangle$ and $\langle S_z(A)\rangle$ may caused by the disappearance of spin S_z =1/2 on $\langle S_z(B)\rangle$ and spin S_z =5/2 on $\langle S_z(A)\rangle$ which is mixed at high temperatures in the range of $T<T_s$ with decreasing temperature. The temperature dependence of the



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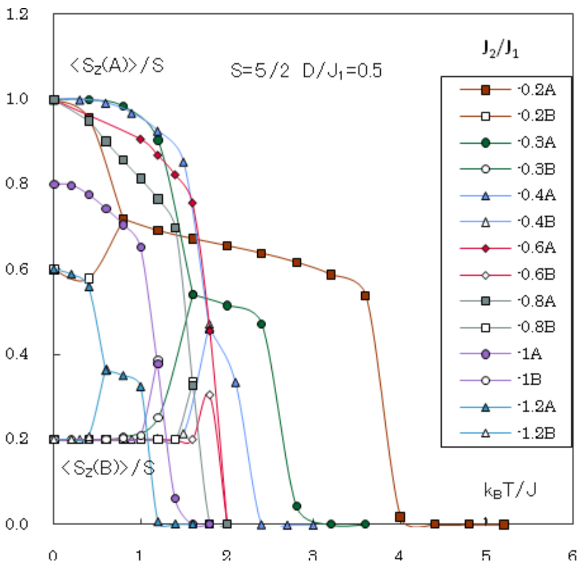

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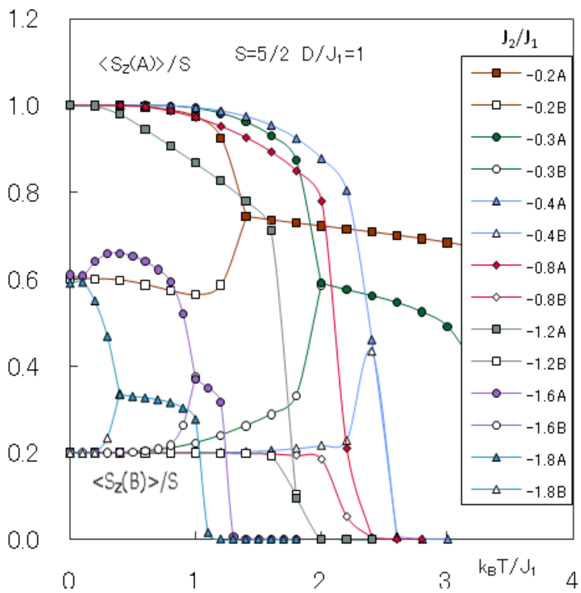
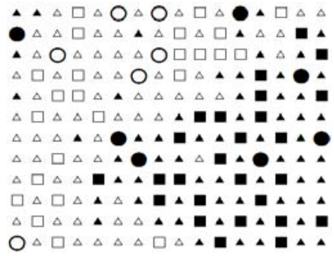


(c)

Fig. 4 The temperature dependence of the sub-lattice magnetizations $<S_z(A)>/S$ and $<S_z(B)>/S$ of Ising spin system of S=5/2 with various negative values of interaction J_2 for (a) D/J_1=0, (b) D/J_1=0.5, (c) D/J_1=1.

spin structure mixed with S_z =1/2 on sub-lattice (B) for Ising spin system with J_2/J_1 = -0.2 and D/J_1 =1 is shown in Fig.6 at the temperatures of T= 5.0J_1/k_B, T=1.6J_1/k_B, T=1.0J_1/k_B and T= 0.2J_1/k_B.



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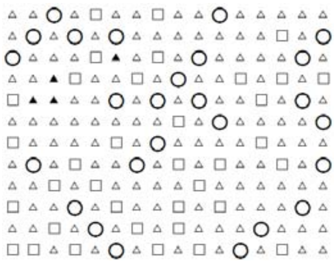

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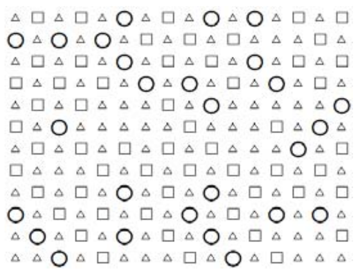

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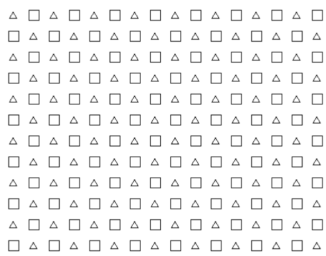
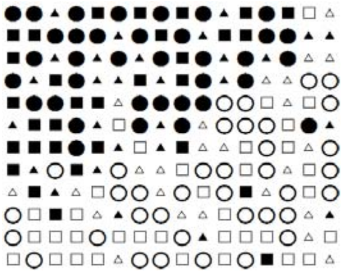


(d)

Fig. 5 The temperature dependence of the spin structure of Ising spin system of S=5/2 with J_2/J_1 =-0.6 and D/J_1 =0 (a) for T=1.4J_1/k_B, (b) for T=0.9J_1/k_B, (c) for T=0.5J_1/k_B, (d) for T=0.1J_1/k_B. Open and closed circle, open and closed square and open and closed triangle denote S_Z=5/2 and -5/2, S_Z=3/2 and -3/2 and S_Z =1/2 and -1/2, respectively.



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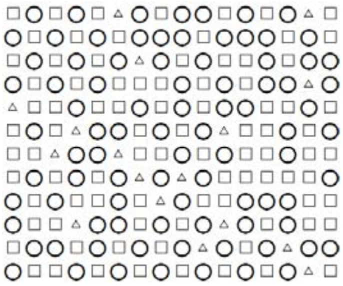

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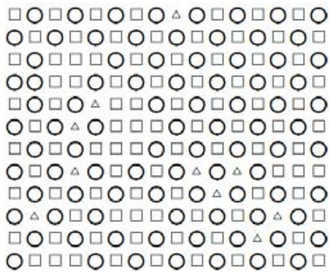

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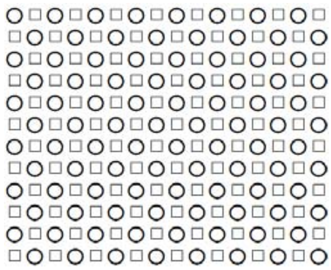
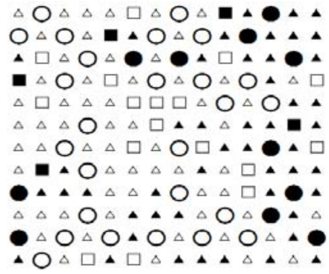


(d)

Fig. 6 The temperature dependence of the spin structure of Ising spin system of *S*=5/2 with J_2/J_1 =-0.2 and D/J_1 =1 (a) for T=5.0J_1/k_B, (b) for T=1.6J_1/k_B, (c) for T=1.0J_1/k_B, (d) for T=0.2J_1/k_B. Open and closed circle, open and closed square and open and closed triangle denote S_Z=5/2 and -5/2, S_Z=3/2 and -3/2 and S_Z =1/2and -1/2, respectively.



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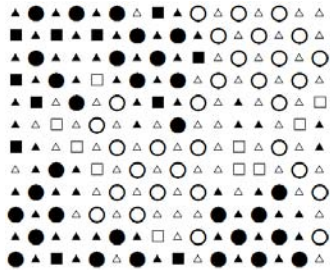

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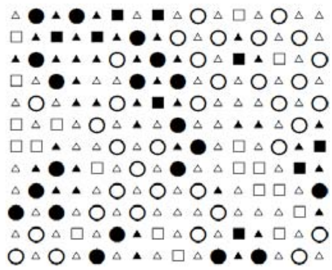

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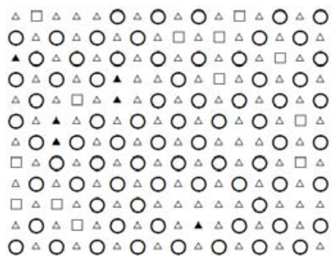

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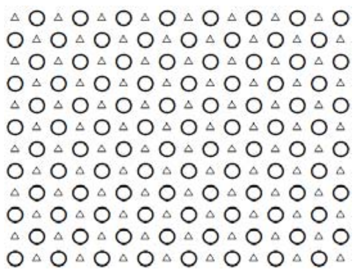


(e)

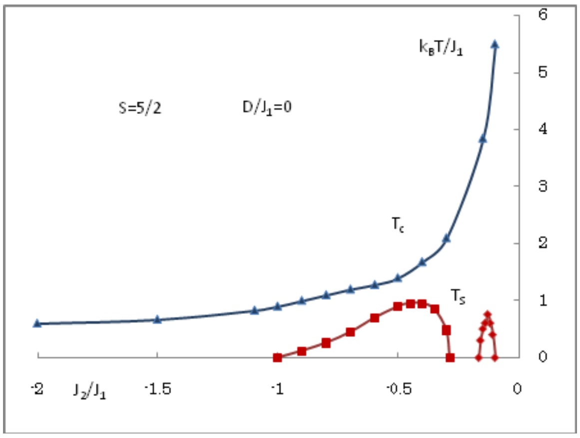
Fig.7 The temperature dependence of the spin structure of Ising spin system of *S*=5/2 with J_2/J_1 =-0.8 and D/J_1 =1 (a)

for T=2.6J_1/k_B, (b) for T=2.4J_1/k_B, (c) for T=2.2J_1/k_B, (d) for T=2.0J_1/k_B, (e) for T=0.4J_1/k_B. Open and closed circle, open and closed square and open and closed triangle denote S_Z=5/2 and -5/2, S_Z=3/2 and -3/2 and S_Z =1/2and -1/2, respectively.

The temperature dependence of the spin structure for system with J_2/J_1 = -0.8 and D/J_1 =1 is shown in Fig.7 for the temperatures of T=2.6$J_1/k_{B,}$ T=2.4$J_1/k_{B,}$ T=2.2J_1/k_B and T= 2.0J_1 /k_B T=0.4J_1/k_B. As can be seen from (b) in Fig.7, two sub-lattices appear at T_c(=2.4J_1/k_B)

3.2 Critical Temperatures T_c and T_s, and Phase Diagram

Next, let us investigate the relation between critical temperatures T_s and T_c. The interaction parameter J_2/J_1-dependences of T_s and T_c are calculated for various values of D and the results for D/J_1=0, 0.5 and 1 are shown by (a), (b) and (c) in Fig.8, respectively. The ranges of the existence of T_s turn out to depend on an anisotropy term D, and expand more widely with increasing D. The two ranges of T_s which correspond to the systems with S_z=5/2 and 3/2, and with S_z=5/2 and 1/2 as the GS spin structure combine under the condition of 0.5 ≦ D/J_1. Furthermore, the value of T_s turns out to coincide with T_c under the condition of -0.7≦ J_2/J_1≦-0.5 for D/J_1 =0.5 and -1.4 ≦J_2/J_1≦-0.4 for D/J_1 =1. Therefore, it is remarkable that under these conditions, two sub-lattice magnetizations <S_z(A)> and <S_z(B)> take different values at the whole temperature range of $T \leqq T_c$.



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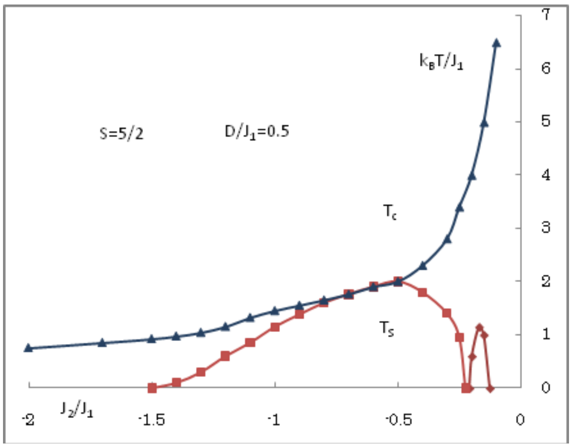
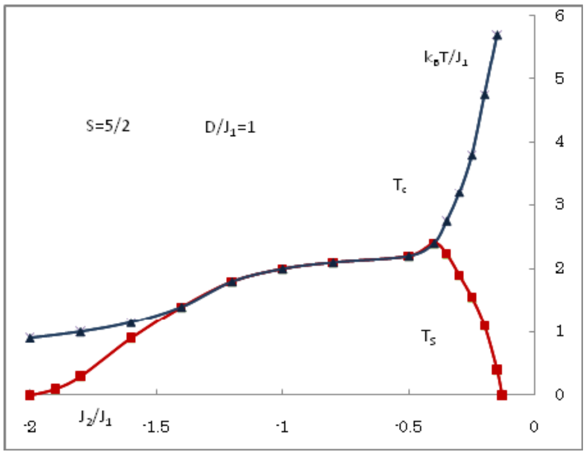


(b)



(c)

Fig.8 The dependence of the Curie temperature T_c and the critical temperature T_s on interaction parameter J_2/J_1 for (a) D/J_1=0, (b) D/J_1=0.5, (c) D/J_1=1, respectively.

Furthermore, we have investigated the phase diagram of the Ising system of S = 5/2. The phase diagram obtained from the MC simulation is shown in Fig.9 for negative interaction parameter (J_2/J_1 < 0) and single-ion anisotropy D/J_1 (-0.5 ≦ D/J_1≦ 1.0). As can be seen from this figure, the spin structure S(c) with S_z=3/2 and 3/2 as a GS structure varnishes for the anisotropy term D in the range of 0.55≦D/J_1. On the other hand, it should be noticed that the range of the spin structure S(d) with S_z=5/2 and 1/2 as a GS structure expands with increasing the anisotropy term D, and this spin structure S(d) as a GS structure varnishes for the anisotropy term D in the range of D/J_1≦-0.2. The ranges of the GS spin structures S(a) with S_z=5/2 and 5/2, the GS spin structure S(b) with S_z=5/2 and 3/2 and the GS spin structure S(e) with S_z=3/2 and 1/2 don't show any significant changes for parameter D.

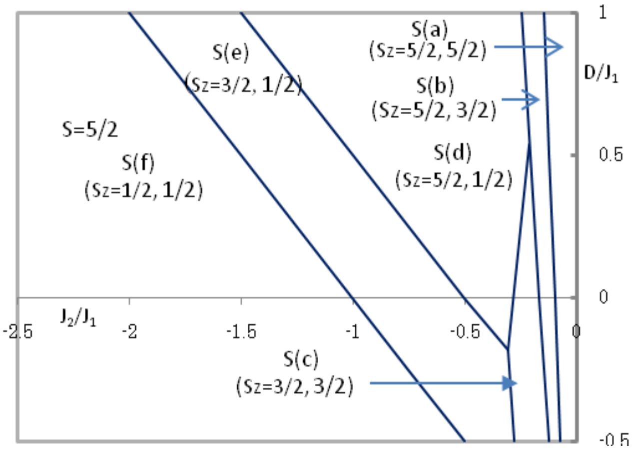


Fig. 9 Phase diagram of Ising spin system with S=5/2 for parameters J_2/J_1 and D/J_1.

4. Results of Simulation and Discussion for Ising Spin System with S=3/2

Next, let us investigate the temperature dependence of the magnetization $<S_z>$, sub-lattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ of the Ising spin system of S=3/2 with and without anisotropy D. The calculated results of magnetization $<S_z>$ for the spin system without D (D=0) are shown in Fig.10.

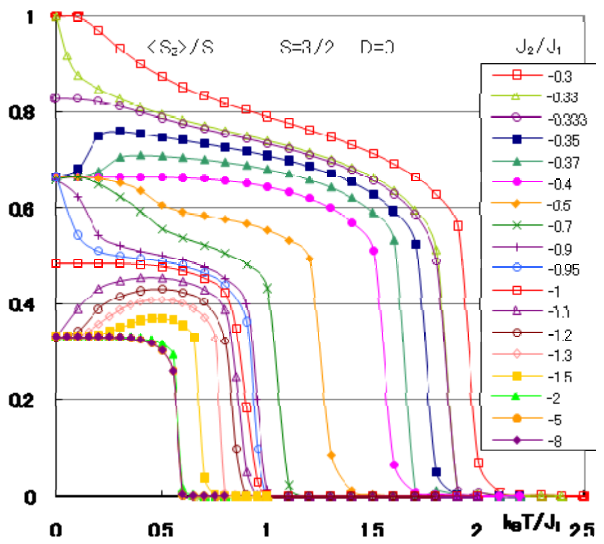
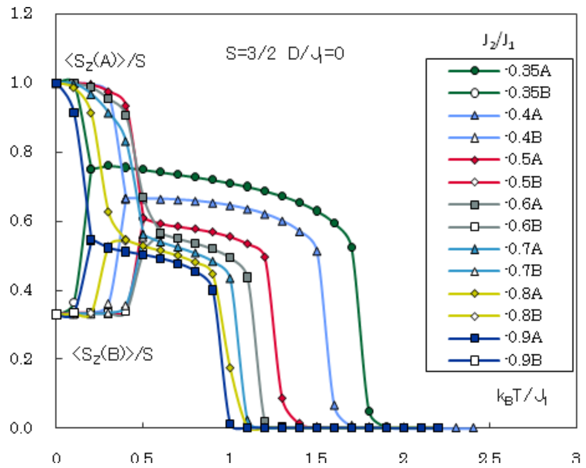
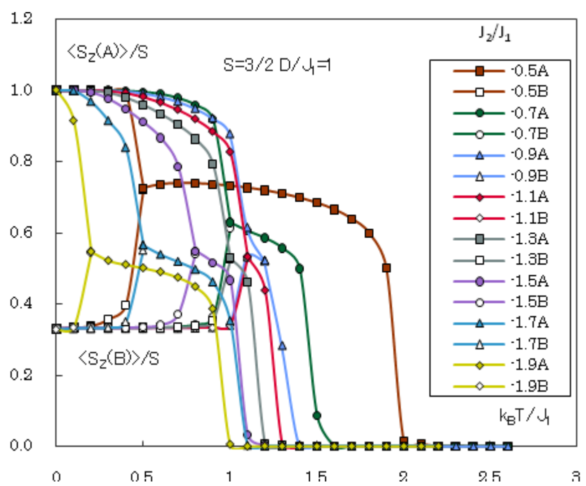


Fig.10 The temperature dependence of the magnetization $<S_z>/S$ of Ising spin system with S=3/2 for various negative values of interaction J_2 (D=0).

The values of $<S_z>$ at T=0 may suggest that the change of the GS spin structure occur under the condition of J_2/J_1 = -1/3 and -1. Furthermore, the value of $<S_z>/S$ at T=0 turns out to be 2/3 in the range of -1< J_2/J_1< -1/3 which corresponds to the GS spin structure S(e) with S_z= 3/2 and 1/2. From the present MC simulation, the GS spin structures are also confirmed to be S(c), S(e) and S(f) in the interaction range of -1/3< J_2/J_1, -1<J_2/J_1 < -1/3 , J_2/J_1 < -1, respectively. These results agree well with those obtained from energy evaluation.



(a)



(b)

Fig. 11 The temperature dependence of the sub-lattice magnetizations $<S_z(A)>/S$ and $<S_z(B)>/S$ of Ising spin system of S=3/2 with various negative values of J_2 for (a) D=0 and (b) D/J_1=1.

The temperature dependence of sub-lattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ of the Ising spin system with S=3/2 are shown by (a) for D =0 and by (b) for D/J_1 =1 in Fig.11. The critical temperature T_s of this spin system turns out to be smaller than the Curie temperature T_c even by introducing anisotropy D in the range of $0 \leqq D/J_1 \leqq 1.0$. The temperature dependences of $<S_z(A)>/S$ and $<S_z(B)>/S$ show normal behaviors at low temperatures of $T<T_c$.

The interaction parameter J_2/J_1-dependences of T_s and T_c are calculated for various values of D and the results for $D/J_1=0$ and 1 are shown by (a) and (b) in Fig.12, respectively. It is confirmed that the value of T_s cannot become equal to T_c even under any condition of J_2/J_1 in the range of $0 \leqq D/J_1 \leqq 1.0$. Therefore, we may conclude that the effect of D is small in this spin system with smaller spin as S=3/2.

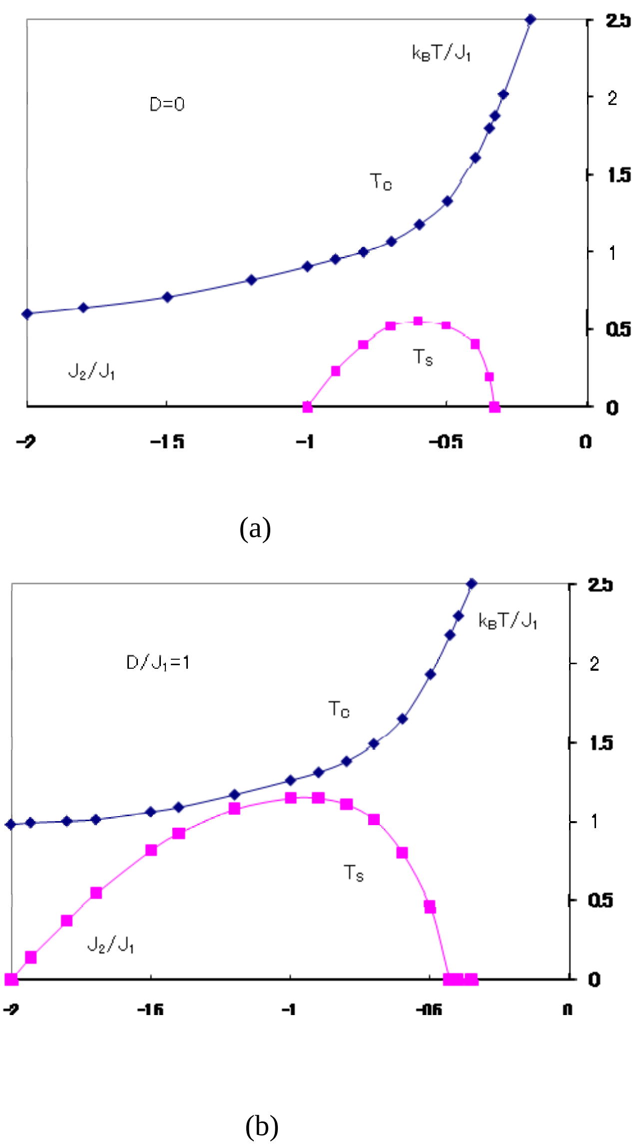


Fig. 12 The dependence of the Curie temperature T_c and the critical temperature T_s on interaction parameter J_2/J_1 for (a) D/J_1=0, (b) D/J_1=1, respectively.

Furthermore, we have investigated the phase diagram of the Ising system of S= 3/2. The phase diagram obtained from the MC simulation is shown in Fig.13 for negative interaction parameter J_2/J_1 in the range of $-2.0 \leqq J_2/J_1 \leqq 0$ and single-ion anisotropy D/J_1 in the range of $-0.5 \leqq D/J_1 \leqq 1.0$.

The range of the GS spin structure S(e) with S_z=3/2 and 1/2 expands with increasing the anisotropy term D. On the other hand, the range of spin structure S(f) with S_z=1/2 and 1/2 reduces with increasing D. It can be said that the anisotropy term D doesn't give any significant effects on the range of the GS spin structures of Ising spin system with small spin like S=3/2.

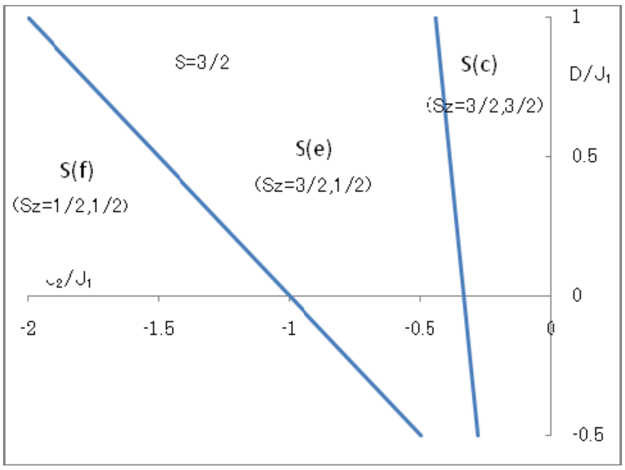


Fig. 13 Phase diagram of Ising spin system with S=3/2 for parameters J_2/J_1 and D/J_1.

5. Concluding Remarks

In the previous section, for the Ising spin systems of S=5/2 and 3/2 with the bilinear exchange interaction $J_1S_{iz}S_{jz}$, the biquadratic exchange interaction $J_2S_{iz}^2S_{jz}^2$ and the single-ion anisotropy D, the magnetization $<S_z>$, sub-lattice magnetizations $<S_z(A)>$ and $<S_z(B)>$, the specific heat C_M, the GS spin structures and phase diagram have been calculated by making use of the MC simulation.

Summarizing the present results on two-dimensional square lattice, we may conclude as follows:

(1) The conditions of the phase transition at T=0 have been obtained for Ising spin systems with S=5/2 and 3/2. The magnetic phase transitions

occur at J_2/J_1 = -1/10, -1/6, -2/7, -1/2, -1 for S=5/2 and J_2/J_1 = -1/3 and -1 for S=3/2. These conditions by the MC simulation are also confirmed by comparison with those obtained from energy evaluation.

(2) The abnormal behaviors of $<S_z>$ at low temperatures for spin systems with S=5/2 and 3/2 may explained by behaviors of $<S_z(A)>$ and $<S_z(B)>$. The temperature dependences of the sub-lattice magnetization shows interesting behaviors especially for $<S_z(A)>$ with J_2/J_1 = -0.6 and D/J_1=0, for $<S_z(A)>$ with J_2/J_1 = -1.6 and D/J_1=1, for $<S_z(B)>$ with J_2/J_1 = -0.2 and D/J_1=1. These interesting behaviors may occur by the mixing effect of S_z with lager spin for $<S_z(A)>$ and the one of S_z with smaller spin for $<S_z(B)>$ at high temperatures in the range of $T \leqq T_s$.

(3) The critical temperature T_s depends largely on the anisotropy parameter D for both spin systems of S=5/2 and 3/2. Especially, the condition of $T_s= T_c$ can appear at the condition of $0.5 \leqq D/J_1$ for system with S=5/2. For this condition of $T_s= T_c$, $<S_z(A)>$ and $<S_z(B)>$ take different values at all temperatures of $T \leqq T_c$.

(4) The magnetic phase diagrams for both spin systems with S=5/2 and 3/2 are obtained for parameters J_2/J_1 and D/J_1. The magnetic phases of S(c) and S(d) disappear under the conditions of $0.55 \leqq D/J_1$ and $D/J_1 \leqq -0.2$ for spin system with S=5/2, respectively. The effect of D on sub-lattice magnetizations $<S_z(A)>$ and $<S_z(B)>$, the critical temperature T_s and the phase diagram of the system with large spin like S=5/2 is larger than that with small spin like S=3/2.

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