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Spin-3/2 Ising Spin System with Biquadratic Interaction and Single-ion Anisotropy

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Abstract

The magnetic properties such as the magnetization $<S_z>$, the specific heat C_M, the Curie temperature T_c, and spin structures of spin S=3/2 Ising spin system with the bilinear exchange interaction $J_1 S_{iz} S_{jz}$, the biquadratic exchange interaction $J_2\ S_{iz}^2 S_{jz}^2$ and the single-ion anisotropy DS_{iz}^2 have been discussed by making use of the Monte Carlo simulation on two-dimensional square lattice. We found characteristic temperature dependences of the magnetization and the specific heat near the phase transition points of J_2/J_1=-1/3 and -1, and those characteristic behaviors are explained by considering two energy levels with low value and small difference, and by the temperature dependence of sublattice magnetizations. Furthermore, it is found that single-ion anisotropy term D gives significant effects on these temperature dependences of sublattice magnetizations and on the conditions of phase transition. The ground state (GS) spin structures for the spin systems only with positive J_2 and only with negative J_2 have confirmed to be random spin arrangements with S_z=±3/2 and S_z=±1/2, respectively.

Key words: biquadratic exchange interaction, Ising model, Monte Carlo simulation, magnetization

1. Introduction

In Heisenberg and Ising spin systems, the existence and the importance of such higher-order exchange interactions as the biquadratic exchange interaction $(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2$, the three-site four-spin interaction $(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)(\boldsymbol{S}_j \cdot \boldsymbol{S}_k)$, the four-site four-spin interaction $(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)$ have been discussed extensively by many investigators[1,2]. Theoretical explanations of the origin of these interactions have been given in the theory of the superexchange interaction, the magnetoelastic effect, the permutation operator, the perturbation expansion, the higher harmonics of oscillatory exchange coupling and the spin-phonon coupling[3].

It was pointed out that the higher-order exchange interactions are smaller than the bilinear ones for the *3d* group ions [3], and comparable with the bilinear ones in the rare-earth compounds [4,5]. On the other hand, in solid helium and in such phenomena as the quadrupolar ordering of molecules in solid hydrogen, in liquid crystals, or the cooperative Jahn-Teller phase transitions,

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the higher-order exchange interactions turned out to be the main ones [6]. Furthermore, the four-site four-spin interaction has been pointed out to be important to explain the magnetic properties of the solid helium [7,8] and the magnetic materials such as NiS_2 and C_6Eu [9].

In the Ising ferromagnet with a spin of $S \geqq 1$, the dependences of the magnetization and the Curie temperature on the biquadratic exchange interaction [10,11] and the three-site four-spin interaction [12] were investigated and the ground state (GS) spin structures were determined by pair-spin and three-spin models approximation. Recently present authors have investigated the effects of the three-site and the four-site four-spin interactions and biquadratic interaction on magnetic properties and the GS spin structure of the Ising ferromagnet [13,14,15,16] with S=1 by making use of the Monte Carlo (MC) simulation.

In the present paper, we extend this MC calculation to spin-3/2 Ising spin system on the two-dimensional square lattice both with the bilinear exchange interaction $J_1 S_{iz} S_{jz}$ and the biquadratic exchange interaction $J_2 S_{iz}^2 S_{jz}^2$, and with the single-ion anisotropy DS_{iz}^2. This model of Hamiltonian for S=1 Ising system is quite famous as so-called Blume-Emery- Griffiths (BEG) model [17] and has been applied for many problems, e.g. super-liquid helium, magnetic material, semiconductor, alloy, lattice gas and so on. In the BEG model, there appear various characteristic spin orders depending on the combinations of parameters J_1, J_2, D and on the lattice dimensionality [18,19,20,21,22].

In the present study, we have investigated the dependences on interaction parameter J_2 and anisotropy parameter D of the magnetization $\langle S_z \rangle$, the magnetic specific heart C_M and the Curie temperature T_c in the spin-3/2 Ising spin system. Furthermore, the changes of sublattice magnetizations $\langle S_z(A) \rangle$ and $\langle S_z(B) \rangle$ and spin arrangements were also calculated by introducing negative interaction J_2 and single-ion anisotropy term D.

Here, we define the following quantities

$$S_z(A) = \frac{2}{N}\sum_{i(A)} S_{iz}\ ,\ S_z(B) = \frac{2}{N}\sum_{j(B)} S_{jz}\ , \qquad (1)$$

A and B represent the two-interpenetrating sublattices, and N is the total number of spins.

In Section 2, the condition of phase transitions and the GS spin structures are obtained by comparison of the energies per one spin calculated from the spin Hamiltonian given for present Ising system. Furthermore, the method of the MC simulation is explained briefly. In Section 3, first we consider the bilinear exchange model coupled only by interaction J_1, and then by adding biquadratic interaction J_2 and anisotropy term D we discuss the effects of those parameters on the magnetic properties and spin ordering of the system. In the latter part of this section, we discuss the effect of J_1 and D on the spin ordering by starting with the system coupled only by interaction J_2. In the last Section 4, new interesting results obtained here are summarized.

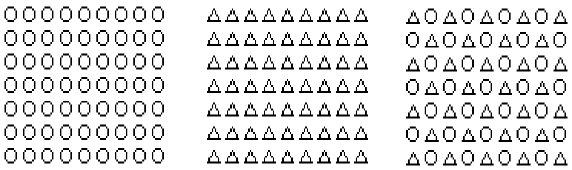
2. Ground State and Methods of Simulation

Let us consider the spin-S=3/2 Ising model described by the following Hamiltonian

$$H = -J_1 \sum_{\langle ij \rangle} S_{iz} S_{jz} - J_2 \sum_{\langle ij \rangle} S^2_{iz} S^2_{jz} - D \sum_i S^2_{iz}\ , \qquad (2)$$

where S_{iz} or S_{jz} = $\pm 3/2, \pm 1/2$. From a consideration of the Hamiltonian (2), magnetic properties and spin arrangements of Ising spin system with two-dimensional square lattice are calculated by the MC simulation. Furthermore, the ground state (GS) spin structures and the conditions of phase transitions can be determined by comparing the energies of various spin structures with each other (see e.g. [11]).

For Ising spin system both with negative J_2 and positive J_1, the energies of various spin structures with low energy have been calculated and compared with each other. The energies E_a and E_b per one spin for ferromagnetic spin structure (a) with S_z= 3/2 and spin structure (b) with S_z= 1/2, and energy E_c for spin structure (c) with S_z= 3/2 and 1/2 shown in Fig.1 are given by $E_a = -9J_1/2 - 81J_2/8$, $E_b = -J_1/2 - J_2/8$, $E_c = -3J_1/2 - 9J_2/8$. By comparing these energies, phase transitions turn out to occur at J_2/J_1=-1/3 and -1, and the GS spin structures are determined as ferromagnetic spin arrangement (a) with S_z= 3/2 in the range of $-1/3 < J_2/J_1$ and ferromagnetic spin arrangement (b) with S_z= 1/2 in the range of $J_2/J_1 < -1$. Furthermore, the spin structure (c) with S_z= 3/2 and 1/2 shown in Fig.1 turns out to become the GS spin structure in the range of $-1 < J_2/J_1 < -1/3$.



(a) (b) (c)

Fig. 1 Spin structures (a), (b) and (c) represent Type-Ⅰ, Type-Ⅱ, Type-Ⅲ, respectively. Circle and triangle denote S_Z =3/2 and S_Z =1/2, respectively.

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=160. 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 input for the calculation at the next point. Thermal averages $<S_z>$ $(=(<S_z(A)+S_z(B)>)/2)$ and 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=160 are given without showing error bars which were found to be negligibly small in our calculation.

3. Results of Calculation and Discussions

3.1 Effects of negative biquadratic interaction J_2 in the system with J_1>0 and D=0

Let us investigate the effects of negative biquadratic exchange interaction J_2 on the magnetization and the magnetic specific heat of the ferromagnetic Ising spin sysytem with positive interaction J_1. For interaction J_2 in the negative range of $-8 \leqq J_2/J_1 \leqq -0.3$ and $-1.1 \leqq J_2/J_1 \leqq -0.33$, the results calculated for magnetization $<S_z>/S$ and magnetic specific heat C_M by making use of the MC simulation are shown in Fig.2 and Fig.3, respectively. We can conclude from the value of $<S_z>$ at low temperature shown in Fig.2 that the phase transitions occur at J_2/J_1=-1/3 and -1, which agree well with those

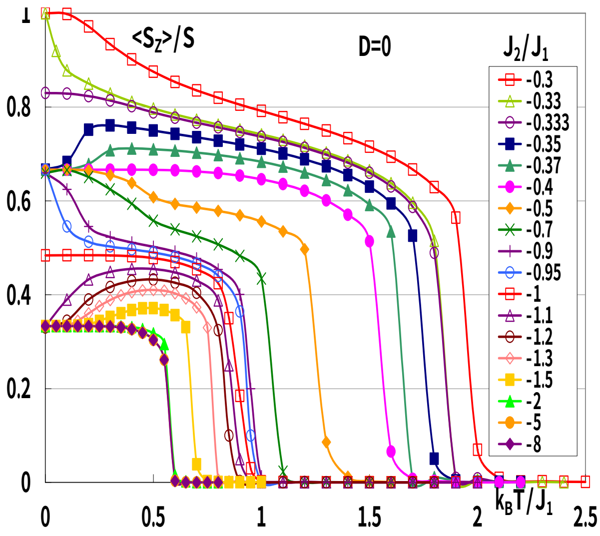


Fig. 2 Temperature dependences of $<S_Z>/S$ for both interactions of fixed positive J_1 and various values of J_2 in the range of $-8 \leqq J_2/J_1 \leqq -0.3$

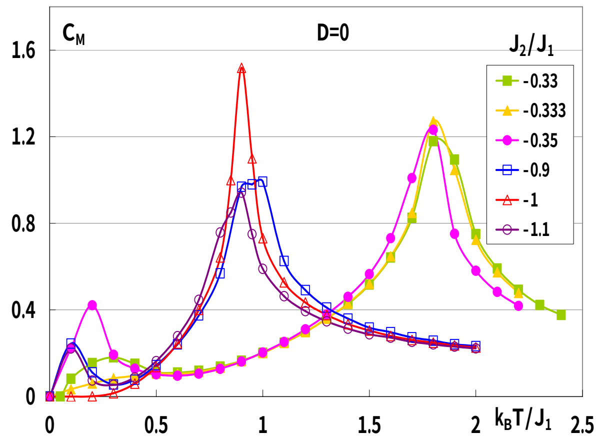


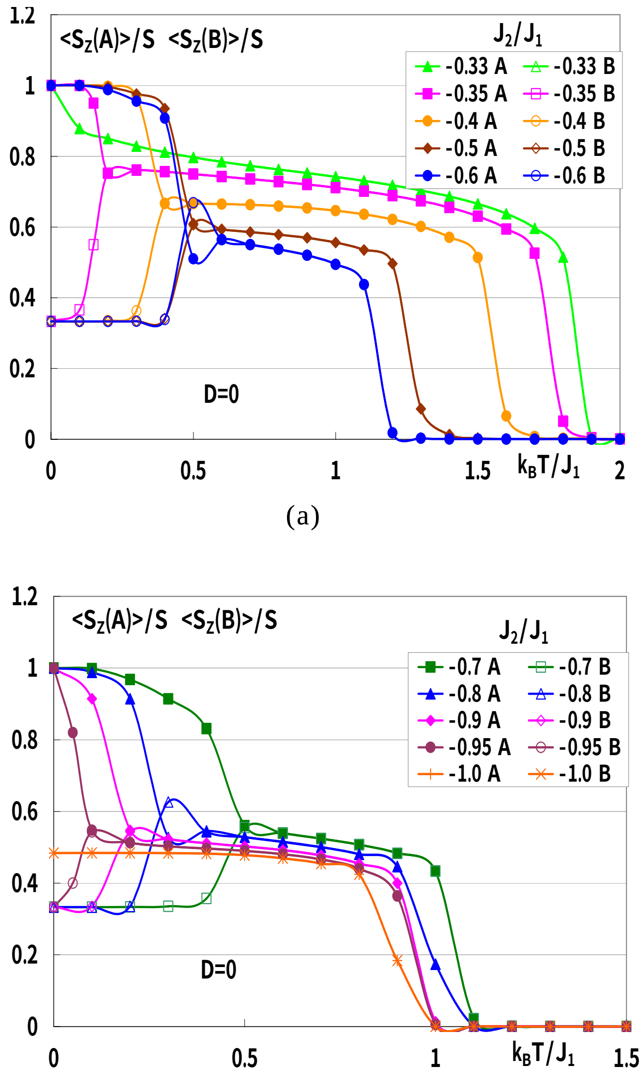
Fig.3 Temperature dependences of C_M for both interactions of fixed positive J_1 and various values of J_2 in the range of $-1.1 \leqq J_2/J_1 \leqq -0.33$

obtained from energy comparison. Furthermore, it is also confirmed that the GS spin structures obtained from this MC simulation coincide completely with those given by energy evaluation for each interaction (J_2/J_1) range.

Near the phase transitions, double peaks are observed on the magnetic specific heat C_M curves shown in Fig.3. These facts may suggest the existence of large change of spin structure at low temperatures in ordered state. The abnormal behaviors of the magnetization $<S_z>$ curves for interaction parameter J_2/J_1 near the phase transitions shown in Fig.2 consistent with the results obtained from magnetic specific heat C_M curves.

It is remarkable that the magnetization $<S_z>$ decreases with decreasing temperature for the interaction J_2 in the ranges of $-0.4<J_2/J_1<-1/3$ and $-2<J_2/J_1<-1$. As can be seen from the behavior of $<S_z>$, the temperature dependence curves of magnetization show almost the same behavior for various values of J_2 in the range of $-8 \leqq J_2/J_1 \leqq -2$. This behavior may be explained by considering the model of the spin ordering by interaction J_1 in the spin system with $S=1/2$($S_z = \pm 1/2$) restricted by negative interaction J_2 of large absolute value. It has also been confirmed by this simulation that there exist only spins of $S_z = \pm 1/2$ in the temperature range of non-zero magnetization for interaction of $J_2/J_1<-2$.

In the interaction range of $-1/3<J_2/J_1<-0.3$, the magnetization curve shows abrupt increase at low temperatures with decreasing temperature. This abrupt increase of $<S_z>$ at low temperatures can be understood by considering the existence of two energy levels of E_a with the lowest value and E_c close to each other near the



(a)

(b)

Fig.4 Temperature dependences of sublattice magnetizations $<S_z(A)>/S$ and $<S_z(B)>/S$ for both interactions of fixed positive J_1 and various values of J_2. (a) and (b) display the sublattice magnetizations in the ranges of $-0.6 \leqq J_2/J_1 \leqq -0.33$ and $-1 \leqq J_2/J_1 \leqq -0.7$, respectively.

condition of phase transition (J_2/J_1=-1/3). In the same way, the behavior of abrupt decreases of $<S_z>$ in the interaction range of $-0.4<J_2/J_1<-1/3$ with decreasing temperature may also be understood by the existence of two energy levels of E_c with the lowest value and E_a

close to each other near the condition of phase transition (J_2/J_1=-1/3). On the other hand, the increase and the decrease of <S_z> with decreasing temperature in the interaction ranges of -1<J_2/J_1<-0.4 and -2<J_2/J_1<-1, respectively may be explained by the existence of two energy levels of E_b and E_c close to each other near the condition of phase transition (J_2/J_1=-1).

In order to investigate more precisely the process of the spin arrangement, the sublattice magnetizations <$S_z(A)$> and <$S_z(B)$> have been calculated in the interaction range of -1≦J_2/J_1≦-0.33. The temperature dependences of <$S_z(A)$>/S and <$S_z(B)$>/S are shown by (a) and (b) in Fig.4 for the ranges of -0.6≦J_2/J_1≦-0.33 and -1≦J_2/J_1≦-0.7,respectively. We define the critical temperature and the magnetization as T_s and <$S_z(s)$> when two sublattice magnetizations begin taking different values with decreasing temperature. The value of T_s increases with decreasing the value of J_2/J_1 from J_2/J_1=-0.35 and takes the maximum value of k_BT_s/J_1=0.55 at J_2/J_1=-0.6. Then, this value becomes small with decreasing J_2/J_1 and zero at J_2/J_1=-1.

The value of <$S_z(s)$>/S at J_2/J_1=-0.4 is about 2/3 which correspond to the average value of <$S_z(A)$>/S=1 and <$S_z(B)$>/S=1/3. In the range of -0.4<J_2/J_1 <-1/3, the value of <$S_z(s)$>/S is larger than this value 2/3. Therefore, as can be seen from this figure the sublattce magnetization <$S_z(A)$>/S makes complete spin arrangement only with S_z/S =1 faster than the sublattce magnetization <$S_z(B)$>/S only with S_z/S =1/3. This fact may lead the decrease of <S_z> with decreasing temperature in this range of -0.4<J_2/J_1 <-1/3.

On the other hand, the value of <$S_z(s)$>/S is smaller than 2/3 in the range of -1<J_2/J_1 <-0.4. Therefore, the sublattce magnetization <$S_z(B)$>/S makes complete spin arrangement only with S_z/S =1/3 faster than the sublattce magnetization <$S_z(A)$>/S only with S_z/S =1. This fact can also explain the abrupt increase of <S_z> at low temperatures with decreasing temperature in this interaction range.

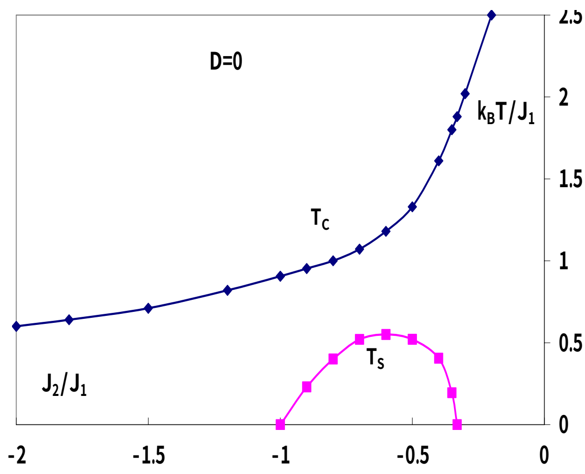


Fig. 5 The dependences of T_c and T_s on the interaction parameter J_2/J_1 in the range of –2≦J_2/J_1≦0.

The dependences on the interaction parameter J_2/J_1 of the Curie temperature T_c, and critical tmprature T_s have been calculated in the negative range of interaction J_2. The results for the interaction J_2 in the range of -2≦J_2/J_1 ≦0 are shown in Fig.5. The existence of T_s turn out to be confined within the range of -1<J_2/J_1<-1/3, where the GS spin structure at T=0 is the one shown in Fig.1. As can be seen from this figure, the T_c and T_s curves are quite separate from each other. The value of T_c is considerably larger than T_s for all values of interaction J_2. From farther calculations in the negative range of J_2, the value of T_c is almost constant for J_2/J_1≦-2.

3.2 Effects of positive single-ion anisotropy D>0 in the system with J_1>0 and J_2<0.

Let us investigate the effects of uniaxial type anisotropy D (D>0) on the magnetic properties and spin structure of the Ising spin system both with interactions J_1 and J_2 . For positive interaction J_2, the anisotropy term DS_{iz}^2 and the biquadratic exchange term $J_2S_{iz}^2S_{jz}^2$ make stable the direction of spins to the z-axis, and these two terms D and J_2 may give almost similar effect on the magnetic properties . Therefore, the temperature dependences of $<S_z>$ and C_M for this system doesn't show large change by introducing anisotropy term D.

On the other hand, for the case of negative J_2, the uniaxial anisotropy term $DS_{iz}^{\ 2}$ has an operation to cancel effects by the biquadratic term $J_2S_{iz}^{\ 2}S_{jz}^{\ 2}$. Therefore, the effect of anisotropy term D may be expected to be large for negative range of J_2, especially near or at the points of phase transition (J_2/J_1=-1/3,-1).

In order to examine the effect of the anisotropy term D, the MC simulation has been carried out for the spin system with fixed positive interaction J_1 and anisotropy term D/J_1=1. The result for magnetization $<S_z>/S$ are shown in Fig.6 for various values of J_2 in the range of -5 $\leqq J_2/J_1 \leqq$-0.3. By the introduction of D, the conditions of phase transition turn out to change from J_2/J_1=-1/3 and -1 for D=0 to J_2/J_1=-0.44 and -2 for D/J_1=1. As can be seen from this figure, the temperature dependence curves of $<S_z>$ for D/J_1=1 decrease with decreasing temperature in the ranges of -0.6<J_2/J_1 <-0.44 and -3<J_2/J_1 <-2.

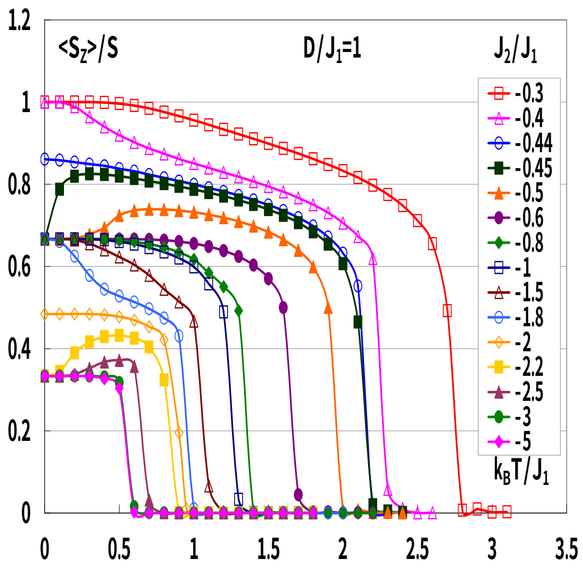
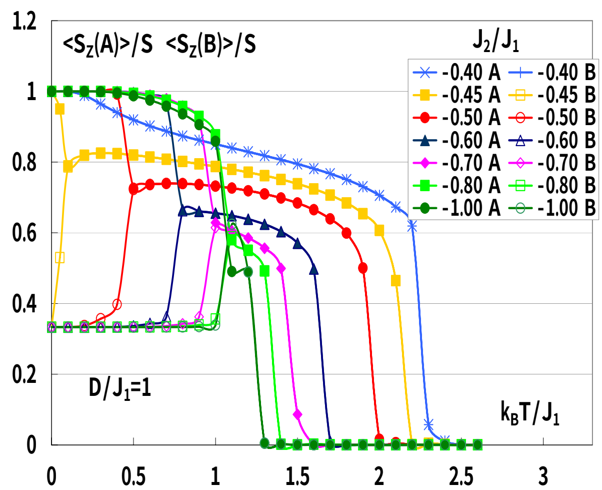


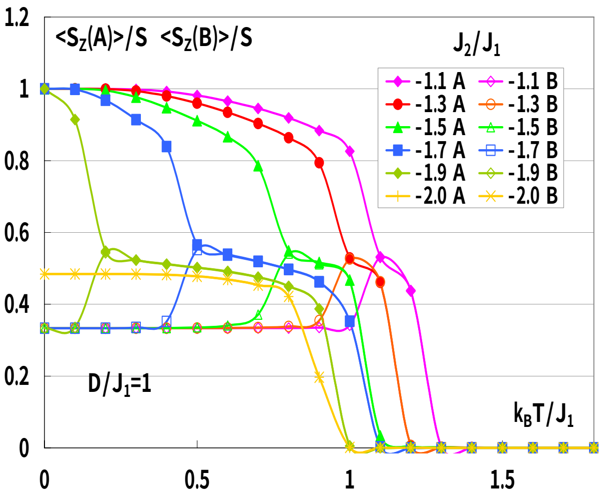
Fig. 6 Temperature dependences of $<S_Z>/S$ of the system with single-ion anisotropy D ($D/\ J_1$ =1) for both interactions of fixed positive J_1 and various values of J_2 in the range of –5$\leqq J_2/J_1 \leqq$-0.3.

Let us calculate the sublattice magnetizations $<S_z(A)>$ and $<S_z(B)>$ to investigate the formation process of spin arrangement. The temperature dependences of $<S_z(A)>/S$ and $<S_z(B)>/S$ are shown by (a) and (b) in Fig.7 for the ranges of -1 $\leqq J_2/J_1 \leqq$ -0.4 and -2 $\leqq J_2/J_1 \leqq$ -1.1,respectively. The value of the critical temperature T_s increases with decreasing interaction J_2/J_1 from J_2/J_1=-0.45, and takes the maximum value of k_BT_s/J_1 =1.15 at J_2/J_1=-1. Then, this value (T_s) becomes small gradually, and zero at J_2/J_1=-2. The value of $<S_z(s)>/S$ at J_2/J_1=-0.6 turns out to become about 2/3 which is average value of S_z/S =1 and 1/3. As can be seen from this figure, the value of $<S_z(s)>/S$ is larger than this value 2/3 in the range of -0.6<J_2/J_1 <-0.44. Therefore, these facts may support the decrease of $<S_z>$ with decreasing temperature in this range of J_2.

For the case of D/J_1=1, the dependences on the interaction parameter J_2/J_1 of the Curie temperature T_c and the critical temperature T_s have been calculated in the negative range of interaction J_2. The results for the interaction J_2 in the range of -2.0$\leqq J_2/J_1 \leqq$-0.3 are shown in Fig.8. As can be seen from this figure, T_s exists for interaction J_2 in more wide range of -2<J_2/J_1 <-0.44, and k_BT_s/J_1 has a maximum values of 1.15 for the interaction J_2/J_1=-1. It should be noted that the curve of T_s for D/J_1=1 approaches more closely to the curve of T_c than the one for D/J_1=0.



(a)



(b)

Fig.7 Temperature dependences of sublattice magnetizations $<S_Z(A)>/S$ and $<S_Z(B)>/S$ of the system with single-ion anisotropy D ($D/ J_1 =1$) for both interactions of fixed positive J_1 and various values of J_2. (a) and (b) display the sublattice magnetizations in the ranges of $-1.0≦J_2/J_1≦-0.4$ and $-2.0≦J_2/J_1≦-1.1$, respectively.

Furthermore, these calculations have been extended for the spin system with larger single-ion uniaxial anisotropy D. For the case of D/J_1=1.5, the

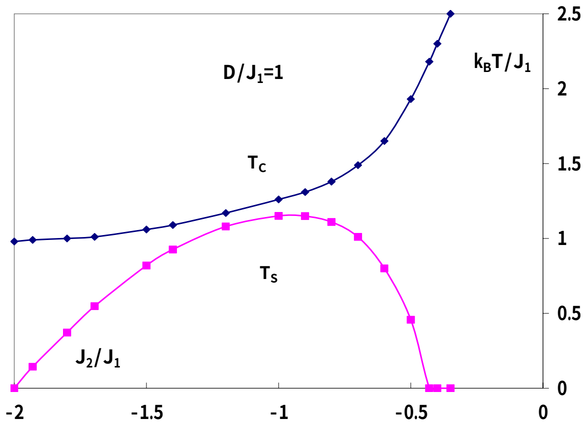


Fig. 8 The dependences of T_c and T_s of the system with single-ion anisotropy D ($D/ J_1 =1$) on the interaction parameter J_2/J_1 in the range of $-2.0≦J_2/J_1≦-0.3$.

dependences on the interaction parameter J_2/J_1 of the Curie temperature T_c and T_s have been calculated, and the results for the interaction J_2 in the range of $-2.5≦J_2/J_1≦-0.4$ are shown in Fig.9. It is quite remarkable that the value of T_s accord exactly with T_c for J_2 in the range of $-1.55≦J_2/J_1≦-1.05$. The region of existence of T_s turns out to become more wide range of $-2.4<J_2/J_1$

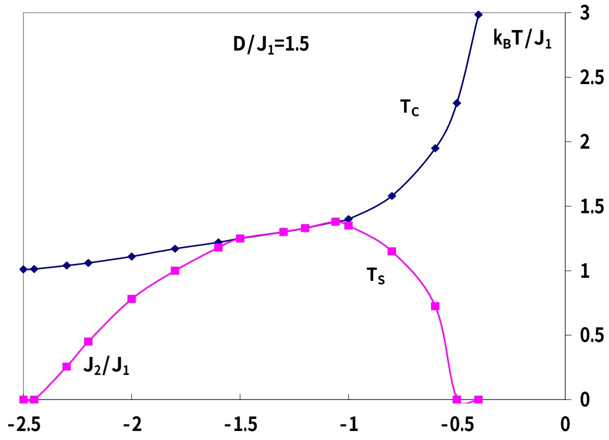


Fig. 9 The dependences of T_c and T_s of the system with single-ion anisotropy D ($D/ J_1 =1.5$) on the interaction parameter J_2/J_1 in the range of $–2.5≦J_2/J_1≦-0.4$.

<-0.5 for anisotropy term of D/J_1=1.5.

The temperature dependences of $<S_z(A)>/S$ and $<S_z(B)>/S$ for anisotropy parameter D/J_1=1.5 and typical values of J_2/J_1 (J_2/J_1 =-1.5, -2.0, -2.5) are shown in Fig.10. It is worth noting that as can be seen from the curve with J_2/J_1 =-1.5, for the interaction J_2 in the range satisfying the condition of T_c=T_s, the temperature dependences of $<S_z(A)>/S$ and $<S_z(B)>/S$ are different from each other in all temperature range below T_c. From

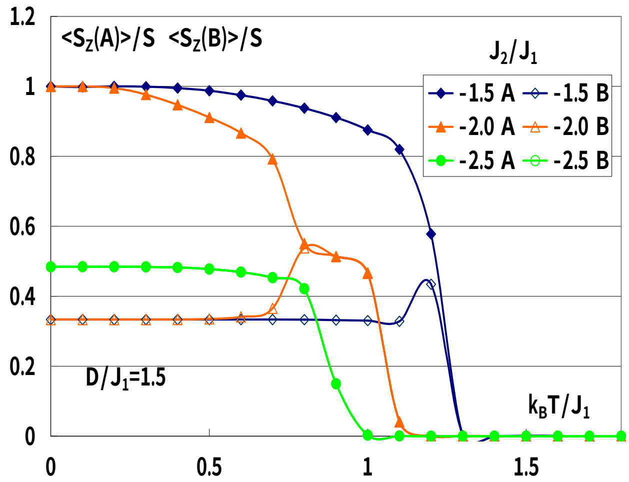


Fig.10 Temperature dependences of sublattice magnetizations $<S_Z(A)>/S$ and $<S_Z(B)>/S$ of the system with single-ion anisotropy D ($D/ J_1 =1.5$) for both interactions of fixed positive J_1 and typical values of J_2 (J_2/J_1=-1.5, -2.0, -2.5).

farther calculation, this range satisfying the condition of $T_c=T_s$ has been confirmed to appear only for anisotropy parameter D of $1.4\leqq D/J_1$.

3.3 Effects of bilinear interaction J_1 and single-ion anisotropy D in the system with J_2

In the Ising spin system only with positive biquadratic exchange interaction J_2, every spin structures not including any spins of $S_z=\pm1/2$ have the same lowest energy and become the GS spin structure. For this biquardatic exchange model, the GS spin structure deduced from the MC simulation at $k_BT/J_2=0.1$ is shown in Fig. 11. This type of spin structure is realized at the temperatures within the range of $k_BT/J_2<1.2$ in our MC simulation. This fixed GS spin structure may be supported by the fact that the value of C_M becomes zero at all temperatures of $k_BT/J_2<1.2$. The total sum of the two-spin correlation $<S_{iz}S_{jz}>$ for all nearest neighboring spin pairs becomes almost zero suggesting random spin arrangement with spins of $S_z=3/2$ and $S_z=-3/2$. In addition, the result that $<S_z>$ is almost zero may show the nearly equal number of spins of $S_z=\pm3/2$, which correspond to the maximum cases in the methods of spin arrangement of $S_z=\pm3/2$.

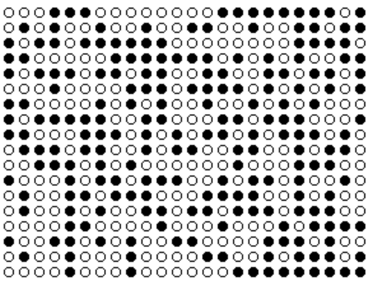


Fig. 11 Spin structure for Ising spin system only with positive interaction J_2. Open and closed circles represent $S_Z=3/2$ and $S_Z=-3/2$, respectively.

In this spin system, let us examine the process and the condition of a construction of ferromagnetic spin ordering by introducing positive bilinear interaction J_1. The temperature dependences of reduced magnetization $<S_z>/S$ for various small positive values of J_1 are shown in Fig.12.

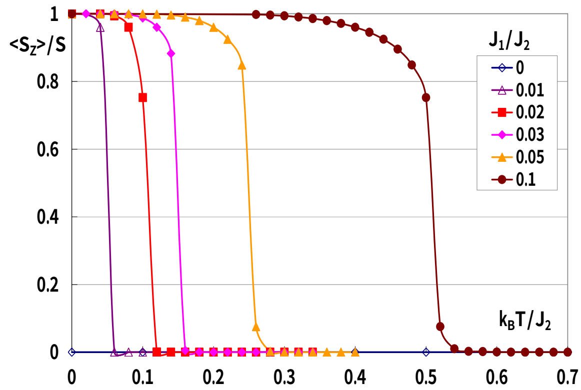


Fig. 12 Temperature dependences of $<S_Z>/S$ for both interactions of fixed positive J_2 and various values J_1 in the range of $0\leqq J_1/J_2\leqq0.1$.

It should be noted that ferromagnetic order can be realized even by introducing such a small value of J_1 as $J_1/J_2=0.01$ and the values of $<S_z>$ is strongly enhanced with increasing the interaction J_1. From further calculation, this rapid increase of $<S_z>$ is confirmed to be led by the direct spin flipping between $S_z=3/2$ and $S_z=-3/2$ with decreasing temperature.

In the same way, by adding negative interaction J_1, the processes of a construction of an antiferromagnetic spin structure on the system with positive J_2 has been investigated. The behavior of sublattice magnetization produced by introducing negative J_1 has been confirmed to be almost the same with the one of the ferromagnetic magnetization for positive J_1 shown in Fig.12.

The positive interactions J_2 and J_1, and the positive anisotropy term DS_{iz}^2 may give almost similar effect on the magnetic properties. Therefore, it has been confirmed that the temperature dependences of $<S_z>$ and C_M for various positive values of J_1 on the system with positive interactions J_2 doesn't show large change by introducing anisotropy term D.

In the Ising spin system only with negative biquadratic exchange interaction J_2, every spin structures not including any spins of $S_z=\pm3/2$ have the same lowest energy and become the GS spin structure. For this biquardatic exchange model, the GS spin structure deduced from the MC simulation at k_BT/J_2=0.1 is shown in Fig. 13. This type of spin structure is realized at the temperatures within the range of $k_BT/J_2<0.2$ in our MC simulation.

Further calculation for the system with negative J_2, positive J_1 and anisotropy term D was not performed, as the discussion for this system has been done in the previous section.

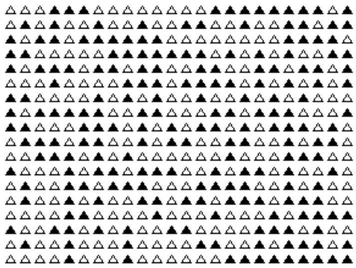


Fig. 13 Spin structure for Ising spin system only with negative interaction J_2. Open and closed triangles represent S_Z =1/2 and S_Z =-1/2, respectively.

4. Conclusions

In the previous section, for the Ising spin system of S=3/2 with both biquadratic and bilinear interactions J_2 and J_1, and with uniaxial anisotropy term D, the magnetization $\langle S_z \rangle$, sublattice magnetizations $\langle S_z(A) \rangle$ and $\langle S_z(B) \rangle$, the magnetic specific heat C_M ,the Curie temperature T_c and the GS spin structures have been calculated by making use of the MC simulation.

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

(1) For the interaction parameter J_2 near the condition of phase transition, the curves of $\langle S_z \rangle$ and C_M of the Ising system with positive J_1 and negative J_2 show characteristic behaviors at low temperatures. These behaviors may be explained by considering two energy levels with low value and small difference, and by the different temperature dependences of two sublattice magnetizations $S_z(A)\rangle$ and $\langle S_z(B) \rangle$.

(2) The anisotropy term D affects largely on the Curie temperature T_c and the sublattice magnetizations $S_z(A)\rangle$ and $\langle S_z(B) \rangle$ of the Ising system with positive J_1 and negative $J_{2.}$ The region satisfying the condition of $T_c=T_s$ exists only for anisotropy parameter D of $1.4 \leqq D/J_{1.}$

(3) The GS spin structure for Ising spin system only with positive J_2 is the one with $S_z=\pm 3/2$ shown in Fig.11, and this spin structure is fixed in the wide range of $k_BT/J_2<1.2$. On the other hand, the GS spin structure only with negative J_2 is one with $S_z=\pm 1/2$ shown in Fig.13, and this spin structure is fixed in the small range of $k_BT/J_2<0.2$. These differences of temperature range of fixed GS spin structure may be explained by the fact that the energy of spin shift between spins of $S_z=\pm 3/2$ is larger than the one between spins of $S_z=\pm 1/2$.

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