Monte Carlo Simulation of Mixed Ising Spin System of S=1and 3/2 with Four-Spin Interaction

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Abstract.

The phase diagram and magnetic properties such as the magnetizations $<S_z>$ and $<R_z>$, the magnetic specific heat C_M, the Curie temperature T_c and the ground state (GS) spin structures of the mixed Ising spin system (S=1and R=3/2) on two-dimensional square lattice with the bilinear exchange interaction $J_1S_{iz}R_{jz}$, four-spin interaction $J_4S_{iz}R_{jz}S_{kz}R_{lz}$ and the single-ion anisotropies DS_{iz}^2 and DR_{jz}^2 have been discussed by making use of the Monte Carlo simulation. In this Ising spin system, we have determined the conditions of phase transitions and phase diagram. Furthermore, it is confirmed that these conditions of phase transition agree well with those obtained from a comparison of energies per one spin for various spin structures with low energy. The characteristic temperature dependence of the magnetizations $<S_z>$ and $<R_z>$ and the ground state (GS) spin structures are investigated for various values of parameters of J_4/J_1 and D/J_1.

Keywords: Ising model; four-spin interaction; mixed spin system; 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 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 have investigated the effects of the three-site and the four-site four-spin interactions on magnetic properties and the ground state (GS) spin structure of the Ising ferromagnet [12,13] with S=1 by making use of

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the Monte Carlo (MC) simulation. Furthermore, we have applied this MC simulation to the Ising spin system of large spin $S = 2$ with interaction J_2, and investigated more precisely the growth of spin ordering and the GS spin structures [14]. We have also developed this MC simulation to the mixed Ising spin system with spins of $S = 1$ and $R=3/2$, and investigated precisely the growth of spin ordering and the ground state (GS) spin structures.

Therefore, in the present study, the effects of the four-site four-spin interaction $J_4S_{iz}R_{jz}S_{kz}R_{lz}$ and the single-ion anisotropies DS_{iz}^2 and DR_{jz}^2 on the magnetizations $\langle S_z\rangle$ and $\langle R_z\rangle$, the magnetic specific heat C_M and the ground state (GS) spin structure of the mixed Ising spin system of $S = 1$ and $R=3/2$ on two-dimensional square lattice are investigated by making use of the MC simulation. Here, spins S and R are situated on each two interpenetrating sub-lattices. The obtained phase diagram is discussed in conjunction with the GS spin structures determined by energy evaluations. The temperature dependences of the magnetizations $\langle S_z\rangle$ and $\langle R_z\rangle$ and the spin structure are also studied for various values of parameters J_4/J_1 and D/J_1.

In Section 2, the spin Hamiltonian is given for present mixed Ising system with $S=1$ and $R=3/2$. Furthermore, the method of the MC simulation is explained briefly. The energies per one spin of spin structures with lower energy are also obtained from this spin Hamiltonian. In Section 3, phase diagram is obtained for parameters J_4/J_1 and D/J_1 by the MC simulation of this Ising system. In the latter part of Section 3, the magnetic properties and the spin ordering are investigated for various temperature. In the last Section 4, new interesting results obtained here are summarized.

2. Spin Hamiltonian , Methods of Simulation and Energy Estimation

The spin Hamiltonian for the present mixed Ising spin system with $S=1$ and $R=3/2$ on two-dimensional square lattice can be written as follows:

$$H = -J_1 \sum_{\langle ij\rangle} S_{iz} R_{jz} - J_4 \sum_{\langle ijkl\rangle} S_{iz} R_{jz} S_{kz} R_{lz} - D\sum_i S^2{}_{iz} - D\sum_j R^2{}_{jz} \qquad (1)$$

Here, $\langle ij\rangle$ and $\langle ijkl\rangle$ denotes the sum on the nearest neighboring spin pairs and four spins of the square on two-dimensional square lattice. Furthermore, S_z and R_z in above expression represent $S_z = \pm 1$, 0 and $R_z = \pm 3/2$, $\pm 1/2$, respectively. From a consideration of the Hamiltonian (1), magnetic properties and spin arrangements of this mixed Ising spin system of $S=1$ and $R=3/2$ 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, J_4 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 magnetizations $\langle S_z\rangle$ and $\langle R_z\rangle$, thermal averages $\langle S_z^2\rangle$ and $\langle R_z^2\rangle$ 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 whole temperature range.

By taking Hamiltonian (1) into consideration, the energies per one spin are obtained for various spin structures with low energy (see e.g. [14]). The GS spin structures are determined for this mixed Ising spin system with interactions J_1 and J_4, and with single-ion anisotropy D by comparing these energies per one spin with each other. The GS spin structures with low energy obtained for this spin system of S = 1 and R = 3/2 with positive interaction J_1 are shown in Fig. 1. The spin structures S(a) ～ S(e) are consisted of two kinds of spins S_z=1 and R_z=3/2, S_z=1and R_z=3/2and 1/2, S_z=1 and R_z=3/2 and -1/2, S_z=1and R_z=3/2 and -3/2, S_z=1 and -1 and R_z=3/2 and -3/2, respectively. Let us define parameters x and y as D/J_1 and J_4/J_1, respectively. The energies per one spin for the spin structures S(a) ～ S(e) of this mixed Ising spin system with S=1 and R=3/2 are given as $E(a) = E_a/J_1 = -13x/8 -9y/2-3$, $E(b) = E_b/J_1 = -9x/8-3y/2-2$, $E(c) = E_c/J_1= -9x/8+3y/2-1$, $E(d) = E_d/J_1 = E(e) = E_e/J_1=-13x/8 +9y/2$, respectively.

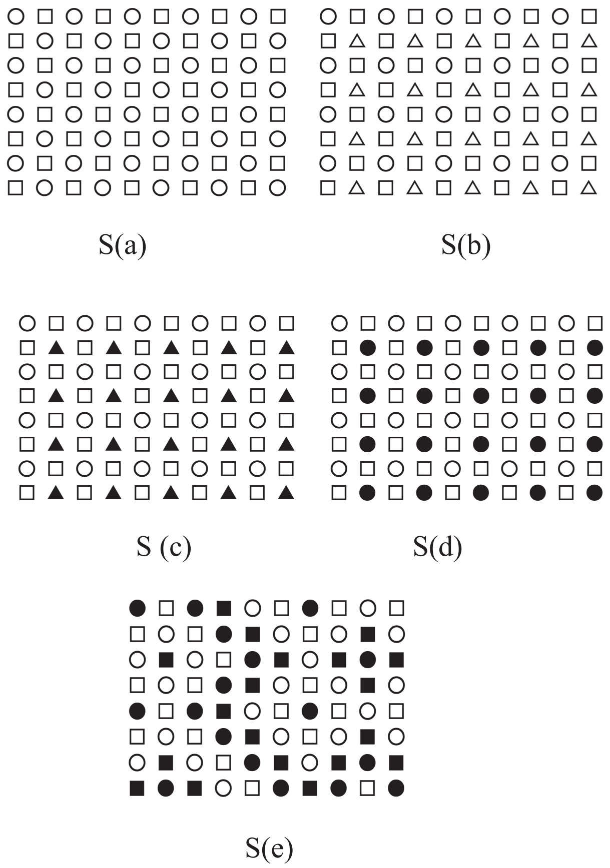


Fig. 1 The GS spin structures S(a), S(b), S(c), S(d) and S(e) for the mixed Ising spin system of S=1 and R=3/2 with interactions J_1, J_4 and anisotropy D. Open and closed circles, and open and closed triangles denote R_Z =±3/2 and R_Z =±1/2, and square and dot denote S_Z =1 and S_Z =0, respectively.

3. Results of Simulation and Discussion

3.1 Phase Diagram of Mixed Ising Spin System

Let us calculate magnetic properties and spin structures by making use of the MC simulation and investigate the condition of phase transitions, and determine the GS spin structures of the Ising spin system with four-spin interaction J_4 in the range of $-1.5 \leqq J_4/J_1 \leqq 1.0$ and the anisotropy D/J_1 in the range of $-1.0 \leqq D/J_1 \leqq 1.0$. In this calculation, the interaction parameter J_1 was treated as a positive constant value. The phase diagram is obtained for this mixed Ising spin system on two-dimensional lattice and the result for both parameters J_4/J_1 in the range of $-1.5 \leqq J_4/J_1 \leqq 0.5$ and D/J_1 in the range of $-0.8 \leqq D/J_1 \leqq 0.2$ is shown in Fig.2.

The GS spin structures of magnetic phases (a) ～ (e) in Fig.2 determined by the MC simulation are confirmed to be the spin structures S(a) ～S(e) shown in Fig.1 obtained by the energy comparison, respectively. For the case of D=0, the conditions of phase transition are determined to be J_4/J_1=-1/3 by this MC simulation. This condition of phase transition for D=0 is confirmed to agree well with that obtained from the equation of $E(a)= E(b)$ given in the previous section under the condition of D/J_1 =0, respectively.

By comparing by the energies $E(a)$ and $E(b)$, and by comparing $E(b)$ and $E(c)$, and by comparing $E(c)$ and $E(d)$, or $E(e)$ given in the previous section, the conditions of phase transition between magnetic phases (a) and (b), between (b) and (c) , between (c)and (d) are obtained as $y= -x/6-1/3$, $y=-1/3$, and $y=x/6-1/3$, respectively. These conditions agree well with those obtained by the MC simulation shown in Fig.2. The condition of phase transition between magnetic phases (d) and (e) is given by the MC simulation as $y=x/4-1/3$. This condition cannot, however, be obtained by the energy comparison as the energies of these magnetic phases have the same energy. The condition of phase transition of y=-1/3 for the positive range of D/J_1 in Fig.2 agrees well with that obtained by the energy comparison of $E(a)$ and $E(e)$.

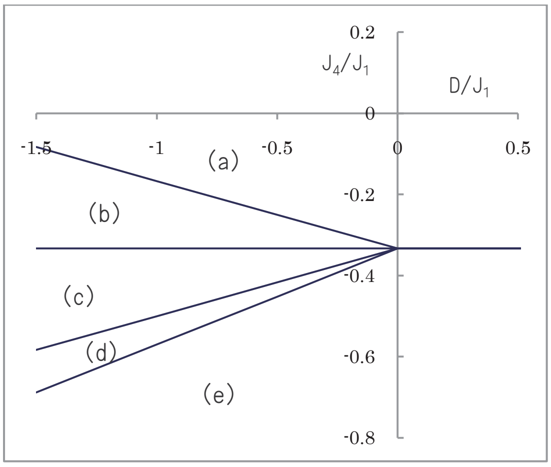


Fig. 2 Phase diagram of mixed Ising spin system on two-dimensional square lattice with exchange parameter $y(J_4/J_1)$ in the range of $-0.8 \leqq y \leqq 0.2$ and anisotropy $x(D/J_1)$ in the range of $-1.5 \leqq x \leqq 0.5$.

3.2 Magnetic Properties of Mixed Ising Spin System of S=1 and R=3/2

(A) Magnetic Properties of Spin System with D/J_1=-0.5

Let us investigate the magnetic properties such as the magnetizations $<S_z>$ and $<R_z>$, and the magnetic specific heat C_M of the mixed Ising spin system of S=1 and R=3/2 with anisotropy D=-0.5 by making use of the MC simulation. The temperature dependences of $<R_z>/R$ and $<S_z>/S$ (=$<S_z>$) of the mixed spin system for various values of interaction J_4 in the range of $-0.8 \leqq J_4/J_1 \leqq -0.2$ are shown in Fig.3 and Fig.4, respectively.

The temperature dependence curves of $<R_z>/R$ for J_4/J_1=-0.2, J_4/J_1=-0.3, J_4/J_1=-0.35 and -0.4, J_4/J_1=-0.45, J_4/J_1=-0.5 correspond to the magnetic phases S(a), S(b), S(c), S(d), S(e), respectively. As can be seen from Fig.3, the values of $<R_z>/R$ at T=0 are 1.0, 2/3, 1/3, 0, 0 for J_4/J_1=-0.2, J_4/J_1=-0.3, J_4/J_1=-0.35 and -0.4, J_4/J_1=-0.45, J_4/J_1=-0.5, respectively. These values of $<R_z>/R$ at T=0 are understood by considering facts that the magnetic phases S(a), S(b), S(c), S(d), S(e) consist of spins R_z=3/2, R_z=3/2 and 1/2, R_z=3/2 and -1/2, R_z=3/2 and -3/2, R_z=3/2 and -3/2, respectively.

The curves for J_4/J_1=-0.25, -0.33 and -0.42 show the temperature dependences correspond to the phase boundary between S(a) and S(b), S(b) and S(c), S(c) and S(d), respectively. For curves with J_4/J_1=-0.3, -0.33, -0.35 -0.4 and -0.42, the values of $<R_z>/R$ show rapid increases in the temperature range just below T_c and these curves complicated behaviors at low temperatures.

Especially, it is interesting that $<R_z>/R$ for J_4/J_1=-0.45 which correspond to the spin structure S(d) takes non-zero value just below T_c and becomes zero at T=0. On the other hand, $<R_z>/R$ for J_4/J_1=-0.5 which correspond to the spin structure S(e) cannot take non-zero value at all temperature range.

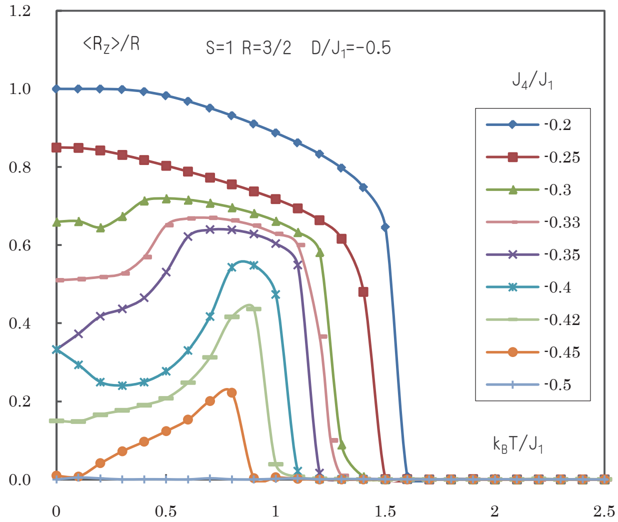


Fig. 3 Temperature dependence of $<R_z>/R$ of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_4 of in the range of $-0.5 \leqq J_4/J_1 \leqq -0.2$.

As can be seen from Fig.4, the values of $<S_z>/S$ at T=0 are all one for J_4/J_1=-0.2～-0.45 which correspond to the spin structures S(a) ～S(d). On the other hand, the values of $<S_z>/S$ are 0 at all temperatures for J_4/J_1=-0.5 which correspond to the spin structure S(e). It is remarkable that the values of $<S_z>/S$ for J_4/J_1=-0.3, J_4/J_1=-0.35 and -0.4 which correspond to the spin structures S(b) and S(c) show rapid increases at different two temperature ranges with decreasing temperature.

Furthermore, it can be seen from Fig.4 that temperature dependences of $<S_z>/S$ for J_4/J_1=-0.45 show rapid increase just below T_c and the value of $<S_z>/S$ gets closer to one with decreasing temperature. On the other hand, $<R_z>/R$ for J_4/J_1= -0.5 which correspond to the spin structure S(e) cannot also take non-zero value at all temperature range.

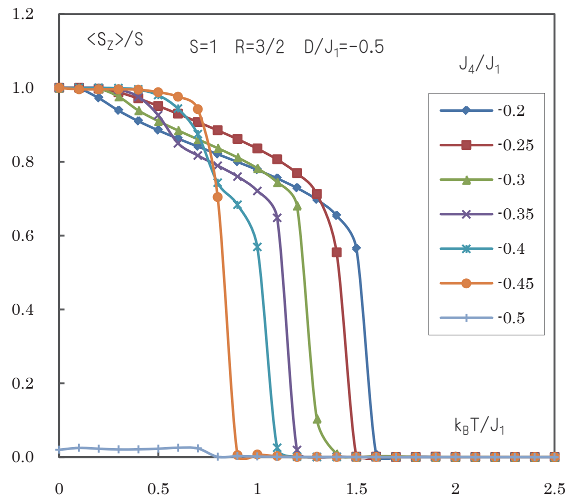


Fig.4 Temperature dependence of $<S_z>/S$ of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_4 of in the range of -0.5≦J_4/J_1≦-0.2.

Furthermore, the temperature dependences of C_M of the mixed spin system for various values of interaction J_4 in the range of -0.5≦J_4/J_1≦-0.2 are shown in Fig.5. As can be seen from Fig.5, the temperature dependence curve of C_M for J_4/J_1=-0.3, -0.35, -0.4 show double peaks. These facts suggest that large change of spin arrangement occurs at low temperatures for these exchange parameters.

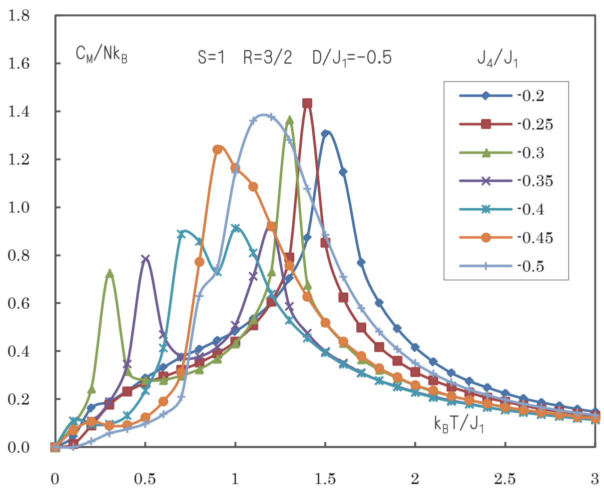


Fig.5 Temperature dependence of C_M of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_4 of in the range of -0.5≦J_4/J_1≦-0.2.

These behaviors of temperature dependence of the magnetic specific heat C_M are consistent with those of the magnetizations $<S_z>$ and $<R_z>$.

(B) Magnetic Properties of Spin System with D/J_1=-1.0

Next, let us investigate the magnetic properties such as the magnetizations $<S_z>$ and $<R_z>$, and the magnetic specific heat C_M of the mixed Ising spin system of S=1 and R=3/2 with anisotropy D/J_1=-1.0 by making use of the MC simulation. The temperature dependences of $<R_z>/R$ and $<S_z>/S$ (=$<S_z>$) of the mixed spin system for various values of interaction J_4 in the range of -0.65≦ J_4/J_1 ≦ -0.15 are shown in Fig.6 and Fig.7, respectively.

The temperature dependence curves of $<R_z>/R$ and $<S_z>/S$ for J_4/J_1=-0.15, J_4/J_1=-0.2, -0.25, -0.3, J_4/J_1=-0.35, -0.4, -0.45, J_4/J_1=-0.55, J_4/J_1=-0.6, -0.65, -0.7 correspond to the magnetic phases S(a), S(b), S(c), S(d), S(e), respectively. The curve for J_4/J_1=-0.5 shows the temperature dependence correspond to the phase boundary between S(c) and S(d), respectively. For curves with J_4/J_1=-0.35, -0.4 and -0.45 which correspond to the spin structure S(c), the values of $<R_z>/R$ show rapid increases in the temperature range just below T_c and these curves show complicated behaviors at low temperatures.

It is noticeable that $<R_z>/R$ for J_4/J_1=-0.55 which correspond to the spin structure S(d) takes non-zero large value just below T_c, and becomes gradually small and takes zero value at T=0. On the other hand, $<R_z>/R$ for J_4/J_1=-0.6 and -0.65 which correspond to the spin structure S(e) take very small value at all temperature range.

It is interesting that the value of $<R_z>/R$ for spin structure S(e) cannot be complete zero in the low temperature range of ordered state. This fact may suggest that complete ordered state of spin structure S(e) cannot be realized with decreasing temperature as many ordered magnetic domains appear independently at different places at high temperatures.

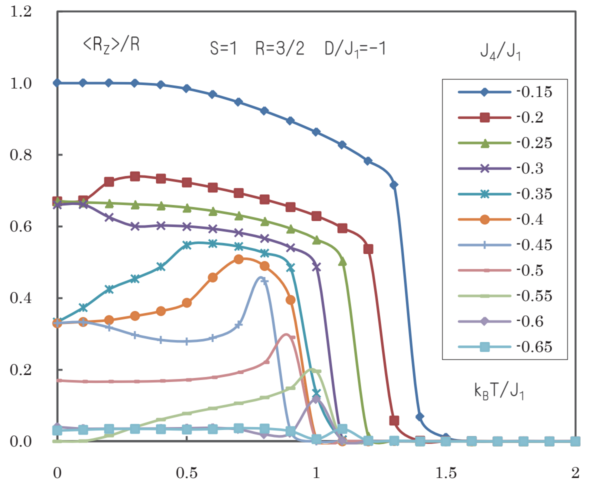


Fig. 6 Temperature dependence of $<R_z^2>/R^2$ of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_4 of in the range of -0. 8≦J_4/J_1≦-0.3.

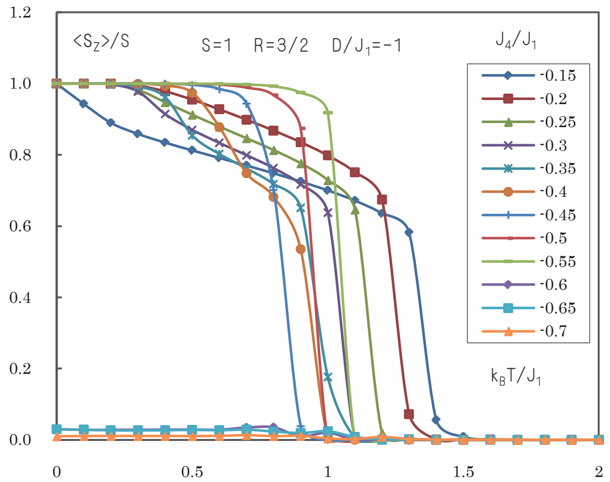


Fig. 7 Temperature dependence of $<R_z^2>/R^2$ of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_4 of in the range of -2.2≦J_4/J_1≦-1.0.

As can be seen from Fig.7, the values of $<S_z>/S$ at T=0 are all one for J_4/J_1=-0.15～-0.55 which correspond to the spin structures S(a) ～S(d). On the other hand, the values of $<S_z>/S$ are 0 at all temperatures for J_4/J_1=-0.6, -0.65 and -0.7 which correspond to the spin structure S(e).

It is remarkable that the temperature dependence curves of $<S_z>/S$ for J_4/J_1=-0.35, J_4/J_1=-0.4 and -0.45 which correspond to the spin structure S(c) show rapid increases at different two temperature ranges with decreasing temperature. It can be seen from Fig.7 that temperature dependences of $<S_z>/S$ for J_4/J_1= -0.55 show rapid increase just below T_c and the value of $<S_z>/S$ gets closer to one with decreasing temperature. On the other hand, $<R_z>/R$ for J_4/J_1=-0.6, -0.65 and -0.7 which correspond to the spin structure S(e) cannot also take non-zero large value at all temperature range.

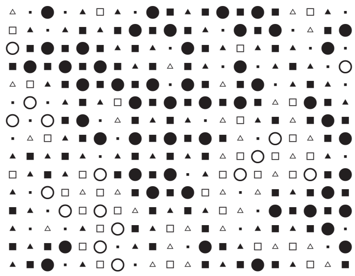
It is interesting that as can be seen from Fig.6 and Fig.7, the Curie temperature T_c takes minimum value at the condition of J_4/J_1=-0.45 which correspond to S(c).

(C) 3.3 Spin Arrangement of Mixed Ising Spin System of S=1 and R=3/2 with *D*/*J*$_1$=-1.0

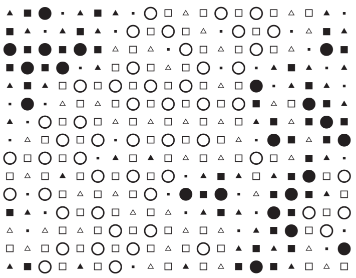
Next, we have investigated the changes of spin structure with different GS spin structure S(a)～S(e) for various values of temperature by making use of the MC simulation and visualized the change of this structure. The changes of spin structure S(a) with J_4/J_1=-0.1 are shown in Fig.8 for various temperatures in the range of 0.1≦ k_BT/J_1≦2.0. For this spin structure, the Curie temperature has been determined to be T_c=1.55J_1 /k_B.

It can be seen from (b) in Fig.8 that the magnetic domains with same sign become large in the paramagnetic state with approaching to the Curie temperature T_c. The rates of occupation of a spin S_z=1 on S-spin site in ordered state below T_c are 65%, 92%, 100%, 100% at temperatures k_BT/J_1=1.5, 1.0, 0.5, 0.1, respectively. On the other hand, the rates of occupation of a spin R_z=3/2 on R-spin site are 55%, 74%, 88%, 100% at temperatures k_BT/J_1=1.5, 1.0, 0.5, 0.1, respectively. It is interesting that the rates of the occupation of both S-spin site and R-spin site are more than 50 % even just below T_c.

It is remarkable that the complete spin arrangement of the S-site can be established at higher temperature (k_BT/J_1=0.5) than that (k_BT/J_1 =0.1) of the R-site. This may be understood by considering that the existence of a spin S_z=0 raises the energy of spin system as the interaction J_1 with positive sign exists.



(a)



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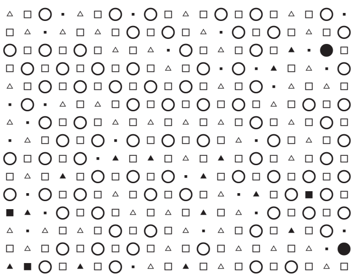

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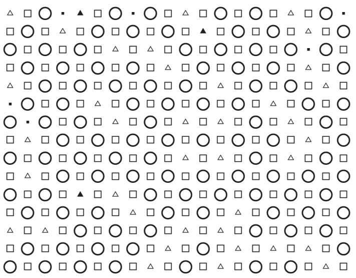

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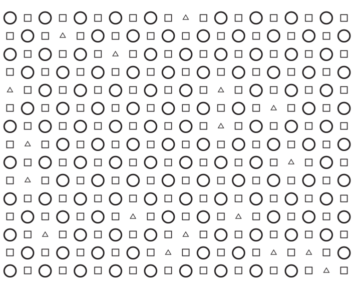

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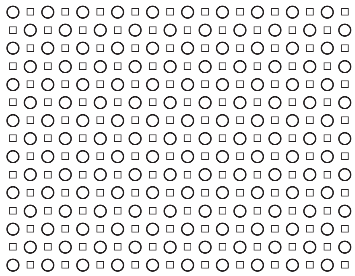


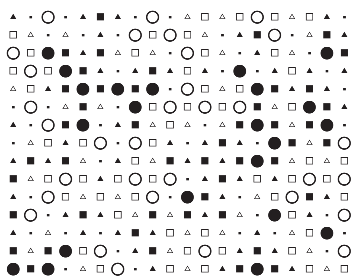
(f)

Fig. 8 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_4/J_1=-0.1 calculated by the MC simulation for various temperatures in the range of 0.1≦k_BT/J_1≦2.0. (a), (b), (c), (d), (e), (f) represent the spin structures at k_BT/J_1= 2.0, 1.6, 1.5, 1.0, 0.5, 0.1, respectively. Open and closed circles, and open and closed triangles denote R_Z =±3/2 and R_Z =±1/2, and square and dot denote S_Z =1 and S_Z =0, respectively.

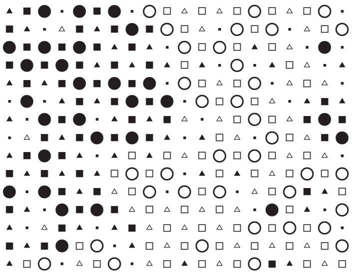
The changes of spin structure S(b) with J_4/J_1= -0.25 are shown in Fig.9 for various temperatures in the range of 0.2≦k_BT/J_1≦1.6. For this spin structure, the Curie temperature has been determined to be T_c=1.15J_1/k_B.

It can be seen from (a) and (b) in Fig.9 that the magnetic domains with same sign at k_BT/J_1=1.2 become larger than that at k_BT/J_1=1.6 in the paramagnetic state. The rates of occupation of a spin S_z=1 on S-spin site in ordered state below T_c are 65%, 81%, 95%, 100% at temperatures k_BT/J_1=1.1, 0.8, 0.4, 0.2, respectively. On the other hand, the rates of occupation of a spin R_z=3/2 on R-spin site are 40%, 50%, 50%, 99% and those of a spin R_z=1/2 on R-spin site are 37%, 37%, 43%, 99% at temperatures k_BT/J_1=1.1, 0.8, 0.4, 0.2, respectively.

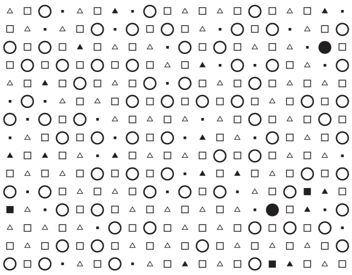
It is remarkable that the complete spin arrangements of the S-site and the R-site can be established at very low temperature (k_BT/J_1=0.1).



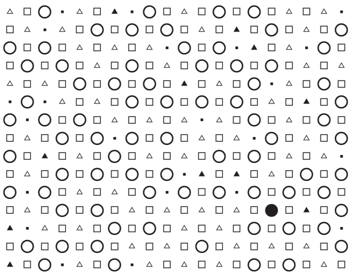
(a)



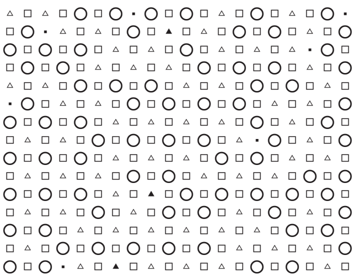
(b)



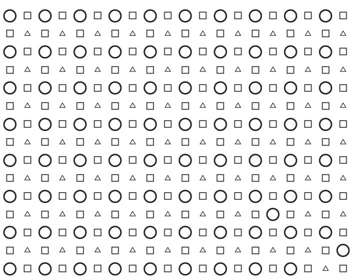
(c)



(d)



(e)



(f)

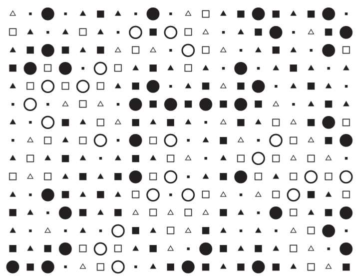
Fig. 9 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_4/J_1=-0.25 calculated by the MC simulation for various temperatures in the range of 0.2≦k_BT/J_1≦1.6. (a), (b), (c), (d), (e), (f) represent the spin structures at k_BT/J_1= 1.6, 1.2, 1.1, 0.8, 0.4, 0.2, respectively.

This may be understood by considering that the energy difference of the spin system by the replacement of R_z=3/2 and R_z=1/2 is small.

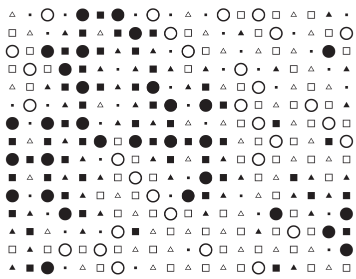
The changes of spin structure S(c) with J_4/J_1= -0.40 are shown in Fig.10 for various temperatures in the range of 0.2≦k_BT/J_1≦1.6. For this spin structure, the Curie temperature has been determined to be T_c=0.9J_1/k_B.

The rates of occupation of a spin S_z=1 on S-spin site in ordered state below T_c are 68%, 100%, 100% at temperatures k_BT/J_1= 0.8, 0.4, 0.2, respectively. On the other hand, the rates of occupation of a spin R_z=3/2 on R-spin site are 45%, 100%, 100% and those of a spin R_z=1/2 on R-spin site are 25%, 88%, 100% at temperatures k_BT/J_1=0.8, 0.4, 0.2, respectively.

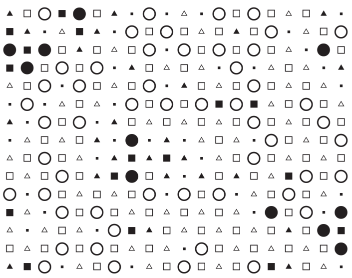
It is remarkable that the complete spin arrangements of S_z=1 on the S-site and of R_z=3/2 on the R-site can be established at high temperature (k_BT/J_1=0.4). On the other hand, the spins of R_z=1/2 on the R-site cannot make a complete spin arrangement even at low temperature (k_BT/J_1=0.2).



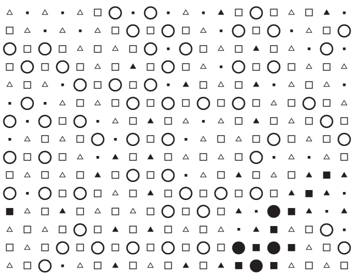
(a)



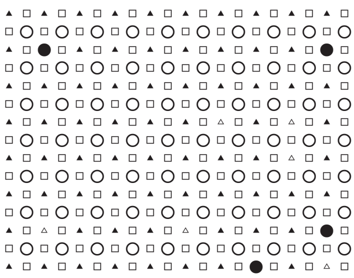
(b)



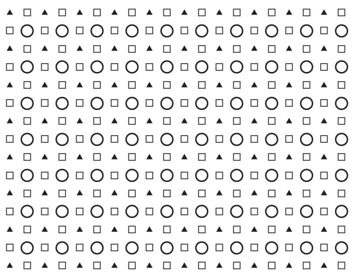
(c)



(d)



(e)



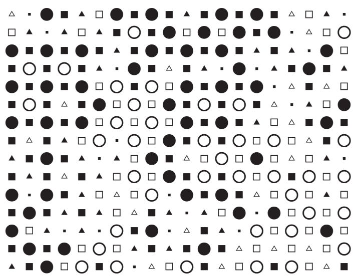
(f)

Fig. 10 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_4/J_1=-0.4 calculated by the MC simulation for various temperatures in the range of 0.2≦k_BT/J_1≦1.6. (a), (b), (c), (d), (e), (f) represent the spin structures at k_BT/J_1= 1.6, 1.2, 1.0, 0.8, 0.4, 0.2, respectively.

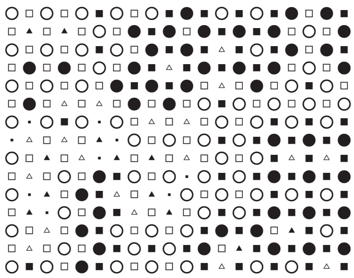
The changes of spin structure S(d) with J_4/J_1= -0.55 are shown in Fig.11 for various temperatures in the range of 0.1≦k_BT/J_1≦1.2. For this spin structure, the Curie temperature has been determined to be T_c =1.05J_1 /k_B.

The rates of occupation of a spin S_z=1 on S-spin site in ordered state below T_c are 98%, 100%, 100% at temperatures k_BT/J_1= 1.0, 0.4, 0.1, respectively. On the other hand, the rates of occupation of a spin R_z=3/2 on R-spin site are 98%, 100%, 100% and those of a spin R_z=1/2 on R-spin site are 70%, 80%, 100% at temperatures k_BT/J_1=1.0, 0.4, 0.1, respectively.

It should be noticed that the rates of the occupation of a spin S_z=1 on S-site and of a spin R_z=3/2 on R-site are both 98 % even just below T_c. The spins of R_z=1/2 on the R-site cannot make a complete spin arrangement even at very low temperature (k_BT/J_1=0.1).



(a)



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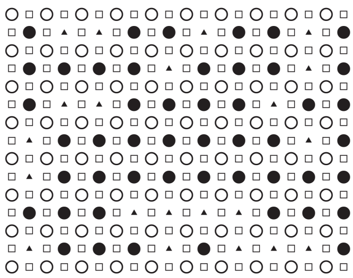
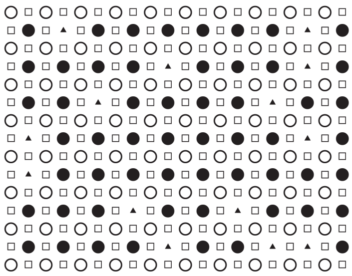
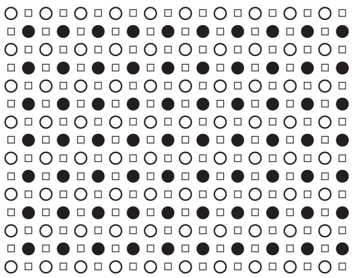


(c)



(d)



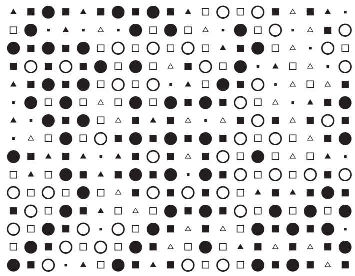
(e)

Fig. 11 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_4/J_1=-0.55 calculated by the MC simulation for various temperatures in the range of 0.1≦k_BT/J_1≦1.2. (a), (b), (c), (d), (e) represent the spin structures at k_BT/J_1= 1.2, 1.1, 1.0, 0.4, 0.1, respectively.

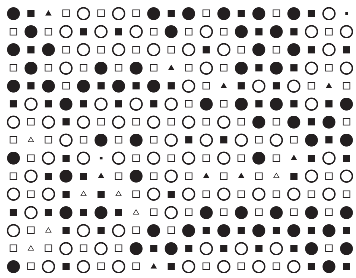
The changes of spin structure S(e) with J_4/J_1= -0.70 are shown in Fig.12 for various temperatures in the range of 0.4≦k_BT/J_1≦2.0. For this spin structure, the Curie temperature may be determined to be T_c=1.9J_1/k_B by judging from the position of the peak of the magnetic specific heat curve.

The rates of occupation of spins S_z=1 or S_z=-1 on S-spin site in ordered state below T_c are 99%, 100%, 100%, 100% at temperatures k_BT/J_1= 1.6, 1.2, 0.8, 0.4, respectively. On the other hand, the rates of occupation of spins R_z=3/2 or R_z=-3/2 on R-spin site are 90%, 98%, 100%, 100% at temperatures k_BT/J_1=1.6,1.2,0.8,0.4, respectively.

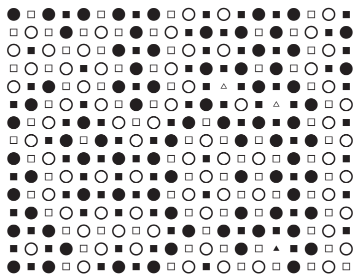
It is remarkable that the rates of occupation of spins S_z=1 or S_z=-1 on S-spin site are nearly 100% even at high temperatures k_BT/J_1= 1.6 just below T_c. Furthermore, this spin structure S(e) turned out not to change its spin arrangement for the wide temperature range of 0.1≦k_BT/J_1≦0.8.



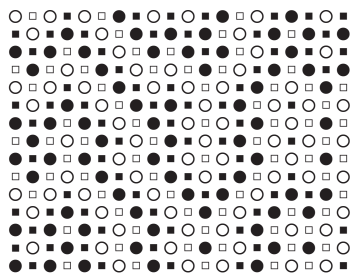
(a)



(b)



(c)



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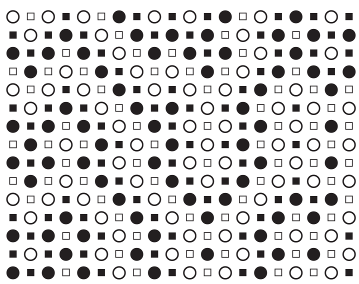

(e)

Fig. 12 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_4/J_1=-0.7 calculated by the MC simulation for various temperatures in the range of $0.4 \leqq k_BT/J_1 \leqq 2.0$. (a), (b), (c), (d), (e) represent the spin structures at k_BT/J_1= 2.0, 1.6, 1.2, 0.8, 0.4, respectively.

4. Concluding Remarks

In the previous section, for the mixed Ising spin system of S=1 and R=3/2 with the bilinear exchange interaction $J_1S_{iz}R_{jz}$, the four-site four-spin interaction $J_4S_{iz}R_{jz}S_{kz}R_{lz}$ and a single-ion anisotropy $D(S_{iz}^2+R_{jz}^2)$, the magnetization $\langle S_z \rangle$ and $\langle R_z \rangle$, the magnetic specific heat C_M, the Curie temperature T_c and the GS spin structures have been calculated for two-dimensional square lattice by making use of the MC simulation.

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

(1) The phase diagram of the ground state of the mixed Ising spin system of S=1 and R=3/2 with interaction J_4/J_1 and anisotropy D/J_1 is obtained by the MC simulation. The conditions of phase transition and the GS spin structures determined by this MC simulation show good agreements with those calculated from the comparison of energies per one spin for various spin structures with low energy.

(2) The new five magnetic phases S(a) ～S(e) are found for parameters J_4/J_1 and anisotropy D/J_1. Especially, two phases S(d) and S(e) have the same energy.

(3) In the magnetic phase S(d) with $S_z=\pm 1$ and $R_z=\pm 3/2$, the non-zero magnetization $\langle S_z \rangle$ exists on S-spin site. On the other hand, the non-zero magnetization $\langle R_z \rangle$ exists only at finite temperature below T_c and become zero at zero temperature (T=0) at R-spin site.

(4) In the magnetic phase S(e) with $S_z=\pm 1$ and $R_z=\pm 3/2$, the non-zero magnetizations $\langle S_z \rangle$ and $\langle R_z \rangle$ cannot exist on S-spin and R-spin sites at all temperature range. The GS spin structure S(e) is made at high temperature and fixed in the wide temperature range.

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