Monte Carlo Simulation of the Blume-Emery-Griffiths Model with Mixed Ising Spin

by

Takashi Iwashita*, Kakuko Uragami*, Yui Ito, Yoshinori Muraoka*****

(Received October 31, 2010)

Abstract.

The phase diagram and magnetic properties such as the magnetizations $<S_z>$ and $<R_z>$, the thermal averages $<S_z^2>$ and $<R_z^2>$, 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 $J_1S_{iz}R_{jz}$, the biquadratic exchange interaction $J_2S_{iz}^2R_{jz}^2$ 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 in the case of D=0 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 $<R_z>$, the thermal averages $<S_z^2>$ and $<R_z^2>$ and spin structures are investigated for various values of parameters of J_2/J_1 and D/J_1.

Keywords: Ising model; biquadratic 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 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].

Therefore, we have developed this MC simulation to the mixed Ising spin system with spins of S = 1 and

*General Education Center, Tokai University
** Department of Environment Conservation Sciences, School of Industrial Engineering, Tokai University
***Department of General Education, Ariake National College of Technology

R=3/2, and investigated precisely the growth of spin ordering and the ground state (GS) spin structures. In the present study, the effects of the biquadratic interaction $J_2S_{iz}^2R_{jz}^2$ and the single-ion anisotropies DS_{iz}^2 and DR_{jz}^2 on the magnetizations $<S_z>$ and $<R_z>$, thermal averages $<S_z^2>$ and $<R_z^2>$, the Curie temperature T_c and 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 $<S_z>$ and $<R_z>$, and the thermal averages $<S_z^2>$ and $<R_z^2>$ are also studied for various values of parameters J_2/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_2/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:

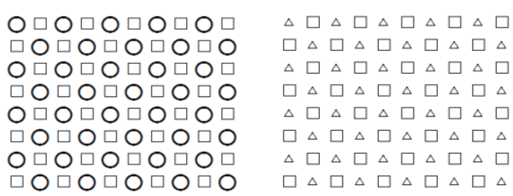
$$H = -J_1\sum_{<ij>} S_{iz}R_{jz} - J_2\sum_{<ij>} S^2{}_{iz}R^2{}_{jz} - D\sum_i S^2{}_{iz} - D\sum_j R^2{}_{jz} \quad (1)$$

Here, $<ij>$ denotes the sum on the nearest neighboring spin pairs 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 $<S_z>$ and $<R_z>$, thermal averages $<S_z^2>$ and $<R_z^2>$ 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_2, and without 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. Let us define parameters x as J_2/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 (D=0) are given as E_a = -9x/2-3 , E_b= -x/2 -1 , E_c =E_d =E_e= 0, respectively. Therefore, by comparing these energies E_a and E_b, and by comparing E_b and E_c or E_d or E_e, the conditions of phase transition are obtained as x=-1/2 and -2 for the case of D=0.



S(a) S(b)

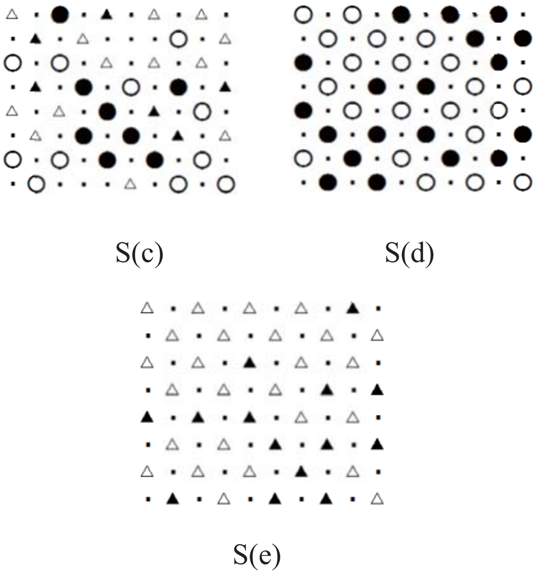


Fig. 1 The GS spin structures S(a), S(b), S(c), S(d) and S(e) for the mixed Ising spin system of *S*=1 and *R*=3/2 with interactions J_1, J_2 and anisotropy *D*. Open and closed circles, and open and closed triangles denote R_Z =±3/2 and R_Z =±1/2, and square and dot denote S_Z =1 and S_Z =0, respectively.

3. Results of Simulation and Discussion

3.1 Phase Diagram of 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 the biquadratic exchange interaction J_2 in the range of $-3.0 \leqq J_2/J_1 \leqq 0$ and the anisotropy D/J_1 in the range of $-0.5 \leqq D/J_1 \leqq 1.0$. 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_2/J_1 and D/J_1 is shown in Fig.2.

The GS spin structures of magnetic phases P(a)～P(c) on the J_2/J_1–axis (*D*=0) determined by the MC simulation are confirmed to be the spin structures S(a)～S(c) shown in Fig.1 obtained by the energy comparison, respectively. For the case of *D*=0, the conditions of phase transition are confirmed to be J_2/J_1=-1/2 and -2 by this MC simulation. The spin structures S(d) and S(e) appear as the GS structure for the case of *D*>0 and *D*<0 in the range of J_2/J_1 with negative small value, respectively. As can be seen from fig.2, it is remarkable that the GS spin structure S(b) disappears for the large anisotropy *D* in the range of D/J_1>1.1.

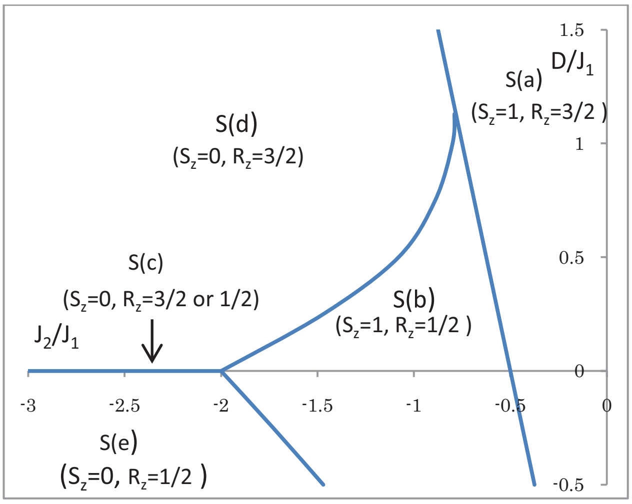


Fig. 2 Phase diagram of mixed Ising spin system on two-dimensional square lattice with exchange parameter $x(J_2/J_1)$ in the range of $-3.0 \leqq x \leqq 0$ and anisotropy $y(D/J_1)$ in the range of $-0.5 \leqq y \leqq 1.5$.

3.2 Magnetic Properties of Mixed Ising Spin System of *S*=1 and *R*=3/2 without Anisotropy *D* (*d*=0)

Let us investigate the magnetic properties such as the magnetizations $<S_z>$ and $<R_z>$, and the thermal averages $<S_z^2>$ and $<R_z^2>$ of the mixed Ising spin system of *S*=1 and *R*=3/2 without anisotropy (*D*=0) by making use of the MC simulation. The temperature dependences of $<R_z>/R$ of the mixed spin system for various values of interaction J_2 in the range of $-0.8 \leqq J_2/J_1 \leqq -0.3$ and $-2.0 \leqq J_2/J_1 \leqq -1.0$ are shown in Fig.3 and Fig.4, respectively. As can be seen from Fig.3, phase transition occurs at J_2/J_1=-1/2. The value 2/3 of $<R_z>/R$ at *T*=0 for J_2/J_1=-1/2 suggests the existence of a mixed spin structure with spins R_z =3/2 and 1/2 of the same number. The inverse temperature dependences of $<R_z>/R$ appear for interaction J_2 in the range of $-1.0<J_2/J_1<-0.5$. This interesting behavior may be understood by considering the reduction of many spins of R_z =3/2 mixed just below the Curie temperature T_c.

It can be seen from Fig.4 that temperature dependences of $<R_z>/R$ show almost same behavior for the interaction J_2 in this range of $-2.0 < J_2/J_1 \leqq -1.0$. It is remarkable that the value of $<R_z>/R$ for the interaction

J_2 in the range of -2.0 < J_2/J_1≦-1 is about 1/3 in the wide temperature range which means that all spins of R-site are R_z=1/2. Both magnetization <R_z> and Curie temperature T_c disappear at the interaction J_2 of J_2/J_1= -2.0. Therefore, phase transition is confirmed to occur at this condition of J_2/J_1=-2.0.

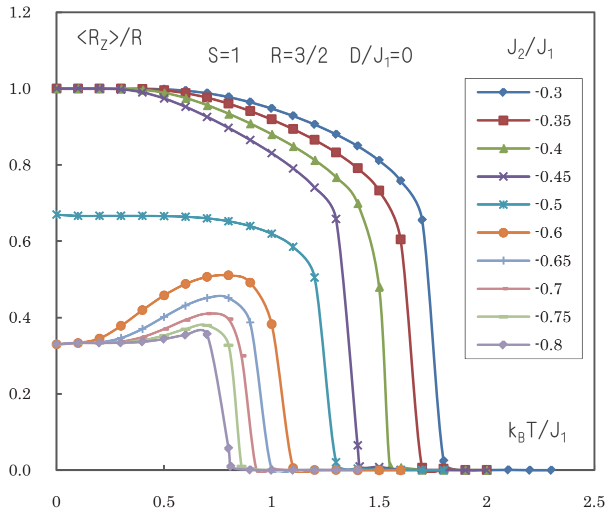


Fig. 3 Temperature dependence of <R_z>/R of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -0.8≦J_2/J_1≦-0.3.

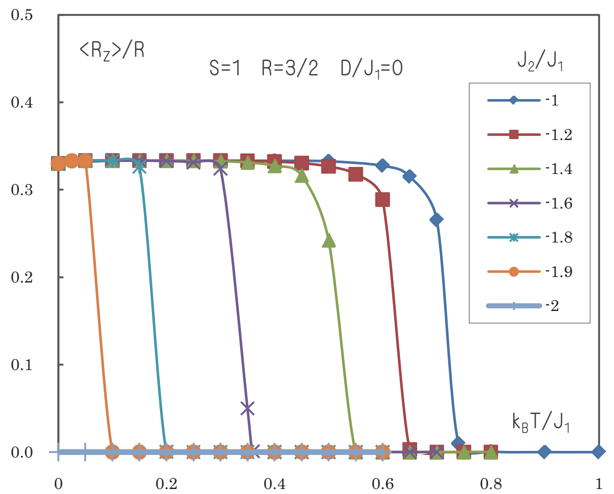


Fig.4 Temperature dependence of <R_z>/R of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -2.0≦J_2/J_1≦-1.0.

The temperature dependences of <S_z> of the mixed spin system for various values of interaction J_2 in the range of -2.0≦J_2/J_1≦-0.2 are shown in Fig.5. Both the magnetization <S_z> and the Curie temperature T_c disappear also at the interaction J_2 of J_2/J_1=-2.0 This condition of J_2/J_1= -2.0 agrees well with that of <R_z>. For these interactions in the range of -2.0≦J_2/J_1≦-0.2, the temperature dependence of the magnetization <S_z> shows almost the same behavior. The behavior of curve of <S_z> for J_2/J_1=-0.6 is, however, different from those for other interaction parameters. This behavior may show the unstable spin state near the phase transition of J_2/J_1= -1/2.

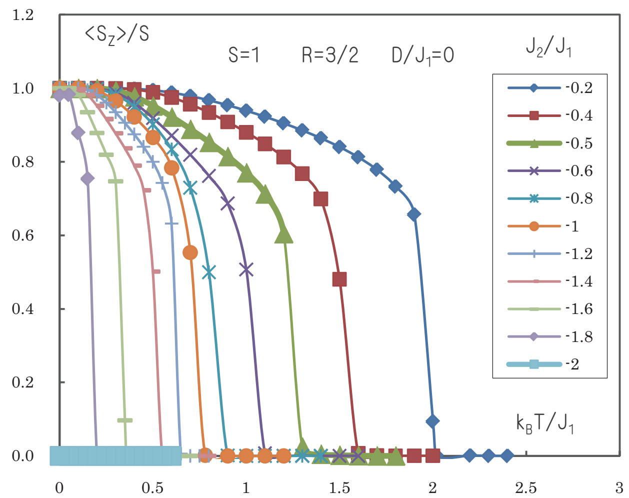


Fig.5 Temperature dependence of <S_z> (=<S_z>/S) of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -2.0≦J_2/J_1≦-0.2.

Next, the temperature dependences of thermal average <R_z^2>/R^2 of the mixed spin system for various values of interaction J_2 in the range of -0.8 ≦J_2/J_1≦-0.3 are shown in Fig.6. The value of <R_z^2>/R^2=0.5555 at T=0 for J_2/J_1=-0.5 suggests that the number of spins R_z=3/2 and 1/2 is equal. It is noticeable that the number of spin of R_z=1/2 is larger than the one of R_z=3/2 at high temperatures for the interaction parameter in the range of -0.8≦ J_2/J_1≦-0.4. The curve of <R_z^2>/R^2 for J_2/J_1=-0.55 shows that the spin R_z=3/2 increases in the temperature range just below T_c. This fact supports the inverse temperature dependence of <R_z>/R for interaction J_2/J_1=-0.55 shown in Fig.3.

Furthermore, the temperature dependences of thermal average <R_z^2>/R^2 of the mixed spin system for various values of interaction J_2 in the range of -2.2≦J_2/J_1≦-1.0 are shown in Fig.7. As can be seen from Fig.7, the ordered state with spins of R_z=1/2 on R-site can established after abrupt decrease of spins of R_z=3/2 at low temperatures. At the condition of J_2/J_1≦-2.0, the number of spins of R_z =3/2 and 1/2 turns out to become almost equal by considering the value of $<R_z^2>/R^2$ at T=0.

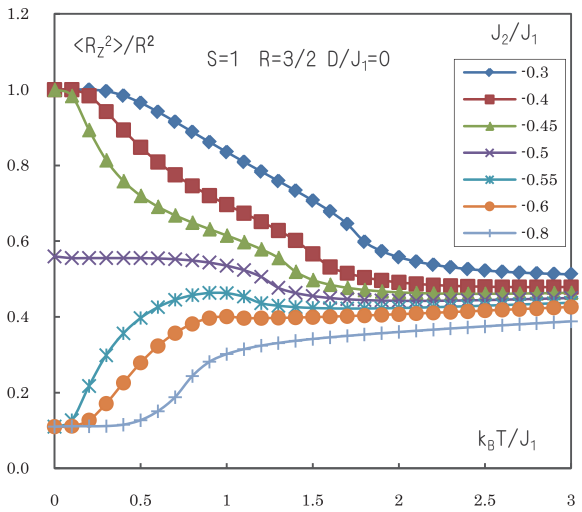


Fig. 6 Temperature dependence of $<R_z^2>/R^2$ of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -0.8≦J_2/J_1≦-0.3.

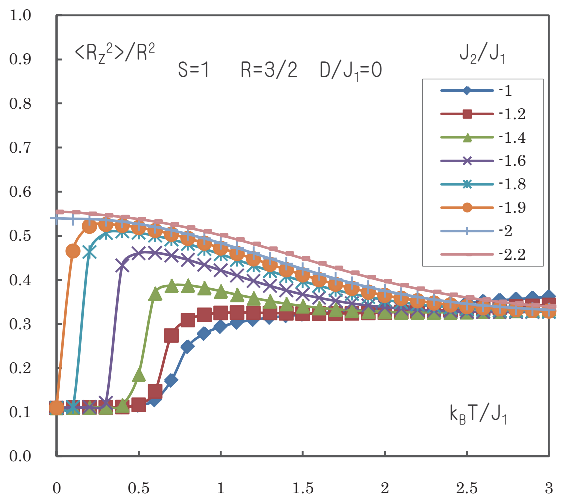


Fig. 7 Temperature dependence of $<R_z^2>/R^2$ of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -2.2≦J_2/J_1≦-1.0.

Furthermore, we have also investigated the temperature dependences of thermal average $<S_z^2>$ of the mixed spin system with S=1 and R=3/2. The calculated results for various values of interaction J_2 in the range of -2.2≦J_2/J_1≦-0.3 are shown in Fig.8. As can be seen from Fg.8, the curves of $<S_z^2>$ show the minimum value for the interaction of -2.0 < J_2/J_1≦-0.6. It is remarkable that this minimum value of $<S_z^2>$ approaches to zero as the interaction J_2 approaches to J_2/J_1=-2.0. The minimum values of $<S_z^2>$ for J_2/J_1=-1.9, -1.95, -1.98 become 0.019, 0.015, 0.012. Therefore, these facts suggest that the rate of spin S_z =1 of S-site is only one or two in the 100 spins for J_2/J_1 in the range of-2.0 < J_2/J_1≦-1.9. It is interesting that the spin structure with spin S_z =0 of large number for J_2/J_1 in the range of-2.0 < J_2/J_1≦-1.9 changes to the one with spin S_z =1 of large number with decreasing temperature of small step.

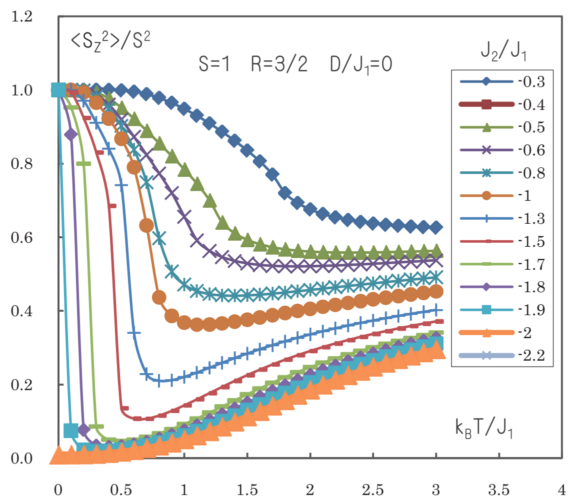


Fig. 8 Temperature dependence of $<S_z^2>$ (=$<S_z^2>/S^2$) of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -2.2≦J_2/J_1≦-0.3.

Next, we have investigated the changes of spin structure for various values of temperature by making use of the MC simulation and visualized the change of this structure. The changes of spin structure of J_2/J_1=-1.9 are shown in Fig.9 for various temperatures. It is confirmed that the spin structure with spin S_z =0 of large number at k_BT/J_1=0.1 change abruptly to the one with spins S_z =1 of large number at k_BT/J_1=0.05, and the same time, the spin structure with mixed spins of R_z=±1/2 and ±3/2 at k_BT/J_1=0.1 also change to the one with spin R_z=1/2 of large number at k_BT/J_1=0.05. The spin structure at k_BT/J_1=0.1 agrees with the one of S(b) in Fig.1.

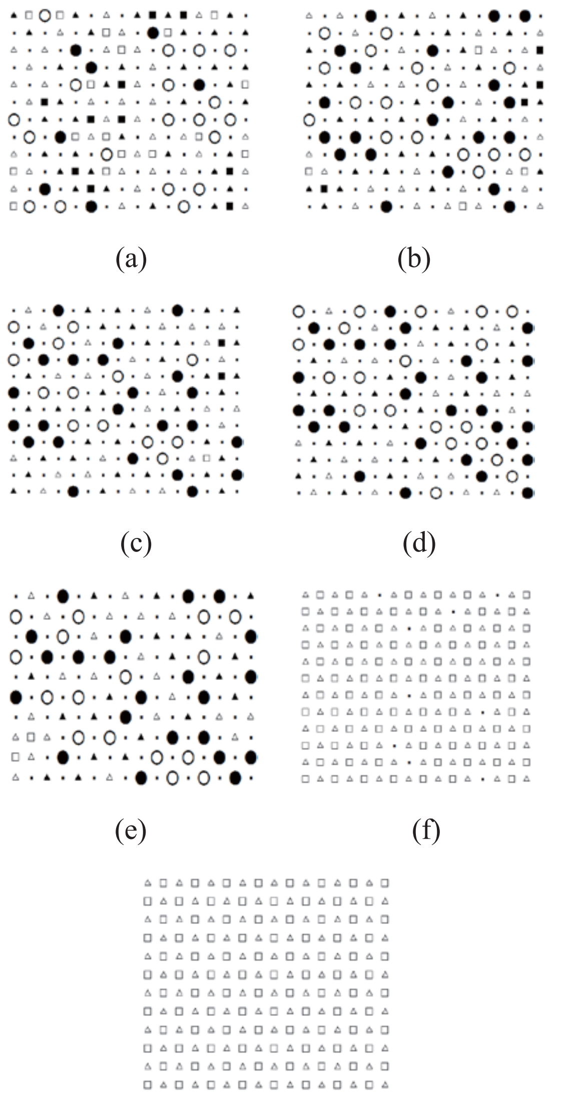


Fig. 9 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_2/J_1=-1.9 calculated by the MC simulation for various temperatures in the range of 0.01 ≦ k_BT/J_1 ≦ 3.0. (a),(b),(c),(d),(e),((f),(g) represent the spin structures at k_BT/J_1=3.0, 2.0, 1.0, 0.3, 0.1, 0.05, 0.01,respectively.

Furthermore, we have investigated the changes of the Curie temperature T_c for various values of interaction parameter J_2/J_1 by making use of the MC simulation. The results for J_2/J_1 in the range -2.0≦J_2/J_1≦0 are shown in Fig.10. From Fig.10, the effects of interaction J_2 on T_c turn out to be large in the phase with S(a) and in the neighborhood of phase transition of J_2/J_1=-0.5. It is remarkable that the change of T_c is small in the range of -1.4≦J_2/J_1≦-0.8. This fact suggests that the GS spin structure in this middle range between two phase transitions of J_2/J_1=-0.5 and J_2/J_1=-2.0 is more stable than the one in the neighborhood of phase transition.

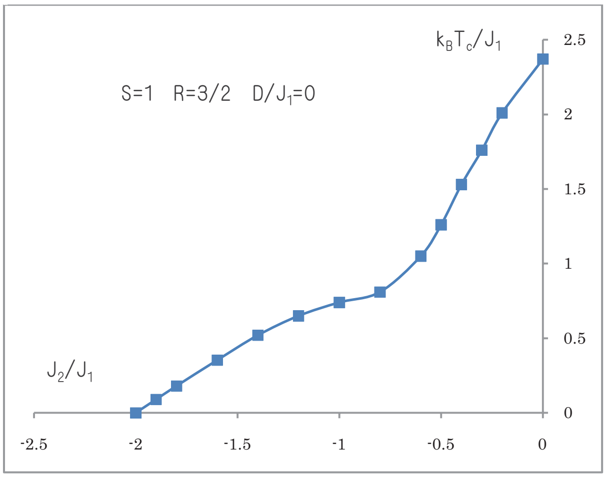


Fig. 10 The change of Curie temperature T_c of the mixed spin system with S=1 and R=3/2 calculated by the MC simulation for various values J_2 of in the range of -2.0≦J_2/J_1≦0

3.3 Magnetic Properties of Mixed Ising Spin System of S=1 and R=3/2 with Anisotropy *D* (*d*≠0)

Next, let us investigate the magnetic properties such as the magnetizations $<S_z>$ and $<R_z>$, and the thermal averages $<S_z^2>$ and $<R_z^2>$ of the mixed Ising spin system of S=1 and R=3/2 with interactions J_1 and J_2 and anisotropy term D by making use of the MC simulation.

The temperature dependences of $<S_z^2>$ for mixed spin system with anisotropy D/J_1=0.25 and various values of interaction J_2 in the range of -1.47≦J_2/J_1≦-1.0 are shown in Fig.11. From the behaviors of $<S_z^2>$ for J_2/J_1=-1.46 and -1.47, phase change turns out to occur at the condition of J_2/J_1=-1.47. As can be seen from Fg.11, the curves of temperature dependence of $<S_z^2>$ have minimum values for the interaction of -1.47< J_2/J_1≦-1.0. It is remarkable that this minimum value of $<S_z^2>$ approaches to zero as the interaction J_2 approaches to J_2/J_1=-1.47. The minimum values of $<S_z^2>$ for J_2/J_1=-1.46 and -1.40 become 0.002 at k_BT/J_1=0.3 and 0.009 at k_BT/J_1=0.4, respectively. Therefore, these facts about $<S_z^2>$ suggest that all spins of S-site are almost S_z=0. Furthermore, these minimum values for D/J_1=0.25 turn out to be smaller than those for D/J_1=0. It should be noted that the sharp increase of $<S_z^2>$ appears for interaction J_2 in the range of

-1.47< $J_2/J_1 \leqq$ -1.2 with decreasing temperature. Especially, the increase of $<S_z^2>$ is very sharp from $<S_z^2> \fallingdotseq 0$ to $0.8<<S_z^2>$ for interaction J_2 in the range of -1.47< $J_2/J_1 \leqq$ -1.3. This fact suggest that the large number of spins of S-site turns from S_z=0 to S_z=1 as the temperature decreases with a small step.

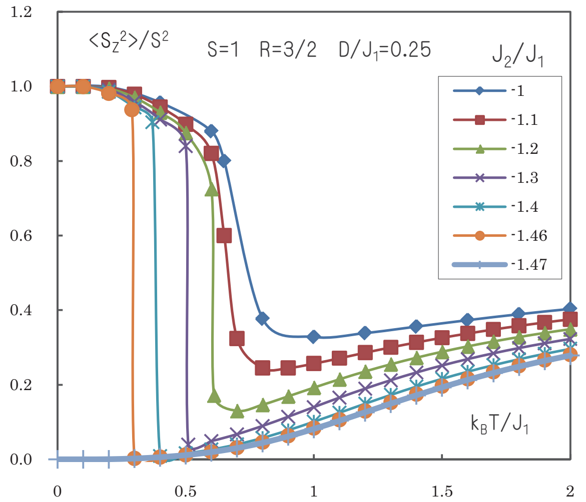


Fig. 11 Temperature dependence of $<S_z^2>$ (=$<S_z^2>/S^2$) of the mixed spin system with S=1 and R=3/2 and D/J_1 =0.25 calculated by the MC simulation for various values J_2 of in the range of -1.47$\leqq J_2/J_1 \leqq$-1.0.

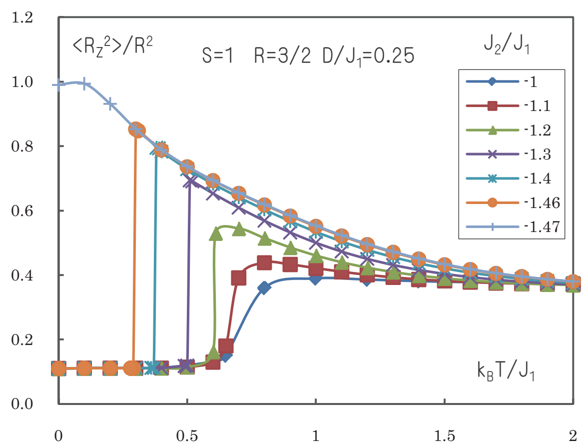
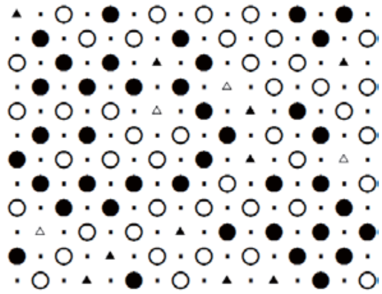


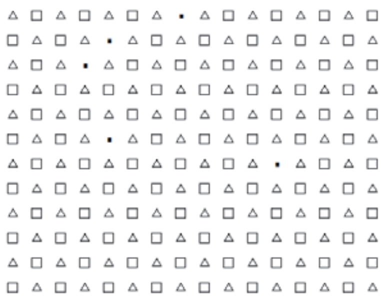
Fig. 12 Temperature dependence of $<R_z^2>/R^2$ of the mixed spin system with S=1 and R=3/2 and D/J_1 =0.25 calculated by the MC simulation for various values J_2 of in the range of -1.47$\leqq J_2/J_1 \leqq$-1.0.

The temperature dependences of $<R_z^2>/R^2$ for mixed spin system with anisotropy D/J_1=0.25 and various values of interaction J_2 in the range of -1.47 $\leqq J_2/J_1 \leqq$-1.0 are shown in Fig.12. It is remarkable that sharp decrease of $<R_z^2>/R^2$ appear for interaction J_2 in the range -1.47< $J_2/J_1 \leqq$-1.2, and especially, the large number of spins of R_z =3/2 on the R-site turn to R_z =1/2 as the temperature decrease with a small step.

As can be seen from Fig.11 and Fig.12, the spins of S-site and R-site change abruptly and make new spin structures at the same temperature. The drastic changes of spin structures from k_BT/J_1=0.3 to k_BT/J_1=0.29 of the Ising spin system with J_2/J_1= -1.46 and D/J_1=0.25 are shown in Fig.13.



(a)



(b)

Fig. 13 Temperature dependence of spin structure of the mixed spin system of S=1 and R=3/2 with J_2/J_1=-1.46 and D/J_1=0.25 calculated by the MC simulation for temperature (a) k_BT/J_1=0.3 and (b) k_BT/J_1=0.29.

The temperature dependences of $<S_z^2>$ for mixed spin system with anisotropy D/J_1=0.5 and various values of interaction J_2 in the range of -1.07 $\leqq J_2/J_1 \leqq$-0.85 are shown in Fig.14. As can be seen from Fg.14, the curves of $<S_z^2>$ show the minimum value for the interaction of -1.07< $J_2/J_1 \leqq$-0.85. The minimum value of $<S_z^2>$ for J_2/J_1=-1.06 is 0.03 at k_BT/J_1=0.5. Therefore, these values suggest that all spins of S-site are not S_z=0 and the spins of S_z=1 are mixed even for interaction J_2 with the condition near phase transition. The increases of $<S_z^2>$ for D/J_1=0.5 are sharp for interaction J_2 of -1.07< $J_2/J_1 \leqq$-1.0.

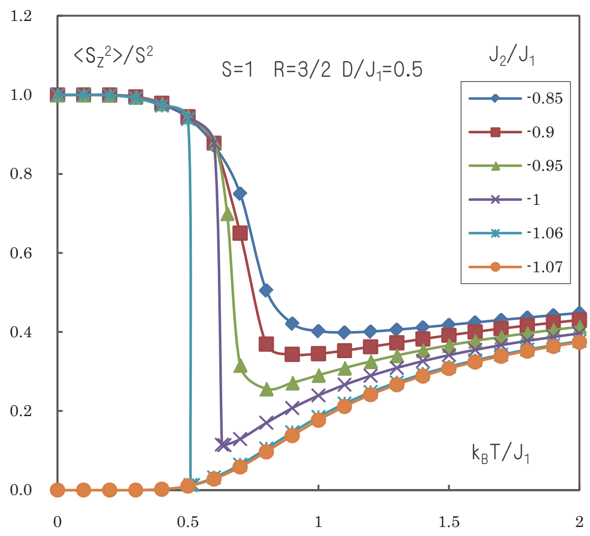


Fig. 14 Temperature dependence of $<S_z^2>$($=<S_z^2>/S^2$) of the mixed spin system with S=1 and R=3/2 and D/J_1=0.5 calculated by the MC simulation for various values J_2 of in the range of -1.07≦J_2/J_1≦-0.85.

The temperature dependences of $<R_z^2>/R^2$ for mixed spin system with anisotropy D/J_1=0.5 and various values of interaction J_2 in the range of -1.07 ≦J_2/J_1≦-0.85 are shown in Fig.15. It is remarkable that sharp decrease of $<R_z^2>/R^2$ appear for interaction J_2 in the range -1.07< J_2/J_1≦-1.0, and especially, all spins of R_z =3/2 on R-site turn to R_z =1/2 as the temperature decrease with a small step.

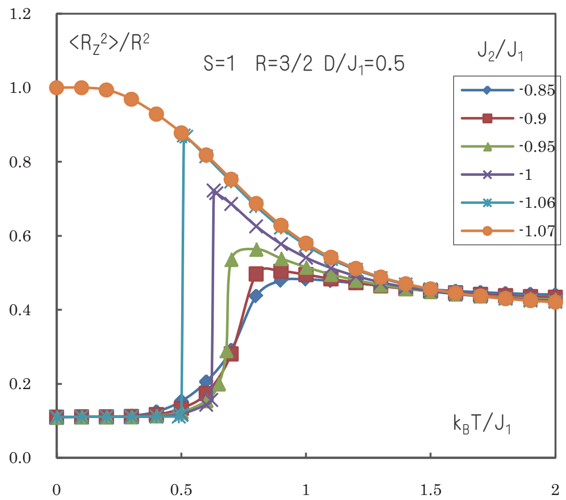


Fig. 15 Temperature dependence of $<R_z^2>/ R^2$ of the mixed spin system with S=1 and R=3/2 and D/J_1 =0.5 calculated by the MC simulation for various values J_2 of in the range of -1.47≦J_2/J_1≦-1.0.

The temperature dependences of $<S_z^2>$ for mixed spin system with negative anisotropy D/J_1= -0.25 and va rious values of interaction J_2 in the range of -1.80≦J_2/J_1≦-1.40 are shown in Fig.16. As can be seen from Fg.15, the curves of $<S_z^2>$ show gentle temperature dependence for the interaction of -1.73≦J_2/J_1≦-1.40. The minimum values of these curves cannot become small. T he minimum value of $<S_z^2>$ for J_2/J_1=-1.70 is 0.105 at k_BT/J_1=0.6.

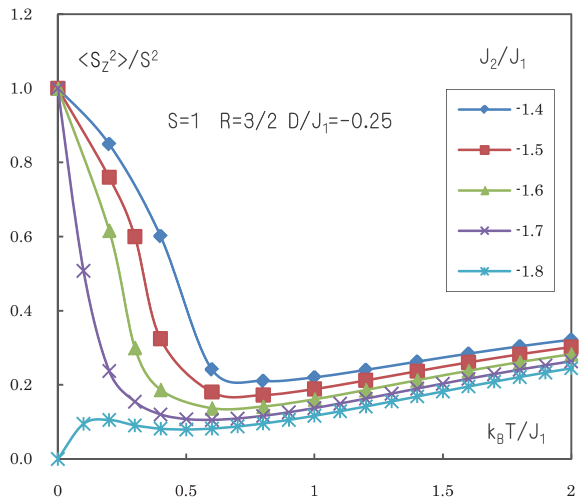


Fig. 16 Temperature dependence of $<S_z^2>$ ($=<S_z^2>/S^2$) of the mixed spin system with S=1 and R=3/2 and D/J_1=-0.25 calculated by the MC simulation for various values J_2 of in the range of -1.8≦J_2/J_1≦-1.4.

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 $J_1S_{iz}S_{jz}$, the biquadratic exchange interaction $J_2S_{iz}^2S_{jz}^2$ and a single-ion anisotropy D, the magnetization $<S_z>$ abd $<R_z>$, the thermal average $\langle S_z^2\rangle$ and $\langle R_z^2\rangle$, 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 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_2/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 for D=0 show good agreements with those calculated from the comparison of energies per one spin for various spin structures with low energy.

(2) The spins S_z = 0 of large number on S-site just above T_c change abruptly to S_z = 1 just below T_c, and the spins R_z=3/2 on R-site just above T_c change abruptly to R_z= 1/2 just below T_c near the condition of phase transition. This abrupt change appears for anisotropy $0 \leqq D/J_1 \leqq 0.5$.

(3) The abrupt change of spin structure on S-site from S_z = 0 to S_z = 1 appears under the condition of $0< J_2/J_1 \leqq 0.3$ and near the phase transition.

(4) Judging from the behavior of interaction J_2/J_1 dependence of the Curie temperature T_c for D=0, the spin structure S(b) may be more stable than the spin structure S(a), and especially, spin structure S(b) become stable in the middle range of $-1.4 \leqq J_2/J_1 \leqq -0.8$.

Refernces

1. M.Blume, V.J. Emerry and Robert B. Griffiths,*Phys. Rev.* A4*, 1071* (1971).
2. H. A. Brown, *Phys. Rev. B* **4**, 115 (1971).
3. J. Adler and J. Oitmaa, *J. Phys. C* **12**, 575 (1979).
4. T. Iwashita and N. Uryu, *J. Phys. C* **17**, 855 (1984).
5. H.H.Chen and P.M.Levy, *J. Phys. Rev*. **7**, *4267* (1973).
6. J.M.Baker, *JRep.Prog. Phys*. 34*, 109* (1971).
7. M. Roger, J. M. Delrieu and J. H. Hetherington, *Phys. Rev. Lett*. **45**, 137 (1980).
8. A.K.McMahan and R.A.Guyer, *Phys. Rev.* **A7***, 1105* (1973).
9. J.H.Hetherington and F.D.C.Willard, *Phys. Rev*. Lett. **35***, 1442*(1975).
10. M.Roger, J.M.Delrieu and A. Landesman, *Phys. Lett.* **62A***, 449* (1977).
11. T. Iwashita, R. Satou, T. Imada and T. Idogaki, *Physica B* **284**, 1203 (2000).
12. T. Iwashita, K. Uragami, K. Goto, K.Kasama and T. Idogaki, *J.Magn.Magn.Mater.* **272**,672 (2004).
13. T. Iwashita, K. Uragami, A.Shimizu, A.Nagaki, T.Kasama and T. Idogaki, *J.Magn.Magn.Mater.* **310**,435 (2007).
14. T. Iwashita and N. Uryu, *J. Phys*. Condens. Matter **3**, 8257 (1991).