Magnetization and ground state spin structures of Ising spin system with four-spin interaction

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Abstract

The magnetization of spin $S(= 1/2$ and $1)$ Ising systems with bilinear and four-site four-spin interactions has been investigated by making use of the Monte Carlo simulation. In low temperature region, the magnetization curves show an anomalous inverse inclination and decrease (increase) with the decrease (increase) of temperature within a certain exchange ratio range. The relation between the value of the magnetization at zero-temperature and the spin structure expected for the ground state is discussed.

Key words: four-site four-spin interaction; Ising model; Monte Carlo simulation; magnetization; ground state

In Heisenberg and Ising ferromagnets, the existence and the importance of such higher-order exchange interactions as $(S_i \cdot S_j)^2$, $(S_i \cdot S_j)(S_j \cdot S_k)$, $(S_i \cdot S_j)(S_k \cdot S_l)$ 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 super exchange interaction, the magnetoelastic effect, the permutation operator, the perturbation expansion and the spin-phonon coupling[3].

In solid helium and some other materials showing such phenomena as quadrupolar ordering of molecules (solid hydrogen, liquid crystals) or the cooperative Jahn Teller phase transitions, the higher-order exchange interactions turned out to be the main ones[4]. In a spin system with a bilinear exchange interaction $J_0(S_i \cdot S_j)$ and a four-site four-spin interaction $J(S_i \cdot S_j)(S_k \cdot S_l)$, the interaction J is expected to have significant effects on magnetic properties, especially in the low temperature region in the case of J not negligible compared to J_0/S^2. Furthermore, the ferromagnetic state established by the interaction J_0 becomes unstable with the introduction of J of a negative sign.

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In the present study, the effects of the four-site four-spin interaction $JS_{iz}S_{jz}S_{kz}S_{lz}$ on the magnetization $\langle S_z \rangle$ of Ising spin systems of $S = 1/2$ and $S = 1$ on two-dimensional square lattice are investigated for negative values of J by using the Monte Carlo(MC) simulation. The obtained characteristic behavior of $\langle S_z \rangle$ is discussed in conjunction with the ground state (GS) spin structures determined by energy evaluations.

The spin Hamiltonian for the present Ising spin system can be written as follows:

$$\mathcal{H} = -J_0 \sum_{<i,j>} S_{iz}S_{jz} - 2J \sum_{<i,j,k,l>} S_{iz}S_{jz}S_{kz}S_{lz}. \quad (1)$$

The coefficient of the second term in this Hamiltonian (1) has been obtained by considering the sum of two terms $(S_{iz} \cdot S_{jz})(S_{kz} \cdot S_{lz})$ and $(S_{iz} \cdot S_{lz})(S_{jz} \cdot S_{kz})$.

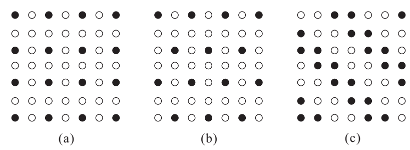

Fig. 1. The spin structures on the two dimensional square lattice. Open and closed circles denote $S_z = 1/2$ and $-1/2$ for $S = 1/2$, and $S_z = 1$ and -1 for $S = 1$.

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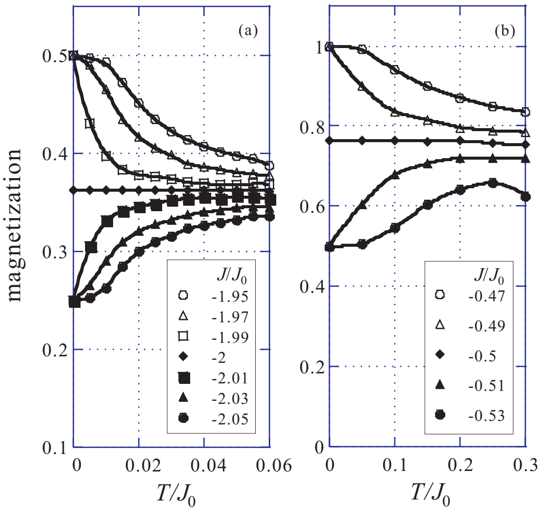

Fig. 2. The temperature dependence of $\langle S_z \rangle$ for (a) $S = 1/2$ in the range of $-2.05J_0 < J < -1.95J_0$, and (b) $S = 1$ in the range of $-0.53J_0 < J < -0.47J_0$.

The GS spin structures and the conditions of GS phase transitions are determined by comparing the energies of various spin structures with each other(see e.g. [5]). For $S = 1/2$ and $S = 1$, we found that the phase changes take place at $J = -2J_0$ and $J = -J_0/2$, respectively. Some typical spin structures which take the lowest energy for $S = 1/2$ for $J < -2J_0$ and for $S = 1$ for $J < -J_0/2$, respectively, are shown in Fig.1. At $J = -2J_0$ for $S = 1/2$ and $J = -J_0/2$ for $S = 1$, a ferromagnetic spin structure, the ones shown in Fig.1 and many other spin structures coexist in the ground state.

On the other hand, MC simulations based on the Metropolis method are carried out assuming periodic boundary condition for two dimensional square lattice with linear lattice size $L = 100$. For fixed values of $|J/J_0|$, we start the simulation at high temperatures adopting a random, a ferromagnetic, and an antiferromagnetic initial configurations, respectively, and gradually lower the temperature. We use the last spin configuration as input for the calculation at the next point. Thermal averages $\langle S_z \rangle$ are calculated using 2×10^5 MC steps per spin (MCS/s) after discarding first 3×10^5 MCS/s. In order to investigate 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.

The temperature dependence of $\langle S_z \rangle$ was calculated for various values of $J(< 0)$ for fixed $J_0(> 0)$. In the calculation, magnetization curves were found to show the same behavior, irrespective of the initial configuration. The results at low temperatures are shown in Fig.2 for $S = 1/2$ and 1 in the vicinity of each GS phase change point $J = -2J_0$ and $-J_0/2$, respectively.

The values of $\langle S_z \rangle$ at $T = 0$ are 0.25 for $S = 1/2$ for $J < -2J_0$ and 0.5 for $S = 1$ for $J < -J_0/2$. These suggest that the spin structures shown in Fig.1 (a), (b) and their mixtures are selectively realized as the GS for both cases of $S = 1/2$ and $S = 1$. In some spin systems, the entropy-induced phase transitions occur due to thermal fluctuations (i.e. entropy effect) while the GS is energetically degenerated[6,7], and it seems likely that the spin structure caused by thermal fluctuations determines the true GS spin structure with decreasing temperature. In the present case, we found they are those having $\langle S_z \rangle = S/4$. The conditions of the GS phase change are consistent with the results obtained from the energy evaluations. At $J = -2J_0$ for $S = 1/2$ and $J = -J_0/2$ for $S = 1$, the value of $\langle S_z \rangle$ at $T = 0$ turns out to be $3S/4$, i.e. a mean value of saturated ferromagnet, S, and those mentioned above, $S/4$.

The behavior of $\langle S_z \rangle$ at low temperatures after undergoing a phase change is very characteristic. As seen in Fig.2, $\langle S_z \rangle$ decrease with decreasing temperature for $S = 1/2$ in the range of $-2.05J_0 < J < -2J_0$ and for $S = 1$ in the range $-0.53J_0 < J < -0.5J_0$. By performing MC simulation for the heating process we confirmed that those behaviors are reversible, i.e. $\langle S_z \rangle$ increases with increasing temperature at low temperatures. These temperature dependences of $\langle S_z \rangle$ are caused by the contribution from spin states with larger total spin due to thermal excitation. Furthermore, e.g. $\langle S_z \rangle$ for $S = 1$ in the range of $-J_0 < J < -0.7J_0$ (not shown in Fig.2) takes almost constant value, $\langle S_z \rangle \sim 0.5$, and shows no apparent temperature dependence in a wide temperature range. The equilibrium of the decrease of $\langle S_z \rangle$ due to the thermal disturbance and the increase owing to the contribution from spin states with larger total spin thermal excitation may bring about this flat behavior of $\langle S_z \rangle$.

These anomalous behaviors are expected to be observed in some real substances such as rare-earth compounds.

References

[1] H.A.Brown, Phys. Rev. B **4** (1971) 115.

[2] J.Adler, J.Oitmaa, J. Phys. C **12** (1976) 2911.

[3] T.Iwashita, N.Uryu, J. Phys. C **17** (1984) 855.

[4] M.Roger, J.M.Delrieu, J.H.Hetherington, Phys. Rev. Lett. **45** (1980) 137.

[5] T.Iwashita, N.Uryu, J. Phys. Condens. Matter **3** (1991) 8257.

[6] S.Watari, S.Miyashita, H.Shiba, J. Phys, Soc. Jpn. **70** (2001) 332.

[7] Y.Miyoshi, T.Idogaki, J. Magn. Magn. Mater. in press.