Reanalysis of a stacked triangular Ising antiferromagnet by use of Monte Carlo simulations

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We have reinvestigated the magnetic properties of a stacked triangular Ising antiferromagnet by use of multi-spin-flip Monte Carlo (MC) simulations with the aid of finite-size-scaling theory. According to our MC results, only one phase transition occurs in this crystal.

In recent years, interest in phase transitions of frustrated Ising-spin systems has been enhanced in connection with experiment.[1-6] Blankschtein *et al.*[2] suggested, from a theoretical speculation together with a Monte Carlo (MC) study, that two phase transitions occur in the stacked antiferromagnetic triangular lattice. We restudy the same problem by the use of multi-spin-flip (MSF) MC method.

The Hamiltonian of the system is written as

$$\mathcal{H} = -J_0 \sum_{\langle i,j \rangle}^{z} S_i S_j + J_1 \sum_{\langle i,j \rangle}^{xy} S_i S_j , \tag{1}$$

where J_0 is the nearest-neighbor (NN) interaction along the z axis and J_1 is the NN interaction in the xy plane (Fig. 1). Here J_0 and J_1 are both positive. $S_i(=\pm 1)$ denotes an Ising spin at site i and the summations run over the NN pairs either along the z axis or in the xy plane.

According to the previous MC simulations,[2,6] there is a sharp peak in the specific heat at the temperature $T \simeq 2.15 J_1/k_B (\equiv T_N)$ in the case of $J_0/J_1 = 0.5$, where k_B denotes the Boltzmann constant, and it is believed that a phase transition occurs at this temperature. Moreover, there is a small peak at the temperature $T \simeq 0.45 J_1/k_B (\equiv T_L)$. Blankschtein *et al.* thought that the second phase transition occurs at $T = T_L$ and the peak is due to the phase transition. In this paper, we show that this peak, which is actually a bump, is not due to the conventional phase transition, but the linear-chain-like excitations.

In this crystal at low temperatures, the correlation in the z direction is extremely larger than that in the xy plane, and hence the conventional single-spin-flip (SSF) MC method may fail to predict the correct behavior of the magnetic property of the crystal.[6] This difficulty can be removed if we use the multi-spin-flip method:[7] Let us consider a spin cluster composed of n spins on a column parallel to the z axis. There are 2^n possible spin states for the cluster. The spin states of the cluster can be determined by the MC method if the configuration of surrounding spins is known. That is, a renewed state of the cluster is chosen among the 2^n states at each MC trial. In our case, $n = L_z$ is the lattice size in the z direction.

We have performed the MSF MC simulations for various values of J_1/J_0. The adopted lattice size was $N = 18^2 \times L_z$. L_z was fixed at the value of 12 because of the limit of machine capacity. The effect of the L_z value will be discussed later in this paper. We assumed the periodic boundary conditions. In our calculation, the MC average was taken over 5000 MC steps per cluster after discarding 5000 MC steps per cluster. We used a cooling process such that the initial spin configuration at the temperature T is inherited from the final configuration at the higher temperature $T + \Delta T$, where $\Delta T = 0.1 J_0/k_B$. The starting temperature was taken at $T = 4.0(2J_0)/k_B$.

In Fig. 2, we show the MSF MC data of the specific heat defined by

$$c = K^2 [\langle (\mathcal{H}/J_0)^2 \rangle - \langle \mathcal{H}/J_0 \rangle^2]/N , \tag{2}$$

where $K = J_0/k_B T$. There is a small bump in the specific heat at $k_B T/(2J_0) \simeq 0.45$. The peak position, the peak

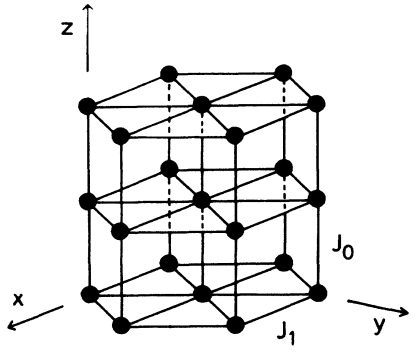

FIG. 1. Lattice structure of a stacked triangular Ising antiferromagnet.

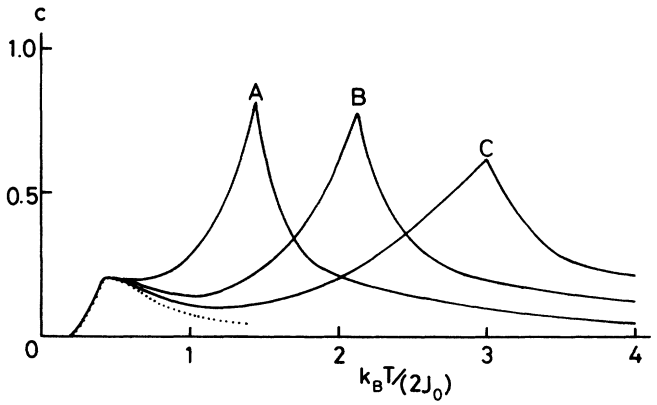

FIG. 2. MC data of the specific heat for various values of J_1/J_0: $J_1/J_0 = 1.0$ (A); 2.0 (B); 3.0 (C); for the dotted line, see text.

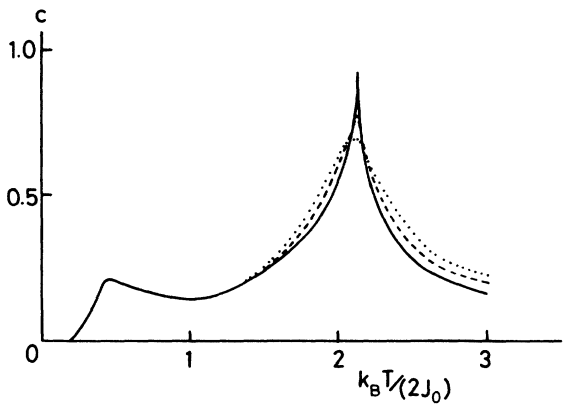

FIG. 3. MC data of the specific heat for various values of the crystal size, $N=L_x^2\times 12$: $L_x=12$ (dotted line), $L_x=18$ (dashed line), and $L_x=24$ (solid line). The value of J_1/J_0 was fixed at 2.0.

height, and the shape of the bump on the low-temperature side are not affected by the change of the J_1/J_0 value, as can be seen from this figure. Hence, we think that this bump is due to the linear-chain-like excitations in the crystal, where the coupling constant of the "linear-chain" is given by J_0. According to Coppersmith,[3] the specific heat of our system is expressed as

$$c=\gamma c_{LC} \tag{3}$$

at low temperature. Here $c_{LC}=K^2/(\cosh K)^2$ represents the specific heat of a free linear chain and γ is a numerical factor where $\frac{1}{3}<\gamma<\frac{2}{3}$. Our MC data at low temperatures are well fitted by Eq. (3) if $\gamma=0.376$ (the dotted line in Fig. 2).

In Fig. 3, we show the MSF MC data of the specific heat for various values of the crystal size: $N=12^2\times 12$, $18^2\times 12$, and $24^2\times 12$. The J_1/J_0 value was fixed at 2.0. The peak at high temperature shows an appreciable change due to the size change. On the other hand, the bump at low temperature does not show any change due to the size change. The above behavior also indicates that the bump is not due to the conventional phase transition. Although we have to perform the MC calculation with increasing lattice size in the z direction, we could not do it because of the limit of the machine capacity. Instead, we perform the calculation for the case $L_z=9$.

In order to see the linear-chain-like excitations in our crystal, we compare the specific heat of our crystal with that of the linear chain at low temperature. The partition function of a linear chain with periodic boundary condition (or ring) with n spins is written as

$$Z(n)=2^n[(\cosh K)^n+(\sinh K)^n], \tag{4}$$

where $K=J_0/k_BT$. On the other hand, the partition function of the linear chain with free ends (or open chain) is written as

$$Z(n)=2^n(\cosh K)^{n-1}. \tag{5}$$

By using the standard formula, we can calculate the specific heat as

$$C=-k_B\frac{d}{dT}\frac{d}{d(1/T)}[\ln Z(n)].$$

The computed specific heat (c) of the linear chain is

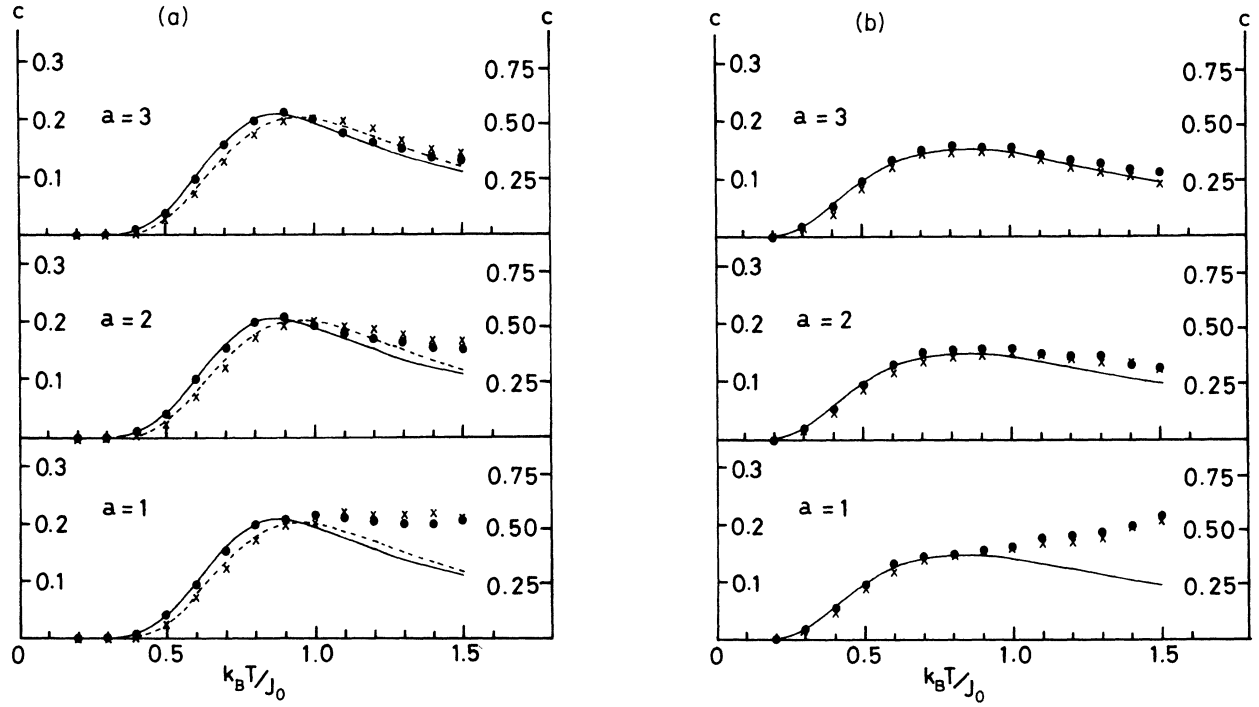

FIG. 4. (a) The specific heat of our crystal with a periodic boundary condition is compared with that of the ring. $a=J_1/J_0$. The scale for the crystal is written on the left ordinate and the scale for the ring on the right ordinate; see text. (b) The specific heat of the crystal with free xy surfaces is compared with that of the open chain. $a=J_1/J_0$; see text.

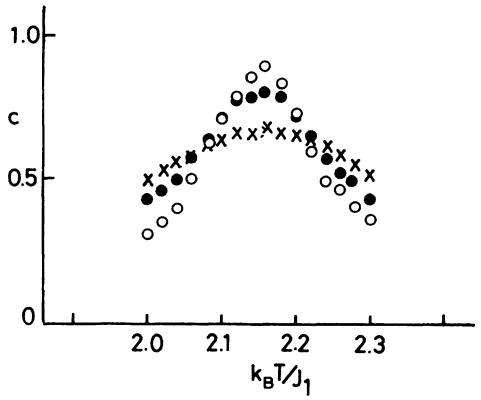

FIG. 5. The specific heat data by the single-spin-flip MC method for various lattice sizes: $N=12^3$ (crosses), 18^3 (filled circles), and 24^3 (open circles). The value of J_1/J_0 was fixed at 2.0.

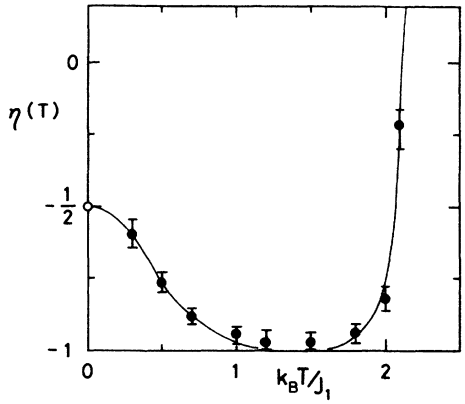

FIG. 6. MC data of $\eta(T)$ defined in Eq. (7) for the case $J_1/J_0=2.0$.

shown in Figs. 4(a) and 4(b). Here $c\equiv C/(nk_B)$. In Fig. 4(a), the solid line and the dashed line denote the specific heat of the ring with $n=12$ and $n=9$, respectively. The solid line in Fig. 4(b) denotes c with an open chain of $n=12$. We note the following two points: (i) For the case of the ring, the peak position depends on the value of n. (ii) For the case of the open chain, the peak position does not depend on the n value but the magnitude of c is given by $c_{LC}(n-1)/n$.

We also show the MC result of specific heat for our crystal in Figs. 4(a) and 4(b). The filled circles denote the MC data for the crystal size $N=18^2\times12$ and the crosses denote the MC data for the crystal size $N=18^2\times9$. The periodic boundary conditions are assumed in Fig. 4(a) and the free xy surfaces are assumed in Fig. 4(b). As can be seen from Figs. 4(a) and 4(b), the MC data for our crystal demonstrates the above-mentioned characteristic features of the specific heat of the linear chain. Hence, we think that the MC calculation again indicates the existence of the linear-chain-like excitations in the crystal.

At a high temperature of $k_BT/(2J_0)\simeq2.15$, where the peak of the specific heat is observed, the SSF excitations will be dominant compared with the linear-chain-like excitations. Hence, we performed the conventional SSF MC simulations in this temperature region. In the SSF calculation, the MC average was taken over 5000 MC steps per spin after discarding 5000 MC steps per spin. The precise MC data of the specific heat for the case of $J_1/J_0=2.0$ are shown in Fig. 5 for various values of the crystal size $N=L^3$: $L=12$ (crosses), $L=18$ (filled circles), and $L=24$ (open circles). According to the finite-size scaling theory,[8] the peak height of the specific heat is given by

$$a_1+a_2L^{\alpha/\nu}, \tag{6}$$

where a_1 and a_2 are some numerical constants and α and ν are the well-known critical indices. By using the MC data in Fig. 5, we find that α/ν is nearly equal to 0.5.

Matsubara and Inawashiro[6] calculated the correlation function in the z direction and they found that T_L is some turning point for the above quantity. In this paper, we compute the correlation function in the xy plane. In our calculation, we adopted the MSF MC method and the assumed number of spins was $60^2\times12$.

It is known that the correlation function $\langle S_0S_r\rangle_{xy}$ in the antiferromagnetic triangular lattice at $T=0$ K is written as $\langle S_0S_r\rangle_{xy}\sim r^{-1/2}\cos(2\pi r/3)$ for large r, where r denotes the distance between spins on the xy plane.[9] In the case of the stacked triangular lattice, we find that the correlation function in the xy plane is, in a good approximation, written as

$$\langle S_0S_r\rangle_{xy}\sim r^{-d+2-\eta(T)}\cos(2\pi r/3)\,, \tag{7}$$

where $d=3$ and $\eta(T)$ is a numerical parameter which is determined by the calculation.

According to the MC calculation, the correlation function for $T>T_N$ is not described by Eq. (7) but it is described by

$$\langle S_0S_r\rangle_{xy}\sim\exp(-\kappa r)\cos(2\pi r/3) \tag{8}$$

for large r, where κ means the inverse of the correlation length. That is, $\eta(T)=\infty$ for $T>T_N$ if we follow the form of Eq. (7). In Fig. 6, we show the computed values of $\eta(T)$ for the case $J_1/J_0=2.0$. We observe two anomalous changes in η: an abrupt drop at $T=T_N$ and a sudden increase at $T=T_L$ toward the ground-state value, $-\frac{1}{2}$. Thus, in the low-temperature region $(0<T<T_L)$, there appear spin states (or *phases*) with various η values, as seen from Fig. 6. We note that the η value at the critical point is -0.75 for the two-dimensional Kosterlitz-Thouless model.[10]

We have seen that the MC data of the specific heat and the correlation function support the existence of phase transition at $T=T_N$. The MC data also indicate some turning point at $T=T_L$ below which the magnetic properties of the crystal are different from those above T_L. We may define this T_L as the temperature below which the linear-chain-like excitations become dominant.

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[1]K. Hirakawa, H. Kadowaki, and K. Ubukoshi, J. Phys. Soc. Jpn. **52**, 1814 (1983); W. B. Yelon and D. E. Cox, Phys. Rev. B **7**, 2024 (1973); D. P. Belanger, A. R. King, V. Jaccarino, and J. L. Cardy, *ibid.* **28**, 2522 (1983), and references therein.

[2]D. Blankschtein, M. Ma, A. N. Berker, G. S. Grest, and C. M. Soukoulis, Phys. Rev. B **29**, 5250 (1984); A. N. Berker, G. S. Grest, C. M. Soukoulis, D. Blankschtein, and M. Ma, J. Appl. Phys. **55**, 2416 (1984).

[3]S. N. Coppersmith, Phys. Rev. B **32**, 1584 (1985).

[4]O. Nagai, Y. Yamada, and H. T. Diep, Phys. Rev. B **32**, 480 (1985).

[5]E. Dubois-Viollete, R. Jullien, and J. P. Carton, J. Phys. (Paris) **45**, 1297 (1984).

[6]F. Matsubara and S. Inawashiro, J. Phys. Soc. Jpn. **56**, 2666 (1987).

[7]O. Nagai, Y. Yamada, K. Nishino, and Y. Miyatake, Phys. Rev. B **35**, 3425 (1987).

[8]M. N. Barber, *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8, p. 145.

[9]J. Stephenson, J. Math. Phys. **11**, 413 (1970).

[10]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).