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Phase transitions of classical *XXZ* model with easy-plane anisotropy on a two-layer triangular lattice

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Abstract

We investigate phase transitions of a classical *XXZ* model with easy-plane anisotropy, on a two-layer triangular lattice with ferromagnetic and antiferromagnetic layers by using Monte Carlo simulations. It turns out that the chirality shows a very steep increase as temperature increases in a temperature range; the value of a critical exponent for this change is estimated. © 2000 Elsevier Science B.V. All rights reserved.

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Magnetic thin films, layered magnets or magnets on superlattices show interesting properties that are different from bulk properties [1–3]. We expect that some systems on a lattice consisting of multi-layers show quite interesting behaviors, which do not exist in a system on a single layer nor in three-dimensional bulk systems [4–13]. Even in a simple magnetic model such as an *XY* model, we may have a completely different nature of phase transitions in systems on a few layers from that in two-dimensional systems or from that in three-dimensional bulk systems [14,15].

In the thermodynamic limit, there is no phase transition in the ferromagnetic classical Heisenberg model on two-dimensional lattices [16]. There is no long-range order but there exists the so-called Kosterlitz–Thouless (KT) type transition in the antiferromagnetic classical Heisenberg model on the triangular lattice [17,18]. As for the KT transition of the *XY* model (the plane rotator model), see for example Refs. [19–21]. In the present Letter, we are interested in phase transitions in an anisotropic classical Heisenberg model with an easy-plane anisotropy, namely a classical *XXZ* model with strong *XY* anisotropy; we simply call this model an *XXZ* model hereafter. For the *XXZ* model, it has been shown that there exist the KT transition and also the chirality transition, when the system is fully frustrated [22,23]. This situation is similar to the *XY* model with full frustration [24–26]. Hence we investigate phase tran-

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sitions for an XXZ model on a two-layer triangular lattice with a ferromagnetic layer and an antiferromagnetic layer.

We consider an XXZ model with an easy-plane anisotropy on a two-layer triangular lattice. Each of two triangular lattices is denoted by Λ_1 and Λ_2, respectively. We assume Heisenberg spins, $\boldsymbol{s}_i$ and $\boldsymbol{t}_i$ for $i \in \Lambda_1$ and Λ_2, respectively, where $N = |\Lambda_1| = |\Lambda_2|$; $N = L \times L$ for each layer and L is the linear size of $\Lambda_k (k = 1,2)$. Then the two-layer triangular lattice is denoted by Λ: $\Lambda = \Lambda_1 + \Lambda_2$ and hence $|\Lambda| = 2N$. The Hamiltonian is given as follows:

$$H = -I \sum_{(i,j)} \left(s_i^x s_j^x + s_i^y s_j^y + \xi s_i^z s_j^z \right) - J \sum_{(i,j)} \left(t_i^x t_j^x + t_i^y t_j^y + \xi t_i^z t_j^z \right) - K \sum_i \left(s_i^x t_i^x + s_i^y t_i^y + \xi s_i^z t_i^z \right), \tag{1}$$

where ξ is an anisotropy parameter with $0 \le \xi < 1$; we assume $\xi = 0.5$ in the present Letter. Here we have assumed that intralayer interactions exist only between spins at nearest-neighbor lattice sites on each of Λ_1 and Λ_2; those interaction constants are denoted by I and J, respectively. The sum with (i,j) indicates a summation over nearest-neighbor pairs of sites on Λ_1 or Λ_2. We have also assumed that interlayer exchange interactions exist only between spins at a site i on Λ_1 and at its corresponding site i on Λ_2; this interaction constant is denoted by K. The sum with i indicates a summation over pairs of sites i on $\Lambda_1 + \Lambda_2$. We assume the periodic boundary conditions for each layer Λ_1 or Λ_2.

We notice that there is a relation:

$$\mathscr{O}(I,J,K) = \mathscr{O}(I,J,-K) \tag{2}$$

for a thermodynamic quantity $\mathscr{O}(I,J,K)$. Then we assume that $K > 0$ without loss of generality. In the present Letter, we investigate the system with $I = -1, K = 1$ and $J > 0$; namely the exchange interactions on the upper layer (Ul) Λ_1 is antiferromagnetic and that on the lower layer (Ll) Λ_2 is ferromagnetic. We investigate the system by Monte Carlo (MC) simulations. Hereafter we just mention only the values of J in order to indicate the system. We have performed our MC simulations for $L = 24, 36$ and 48. We have used random spin configurations as initial spin configurations in our MC simulations. A MC average, $\langle \mathscr{O} \rangle$, for a quantity $\mathscr{O}$ is calculated by

$$\langle \mathscr{O} \rangle = \frac{1}{n - n_0} \sum_{t = n_0 + 1}^{n} \mathscr{O}(t), \tag{3}$$

where we choose $n_0 = 2.5 \times 10^5$ MC steps, $n = 5 \times 10^5$ MC steps, and also $n_0 = 5 \times 10^5$ MC steps and $n = 10^6$ MC steps, depending upon the system size and the values of temperature. We set the Boltzmann constant k to 1 throughout the present Letter.

We have calculated the internal energy, the specific heat, the chirality and Binder parameters. The internal energy is given as

$$E = \frac{1}{2N} \langle H \rangle. \tag{4}$$

The specific heat is obtained by

$$C = \frac{1}{2NT^2} \left\{ \langle H^2 \rangle - \langle H \rangle^2 \right\}. \tag{5}$$

The chirality is defined for a smallest up-triangle, namely an elementary upward triangle on each plane. For example, the chirality, κ_{ijk}^s, on Λ_1 plane is given as follows:

$$\kappa_{ijk}^s = \frac{2}{3\sqrt{3}} \left(\boldsymbol{s}_i \times \boldsymbol{s}_j + \boldsymbol{s}_j \times \boldsymbol{s}_k + \boldsymbol{s}_k \times \boldsymbol{s}_i \right) \cdot \boldsymbol{e}_z, \tag{6}$$

where $\boldsymbol{e}_z$ is the unit vector of z-component in the spin space. A set of sites $\{i,j,k\}$ expresses three sites labeled counterclockwise on an up-triangle of lattice Λ_1. In a similar way, we define the chiralities κ_{ijk}^t on lattice Λ_2. The averaged chirality for the whole system is defined by

$$\kappa = \tfrac{1}{2} (\kappa_s + \kappa_t), \tag{7}$$

where

$$\kappa_s = \frac{1}{N} \sum_{(ijk)} \left\langle \kappa_{ijk}^s \right\rangle, \quad \kappa_t = \frac{1}{N} \sum_{(ijk)} \left\langle \kappa_{ijk}^t \right\rangle. \tag{8}$$

The sum with (ijk) in Eq. (8) is taken over all the elementary up-triangles on the lattice Λ_1 or Λ_2. The Binder parameter is defined as

$$U_\sigma(M) = 1 - \frac{\left\langle \left(\boldsymbol{M}_\sigma^2 \right)^2 \right\rangle}{3\left\langle \boldsymbol{M}_\sigma^2 \right\rangle^2}. \qquad (9)$$

Here we have

$$\boldsymbol{M}_\sigma = \sum_{i \in \Lambda} \boldsymbol{\sigma}_i, \qquad (10)$$

where $\boldsymbol{\sigma}_i$ is either $\boldsymbol{s}_i$ or $\boldsymbol{t}_i$.

The specific heat C is shown in Fig. 1 for $J = 0.10, 0.18, 0.30$ and 0.5 as functions of temperature. We see two peaks in the specific heat for those values of J except $J = 0.10$. From the behaviors of the specific heat, there are two critical values for J, namely J_{c1} and J_{c2}; J_{c1} is estimated as 0.17 and J_{c2} as 0.35. We find only one sharp peak for $J < J_{c1}$. There are two sharp peaks for $J_{c1} < J < J_{c2}$; although we do not show here, we find that these two peaks show size-dependencies for data by $L = 24,36$ and 48. The peak near $T = 0.4$ is sharp as we see; we denote the peak temperature for this sharp peak by T_{ch} and notice that the values of T_{ch} do not depend much on the value of J. The peak temperature for the other sharp peak of the specific heat is denoted by T_{cl}. We have a sharp peak and a broad peak for $J > J_{c2}$. We denote the peak temperature for this sharp peak by T_{ch} and notice that the values of T_{ch} do not depend much on the value of J for $J > J_{c2}$, too. On the other hand, a broad peak at temperature higher than T_{ch} shows no size dependence, and then it is reasonable to think that the transition for this broad peak is of the Kosterlitz–Thouless type. We denote this peak temperature by T_{KT}. Although we need more comprehensive calculations in order to estimate T_{KT}, for example, by calculating the helicity modulus, we estimate it here by the peak temperature

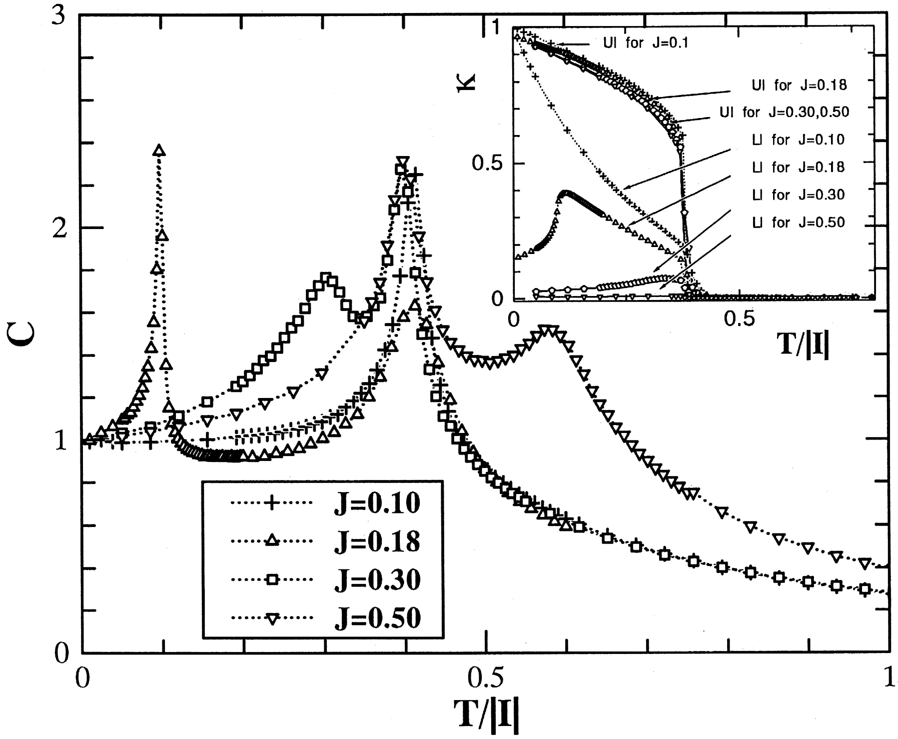

Fig. 1. The specific heat as functions of temperature for $J = 0.1, 0.18, 0.3$ and 0.5. In the inset, we show the chirality on the upper layer (Ul) and on the lower layer (Ll) for $J = 0.1, 0.18, 0.3$ and 0.5.

because we are not interested in estimation of T_{KT} in the present Letter. In the inset of Fig. 1, we show behaviors of the chirality, κ_s and κ_t. We see clearly that the chirality for $J=0.18$ increases steeply just below $T/|I|=0.1$, as temperature increases. The chirality for $J=0.30$ shows a similar behavior as that for $J=0.18$, although the increasing seems not so steep; this is due to the finite size effect. The chirality becomes zero at T_{ch} as the temperature increases.

We estimate roughly the values of T_{cl}, T_{ch} and T_{KT} by using the system with $L=24$ from the peak temperature of the specific heat. In Fig. 2, we give a phase diagram in the J versus temperature plane; we denote the paramagnetic phase by P, the KT phase by KT and the chiral phase by C. In the chiral phase, we see a critical line between $J_{c_1}<J<J_{c_2}$ which terminates at a low temperature; this is a critical end point.

In order to investigate the nature of the phase transition at temperatures where the sharp peaks are observed in the specific heat between $J_{c_1}<J<J_{c_2}$, we have to estimate the critical temperature as precise as possible. For this purpose, we calculate the Binder parameters. Some results are shown in Figs. 3 and 4; we have estimated as $T_{ch}=0.3928$ and $T_{cl}=0.0970$, respectively, for $J=0.18$. We have found that the Binder parameters for each layer show more clearly the behaviors of crossing than the Binder parameter for the whole system. We make finite-size scaling analyses for the specific heat and the chirality (in the inset) at $T_{ch}=0.3928$ in Fig. 5 and $T_{cl}=0.0970$ in Fig. 6, respectively. From the finite-size scaling analyses for the specific heat and the chirality at T_{ch}, we have found that the values of critical exponents, ν, α and β are 1.00 ± 0.05, 0(ln) and 0.125 ± 0.05, respectively. In order to investigate the behavior of the chirality at T_{cl}, we define the critical exponent β as follows:

$$\kappa_t \sim \kappa_t^{(c)} - a(T_{cl}-T)^{\beta} \quad (T \lesssim T_{cl}), \tag{11}$$

where $\kappa_t^{(c)}$ is the maximum value of the chirality κ_t on the ferromagnetic layer (Ul) and a is a constant.

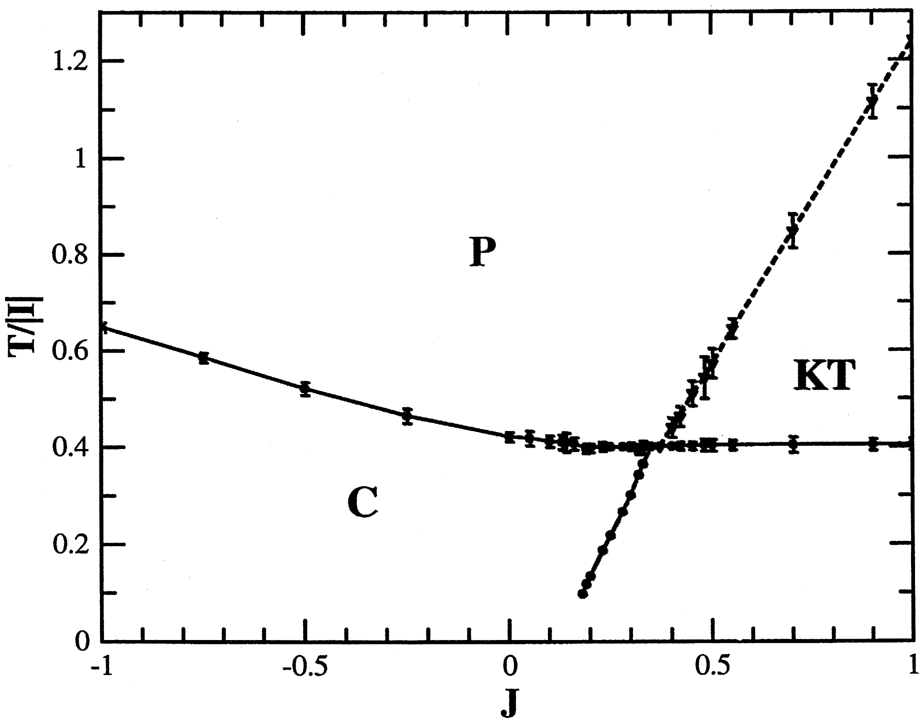

Fig. 2. Phase diagram in J versus $T/|I|$ plane.

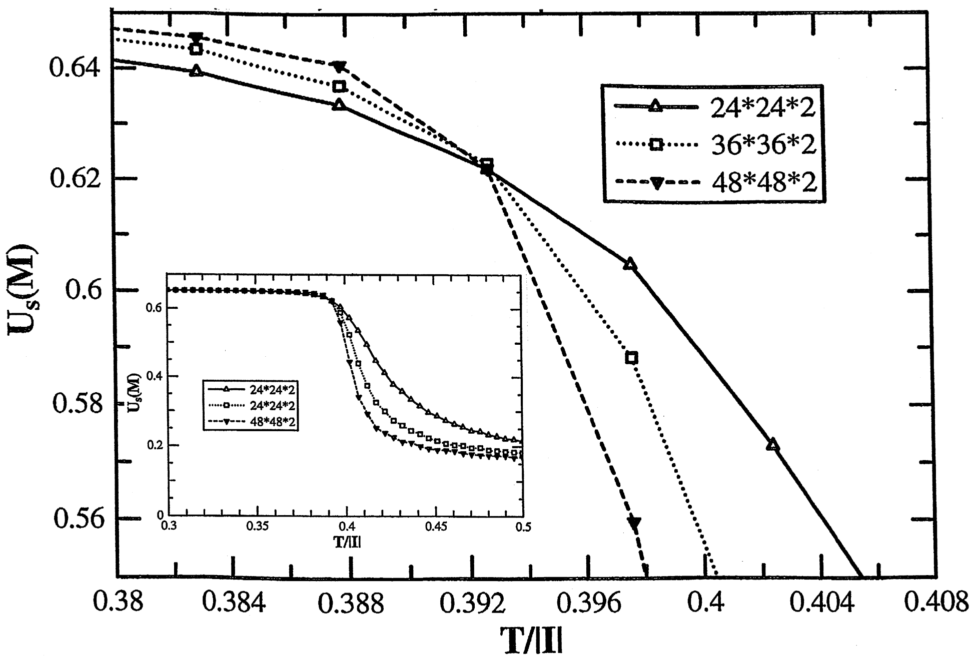

Fig. 3. Binder parameter for determination of critical temperature T_{cl}. In the inset, we show the whole behavior of the Binder parameter for the lower layer.

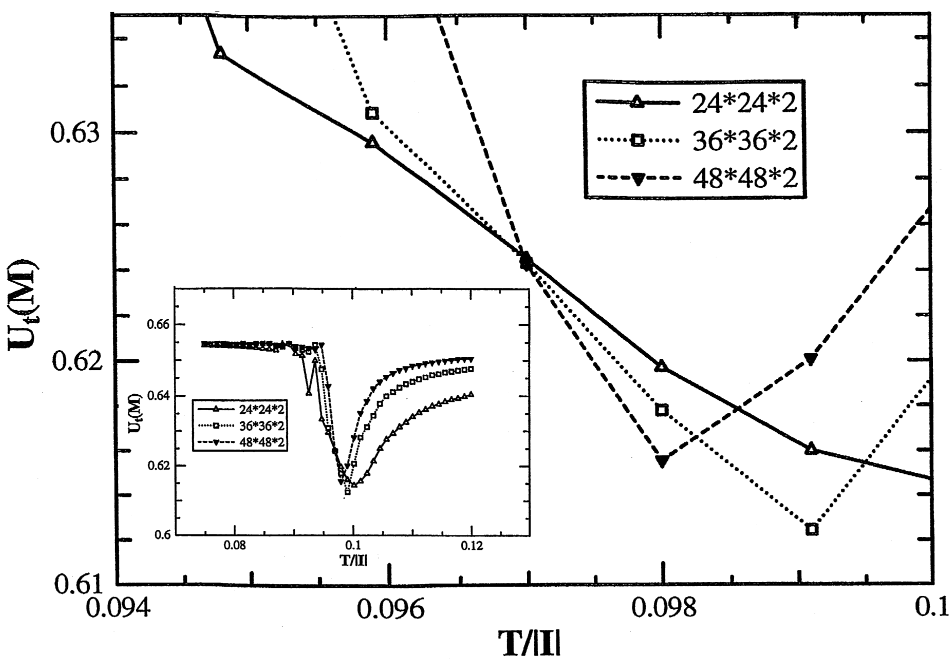

Fig. 4. Binder parameter for determination of critical temperature T_{ch}. In the inset, we show the whole behavior of the Binder parameter for the upper layer.

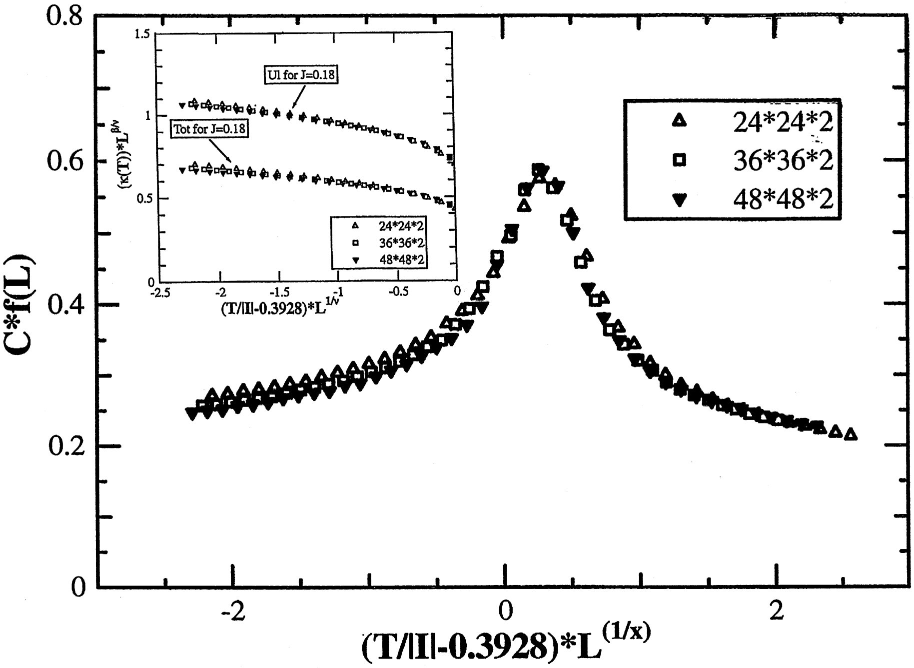

Fig. 5. Finite-size scaling analysis of the specific heat C for the system with $I=-1, K=1, \xi=0.5$ and $J=0.18$ near T_{ch}. In the set, we show a finite size scaling analysis of the chirality for the upper layer (Ul) and that for the whole system (Tot).

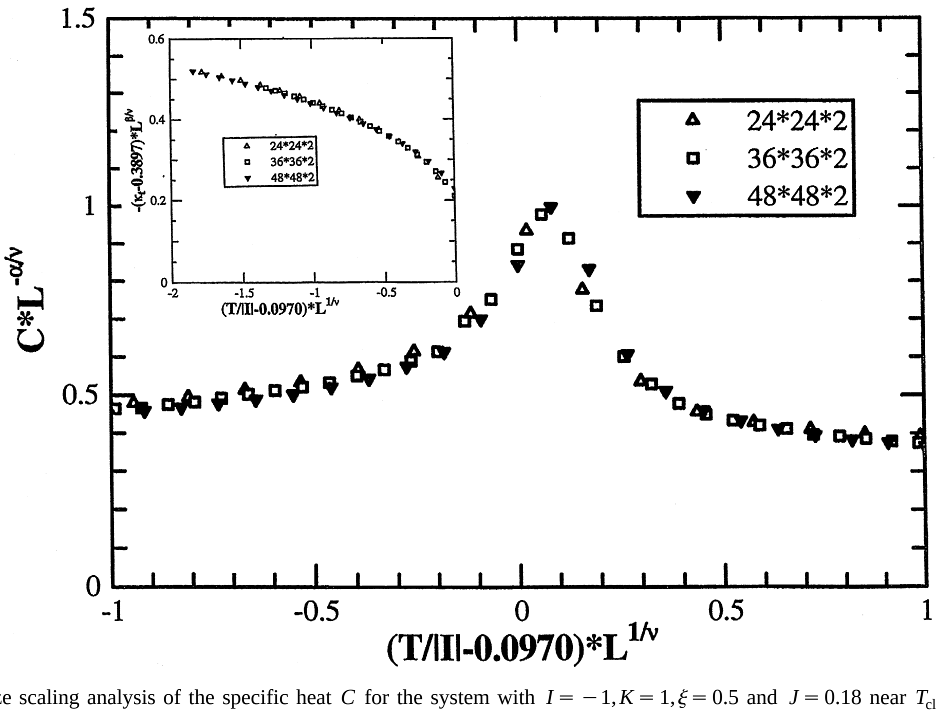

Fig. 6. Finite-size scaling analysis of the specific heat C for the system with $I=-1, K=1, \xi=0.5$ and $J=0.18$ near T_{cl}. In the set, we show a finite size scaling analysis of the chirality for the upper layer.

We have found that the values of ν and β are 0.875 ± 0.05 and 0.255 ± 0.05, respectively. The errors for the values of critical exponents are estimated by the fitness for the finite-size scaling. We believe that this critical behavior is a new finding for the *XXZ* model. We found a similar behavior in the two-layer *XY* model and in the three layer *XY* model [14,15]. In this way, we think that this quite new critical behavior occurs commonly in the *XY* model and also in the *XXZ* model of lattices consisting with layers when there is competing of ordering among ferromagnetic planes and frustrated planes. We have the chirality transitions similar to that in the *XY* model on the antiferromagnetic triangular lattice for $J < J_{c_1}$. For $J > J_{c_2}$, we also have a chirality transition from the KT phase to the chirality phase.

In conclusion, we have investigated critical phenomena and a phase diagram for an *XXZ* model with anisotropy parameter $\xi = 0.5$ on a two-layer triangular lattice with a ferromagnetic layer and an antiferromagnetic layer. The interlayer interaction constant is assumed to be ferromagnetic without loss of generality. We have constructed the phase diagram in an interaction parameter versus temperature plane. We have found that there are three phases, namely the paramagnetic phase, the Kosterlitz–Thouless (KT) phase and the chirality phase and that there is a critical line in the chirality phase in some range of interaction parameters for the ferromagnetic layers. Similar behaviors are also found for the system with other values of the anisotropy parameter, $\xi =$ 0, 0.7 and 0.9. In order to clarify the critical behaviors of the system, we have made finite-size scaling analyses for the specific heat and the chirality at a range of interaction parameters in which the critical line appears in the chirality phase. When we compare the obtained values of critical exponents and the phase diagram with those for the two-layer and the three-layer systems of the *XY* model investigated previously, we find that the present system belongs to the same universality class as that for those *XY* models. We will discuss elsewhere details of the finite-size analyses for the chirality, the specific heat and the susceptibility of the present system with several values of ξ. It is also interesting to investigate crossover effects as the strength of the coupling K varies. This is left as a future problem.

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