

Anisotropic antiferromagnetic XY -model of classical Heisenberg spins on a triangular lattice

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We obtain a phase diagram of an anisotropic antiferromagnetic XY -model of classical Heisenberg spins on a triangular lattice by calculating the average values of x -component and y -component of spins, the chirality, angles between averaged spins on sublattices and the specific heat by means of Monte Carlo simulations. It turns out that the system has two phase transition temperatures: one for the Kosterlitz–Thouless-type phase transition and the other for the Ising-type phase transition. These two phase transition temperatures are merged into one in the isotropic XY -model. We find that the chirality is a good order parameter at low temperatures even in the system with anisotropic interaction. For the system with isotropic interaction, the 120 degree structure persists as far as the chirality is non-zero.

1. Introduction

The nature of an antiferromagnetic plane rotator model on the triangular lattice was investigated by Miyashita and Shiba [1] by Monte Carlo simulations. They showed that there are two phase transition temperatures in the system, namely $kT_c/J \sim 0.513$ and $kT_{KT}/J = 0.502 \pm 0.002$, where k is the Boltzmann constant and J is the exchange interaction; T_{KT} is the temperature for the Kosterlitz–Thouless (KT)-type phase transition [2] and T_c is that for the Ising-type phase transition due to the order-disorder transition of chirality [3]. Before Miyashita and Shiba [1], Garel and Doniach [4] argued that there are the Ising-type phase transition and the XY -type phase transition in a two-dimensional XY helimagnets. The frustrated continuous spin systems have

extensively been investigated by many authors [5–21] stimulated by those investigations [1–4]. Berge et al. [15] studied a classical XY-model on a uniformly frustrated square lattice by Monte Carlo simulations; the nearest-neighbor interaction is equal to J for positive bonds and equal to $-\eta J$ for negative bonds. They found the Ising-type phase transition and the KT-type phase transition for $\eta > 1/3$. The transition temperature for the KT-type phase transition is higher than that for the Ising-type phase transition and these two transitions are merged into a single one of dominant Ising character at $\eta = 1$. The anisotropic antiferromagnetic Heisenberg model on the triangular lattice has been investigated by Miyashita and Kawamura [8]. When the exchange interaction between x -component of spins and between y -component of spins is denoted by J_{xy} and that between z -component of spins by J_z , they showed a roughly estimated phase diagram in which there are two phase transitions for $J_z/J_{xy} > 1$ and one phase transition for $0 \leq J_z/J_{xy} \leq 1$. But they did not state whether there are two phase transitions or one phase transition for the XY-model of classical Heisenberg spins. In these situations, we think that the problem whether there are two phase transition temperatures or one phase transition temperature in the plane rotator model and in the XY-model of Heisenberg spins on the triangular lattice is still unsettled.

The plane rotator model and the XY-model of classical Heisenberg spins have the same symmetry properties in the ground state and then are expected to belong to the same universality class. We then expect that the system with isotropic XY-interaction of Heisenberg spins has the two phase transition temperatures if the system with the plane rotator model does. Horiguchi et al. [22–25] investigated an antiferromagnetic Ising model of infinite spins on the triangular lattice and showed that the system has at least a phase transition, whose nature is not clarified yet. Namely we have the low-temperature phase for $kT/J \leq 0.1$, in which we have a stable sublattice ordering, and the middle temperature phase for $0.1 \leq kT/J \leq 0.46$, in which there is a strong sublattice switching, and the paramagnetic phase for $kT/J \geq 0.46$ [23,25]. This model is considered as the system of antiferromagnetic interaction between only x -component of spins of classical Heisenberg spins. In this way, the anisotropic antiferromagnetic XY-model of classical Heisenberg spins on the triangular lattice is a nice model to investigate nature of the phase transitions in the XY-model of classical Heisenberg spins and also the Ising model of infinite spins.

In the present paper, we investigate the system with anisotropic antiferromagnetic XY-model of classical Heisenberg spins on the triangular lattice by using Monte Carlo simulations. The aim of the present paper is to find the phase diagram of the system with anisotropic XY-interaction. By using the obtained phase diagram, we discuss the nature of the phase transition occurring

at $kT/J \sim 0.46$ of the system of infinite Ising spins and show that there is only one phase transition temperature for the system with isotropic XY-interaction.

In section 2, we give the ground state properties of the system. We give the results obtained by Monte Carlo simulations and discussions for the results in section 3. The concluding remarks are given in section 4.

2. Ground state properties

The system which we investigate in the present paper is an anisotropic antiferromagnetic XY-model of classical Heisenberg spins on the triangular lattice Λ . The Hamiltonian of the system is given as follows:

$$H = \sum_{\langle ij \rangle} \{ J_x S_i^x S_j^x + J_y S_i^y S_j^y \}, \quad (1)$$

where S_i^x and S_i^y are the x -component and the y -component, respectively, of the classical Heisenberg spin S_i at a site $i \in \Lambda$; namely we have

$$S_i = (S_i^x, S_i^y, S_i^z), \quad |S_i| = 1. \quad (2)$$

The summation with respect to $\langle ij \rangle$ means that the sum is taken over all the nearest-neighbor pairs of lattice sites of Λ . We assume that $J_x > 0$ and $0 \leq J_y \leq J_x$.

The partition function of the system is given by

$$\begin{aligned} Z &= \int_0^\pi \int_0^{2\pi} \sin \theta_1 d\theta_1 d\phi_1 \cdots \int_0^\pi \int_0^{2\pi} \sin \theta_N d\theta_N d\phi_N \\ &\quad \times \prod_{\langle ij \rangle} \exp(-K_x \sin \theta_i \cos \phi_i \sin \theta_j \cos \phi_j - K_y \sin \theta_i \sin \phi_i \sin \theta_j \sin \phi_j) \end{aligned} \quad (3)$$

in terms of the polar coordinates when we put

$$S_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i). \quad (4)$$

In eq. (3), we put $K_x = \beta J_x$, $K_y = \beta J_y$ and $\beta = 1/kT$ as usual. The total number of lattice sites is denoted by N : $N = |\Lambda|$. When J_y is equal to zero, we have

$$Z = (2\pi)^N \int_{-1}^1 dx_1 \cdots \int_{-1}^1 dx_N \prod_{\langle ij \rangle} \exp(-K_x x_i x_j), \quad (5)$$

which is the partition function for the Ising model of infinite spins [23]. Hence we are able to investigate the natures of both systems of isotropic XY-model and of Ising model of infinite spins by changing the parameter $\gamma = J_y/J_x$.

We divide the lattice Λ into three equivalent sublattices Λ_1, Λ_2 and Λ_3 as usual: $\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3$. By using the result obtained by Karl [27], we may get ground state configurations by minimizing the following energy:

$$\begin{aligned} \tilde{E} &= E/J_x = E(\theta_1, \theta_2, \theta_3, \phi_1, \phi_2, \phi_3)/J_x \\ &= \sin \theta_1 \cos \phi_1 \sin \theta_2 \cos \phi_2 + \sin \theta_2 \cos \phi_2 \sin \theta_3 \cos \phi_3 \\ &\quad + \sin \theta_3 \cos \phi_3 \sin \theta_1 \cos \phi_1 + \gamma(\sin \theta_1 \sin \phi_1 \sin \theta_2 \sin \phi_2 \\ &\quad + \sin \theta_2 \sin \phi_2 \sin \theta_3 \sin \phi_3 + \sin \theta_3 \sin \phi_3 \sin \theta_1 \sin \phi_1), \end{aligned} \tag{6}$$

where θ_i and ϕ_i are angles at a lattice site belonging to sublattice Λ_i and the lattice sites 1, 2, and 3 are nearest-neighbors of each other. By putting a partial derivative of $E(\theta_1, \theta_2, \theta_3, \phi_1, \phi_2, \phi_3)$ in terms of θ_1 zero, we may choose $\theta_1 = \pi/2$ as a solution. In the same way, we have $\theta_2 = \theta_3 = \pi/2$. This solution means that the spins are in the xy -plane in the three dimensional spin space and the XY-model of classical Heisenberg spins has the same symmetry properties of those in the plane rotator model in the ground state. We can confirm that $\theta_1 = \theta_2 = \theta_3 = \pi/2$ hold even at finite temperatures by Monte Carlo simulations in the next section.

Now we have

$$\begin{aligned} \tilde{E} &= \cos \phi_1 \cos \phi_2 + \cos \phi_2 \cos \phi_3 + \cos \phi_3 \cos \phi_1 \\ &\quad + \gamma(\sin \phi_1 \sin \phi_2 + \sin \phi_2 \sin \phi_3 + \sin \phi_3 \sin \phi_1). \end{aligned} \tag{7}$$

By taking the stationary condition of the energy for ϕ_1, ϕ_2 and ϕ_3 , we have

$$\begin{aligned} \sin \phi_1(\cos \phi_2 + \cos \phi_3) &= \gamma \cos \phi_1(\sin \phi_2 + \sin \phi_3), \\ \sin \phi_2(\cos \phi_3 + \cos \phi_1) &= \gamma \cos \phi_2(\sin \phi_3 + \sin \phi_1), \\ \sin \phi_3(\cos \phi_1 + \cos \phi_2) &= \gamma \cos \phi_3(\sin \phi_1 + \sin \phi_2). \end{aligned} \tag{8}$$

We set $\phi_1 = 0$ without loss of generality and then we obtain $\phi_3 = -\phi_2$ or $\phi_3 = \phi_2 \pm \pi$ from the first equation of eq. (8). By putting $\phi_2 = \phi_0$, we have

$$\tilde{E} = (1 + \gamma) \left(\cos \phi_0 + \frac{1}{1 + \gamma} \right)^2 - \gamma - \frac{1}{1 + \gamma} \tag{9}$$

for the case of $\phi_3 = -\phi_2$ and

$$\tilde{E} = -(1 - \gamma) \cos^2 \phi_0 - \gamma \tag{10}$$

for the case of $\phi_3 = \phi_2 \pm \pi$. In this way we have the ground state energy

$$\tilde{E} = -\gamma - \frac{1}{1+\gamma}, \quad (11)$$

where its corresponding ground state configuration is given as follows:

$$\theta_1 = \theta_2 = \theta_3 = \pi/2, \quad \phi_2 - \phi_1 = \phi_0, \quad \phi_3 - \phi_1 = -\phi_0, \quad (12)$$

where

$$\cos \phi_0 = -\frac{1}{1+\gamma}. \quad (13)$$

We notice that eq. (13) satisfies the rest of equation of eq. (8).

3. Monte Carlo simulations

In the present paper, we use the Monte Carlo (MC) procedure which has been given in detail in ref. [26]. Our MC simulations were carried out for the systems of N lattice sites with $L = 36, 48$ and 108 , where $N = L^2$. Periodic boundary conditions have been imposed to the system and random spin configurations have been taken as an initial spin configuration. The data shown in the following figures are those obtained by the long time average of data up to n MC steps after n_0 MC steps and we choose $n_0 = 10000$ and $n = 30000$ and also $n_0 = 3000$ and $n = 12000$. A MC average for a quantity X is defined by

$$\langle X \rangle = \frac{1}{n - n_0} \sum_{t=n_0+1}^n X(t). \quad (14)$$

First we show the internal energy defined by eq. (6) in fig. 1 for the system with $L = 36$ for $\gamma = 0.2, 0.5, 0.8$ and 0.9 , where γ is defined in section 2: $\gamma = J_y/J_x$. The values plotted at $T = 0$ are those obtained in section 2.

We calculate the MC average of the quantities defined by

$$s_l^\alpha = \frac{3}{N} \sum_{i \in \Lambda_l} S_i^\alpha \quad (15)$$

for $l = 1, 2$ and 3 and $\alpha = x, y$ and z . We found that the value of $\langle s_l^z \rangle$ is always negligibly small. This is consistent with the symmetry properties in the ground state. In figs. 2, 3 and 4, we give $\langle s_l^x \rangle$ and $\langle s_l^y \rangle$ for $\gamma = 1, 0.5$ and 0.2 , respectively. In each figure, the circles show quantities for sublattice Λ_1 , the

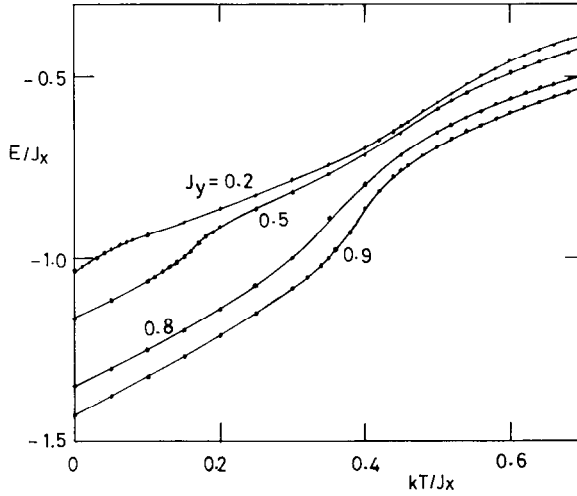


Fig. 1. The internal energy as a function of temperature for $\gamma = 0.2, 0.5, 0.8$ and 0.9 , where $\gamma = J_y/J_x$.

diamonds those for Λ_2 and the squares those for Λ_3 . The data do not show smooth behaviors because of finite size of the system and finite MC steps. We think the irregular behaviors at not very low temperatures are due to the sublattice switching [25]. Despite these irregular behaviors, we consider that these data contain some useful information. When we look at these figure carefully, we find that the behavior of $\langle s_i^x \rangle$ and that of $\langle s_i^y \rangle$ are different. Namely at very low temperatures, the values of $\langle s_1^x \rangle$, $\langle s_2^x \rangle$ and $\langle s_3^x \rangle$ are close to 1 , $-1/(1 + \gamma)$, and $-1/(1 + \gamma)$, respectively, and those of $\langle s_1^y \rangle$, $\langle s_2^y \rangle$ and $\langle s_3^y \rangle$ close to 0 , $\sqrt{\gamma(2 + \gamma)}/(1 + \gamma)$ and $-\sqrt{\gamma(2 + \gamma)}/(1 + \gamma)$, respectively. These values are those at the ground state obtained in the section 2. When the temperature rises, those quantities show irregular behaviors and shrink to zero at temperatures T_x and T_y , which seem to be equal for $\gamma = 1$ but are different for $\gamma \neq 1$.

In order to see the meaning of T_y , we define the chirality

$$K_{ijk} = [S_i \times S_j + S_j \times S_k + S_k \times S_i]_z, \tag{16}$$

where sites $\{i, j, k\}$ are allocated counterclockwise on each upward elementary triangle of the lattice Λ . Here $[A]_z$ denotes the z -component of the vector A . The average of K_{ijk} , $\kappa = \langle K_{ijk} \rangle$, is given in fig. 5 for $\gamma = 1, 0.5$ and 0.2 , in which the squares show the date for $L = 36$ and the circles those for $L = 48$. We find that κ is non-zero for $T < T_y$ and zero for $T > T_y$. Thus T_y is the critical temperature T_c for the order-disorder transition of the chirality; we now use T_c

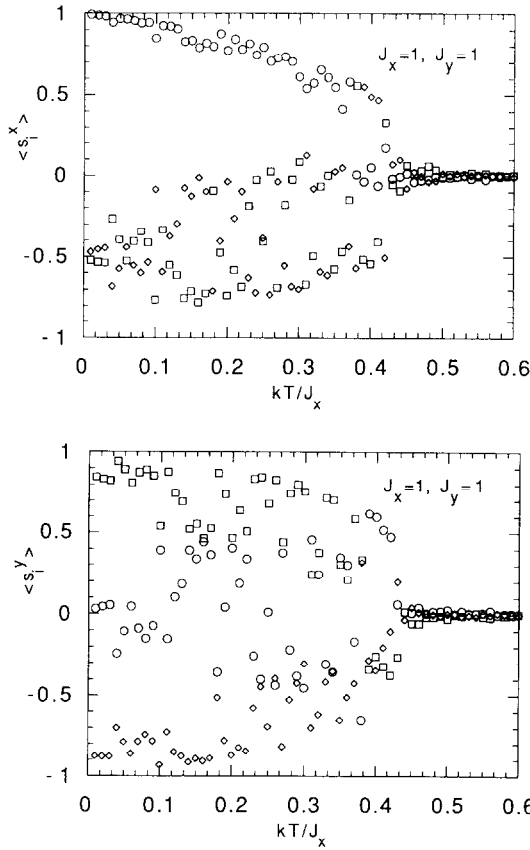


Fig. 2. $\langle s_i^x \rangle$ and $\langle s_i^y \rangle$ as functions of temperature for $i=1, 2$ and 3 and for $\gamma=1$, where $\gamma=J_y/J_x$. The circles show $\langle s_1^\alpha \rangle$, the diamonds $\langle s_2^\alpha \rangle$ and the squares $\langle s_3^\alpha \rangle$ for $\alpha=x$ and y .

for T_y . In order to investigate spin configurations at finite temperatures when $|\langle s_l \rangle|$ and $|\langle s_m \rangle|$ are not zero, we define the angles ζ_{lm} between $\langle s_l \rangle$ for $l \in A_l$ and $\langle s_m \rangle$ for $m \in A_m$ by

$$\cos \zeta_{lm} = \frac{\langle s_l \rangle \cdot \langle s_m \rangle}{|\langle s_l \rangle| |\langle s_m \rangle|}, \quad (17)$$

where (l, m) is $(1, 2)$, $(2, 3)$ or $(3, 1)$. We choose ζ_{lm} as $0 \leq \zeta_{lm} \leq 2\pi$. ζ_{lm} are given in fig. 6 for $\gamma=1$ and 0.5 , in which the filled squares show the data for ζ_{12} , the filled diamonds those for ζ_{23} and the filled circles those for ζ_{31} when $\gamma=1$ and the open squares show the data for ζ_{12} , the open diamonds those for ζ_{23} and the open circles those for ζ_{31} when $\gamma=0.5$. We see the 120 degree structure persists up to T_c for $\gamma=1$. For $\gamma=0.5$, we see that ζ_{12} and ζ_{31} are

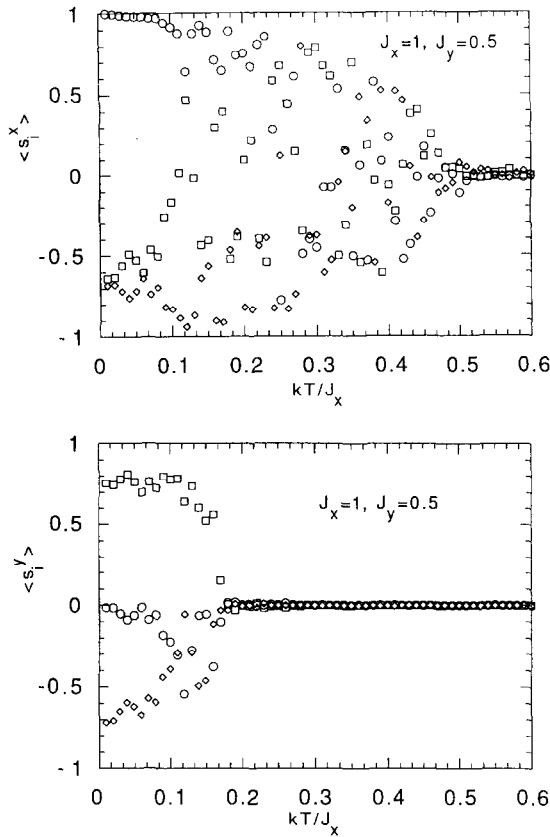


Fig. 3. $\langle s_i^x \rangle$ and $\langle s_i^y \rangle$ as functions of temperature for $i=1, 2$ and 3 and for $\gamma=0.5$, where $\gamma = J_y/J_x$. See the figure caption of fig. 2.

about 132 degree and ζ_{23} are about 96 degree at low temperatures and this structure disappears at T_c . We see the collinear structure for $T_c < T < T_x$ for $\gamma = 0.5$ in fig. 6. For $T > T_x$, we can not obtain a definite conclusion from ζ_{lm} because the values of $|\langle s_i \rangle|$ and $|\langle s_m \rangle|$ are very small.

In order to see the nature of the phase transition occurring at T_x , we give the specific heat in fig. 7 for $\gamma = 0.2$, where the circles show the data for $L = 36$ and the crosses those for $L = 108$. We see that there is no size dependence for the height of a peak at T_x . Then we think that the phase transition occurring at T_x is a KT-type phase transition. However we need more extensive investigation in order to clarify this nature of phase transitions at T_x and T_c by using a finite size analysis. This will be given elsewhere [28].

When we look carefully at the behaviors of $\langle s_i^x \rangle$ in fig. 4, we find that there

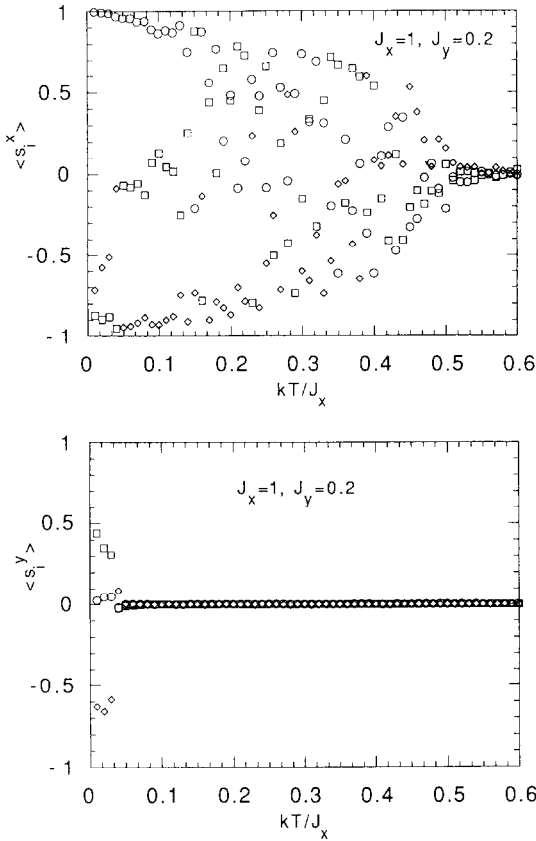


Fig. 4. $\langle s_i^x \rangle$ and $\langle s_i^y \rangle$ as functions of temperature for $i=1, 2$ and 3 and for $\gamma=0.2$, where $\gamma=J_y/J_x$. See the figure caption of fig. 2.

exists some temperature T_0 and there is a stable sublattice structure, namely $\langle s_3^x \rangle \sim -\langle s_1^x \rangle$ and $\langle s_2^x \rangle \sim 0$, for $T_c < T < T_0$. In order to see how a sublattice structure is stable, we define the sum of the maximum value of $\langle s_i^x \rangle$ for $l=1, 2$, and 3 and the minimum value of $\langle s_i^x \rangle$ for $l=1, 2$, and 3 :

$$V = 3[\max\{\langle s_i^x \rangle | i = 1, 2, 3\} + \min\{\langle s_i^x \rangle | i = 1, 2, 3\}] . \tag{18}$$

We think that V plays a role of a measure for a stability of sublattice fluctuations and hence we compare V with kT/J_x in fig. 8 for $\gamma=0.2$. There is a stable sublattice structure similar to the one appearing in the antiferromagnetic Ising model of infinite spin on the triangle lattice for $T_c < T < T_0$ and the sublattice structure is not stable for $T > T_0$. At T_0 , there is no remarkable

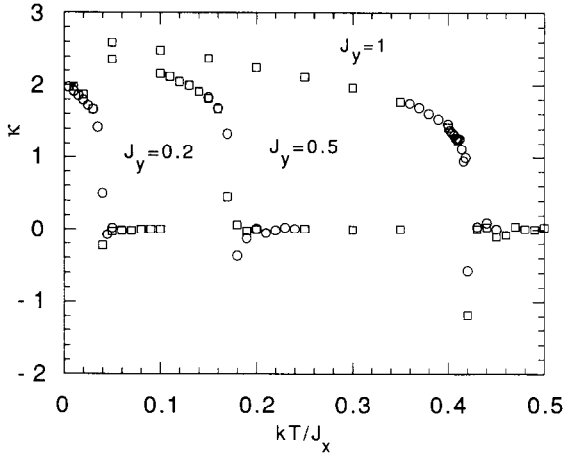


Fig. 5. The chirality as a function of temperature for $\gamma = 1, 0.5$ and 0.2 , where $\gamma = J_y/J_x$. The squares show the data for $L = 36$ and the circles those for $L = 48$.

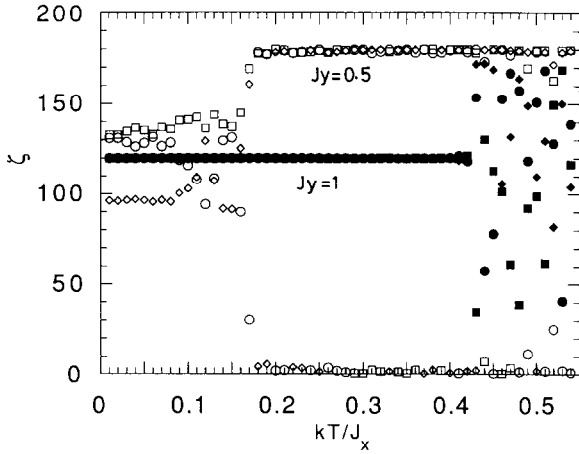


Fig. 6. The angles between $\langle s_i \rangle$ and $\langle s_m \rangle$ as functions of temperature. The filled squares show the data for ζ_{12} , the filled diamonds those for ζ_{23} and the filled circles those for ζ_{31} and for $\gamma = 1$, where $\gamma = J_y/J_x$. The open squares show the data for ζ_{12} , the open diamonds those for ζ_{23} and the open circles those for ζ_{31} and for $\gamma = 0.5$, where $\gamma = J_y/J_x$.

change in the behavior of the specific heat. This situation is also similar to the one occurring in the antiferromagnetic Ising model of infinite spin on the triangular lattice [23,25].

Finally, we find the phase diagram by using the results for the average values of x -component and y -component of spins, the chirality, the angles between the averaged spins on the sublattices and the specific heat obtained in the

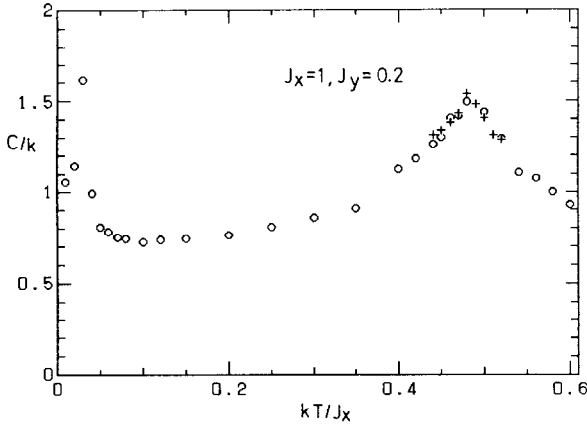


Fig. 7. The specific heat as a function of temperature for $\gamma = 0.2$, where $\gamma = J_y/J_x$. The circles show the data for $L = 36$ and the crosses those for $L = 108$.

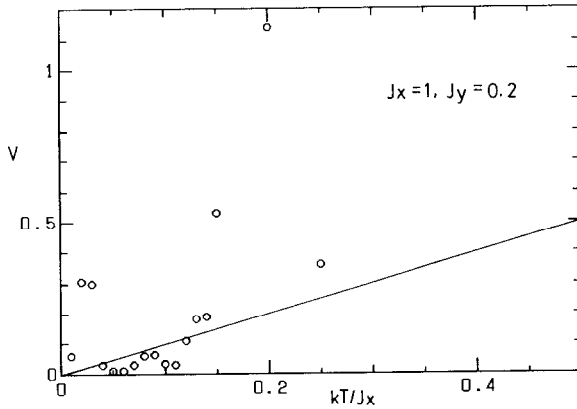


Fig. 8. V defined in eq. (18) as a function of temperature for $\gamma = 0.2$, where $\gamma = J_y/J_x$. V is compared with kT/J which is shown by a solid line.

present MC simulations for various values of J_y from 0.0 to 1.0 with an increment of 0.1. We give it in fig. 9 where the squares show the results for T_x and the circles those for T_c and the diamonds those for T_0 . The error bars are estimated by fluctuations of the values of these temperatures obtained from several kind of quantities. We expect a KT-type phase transition at T_x and the Ising-type phase transition at T_c . There is a stable sublattice structure for $T_c < T < T_0$, but there occur sublattice switchings and then the values of $\langle s_i^x \rangle$ for $i = 1, 2$ and 3 show strong fluctuations for $T > T_0$. It is still an open question whether T_0 is a transition temperature or not and what type of phase transition occurs if T_0 is a transition temperature.

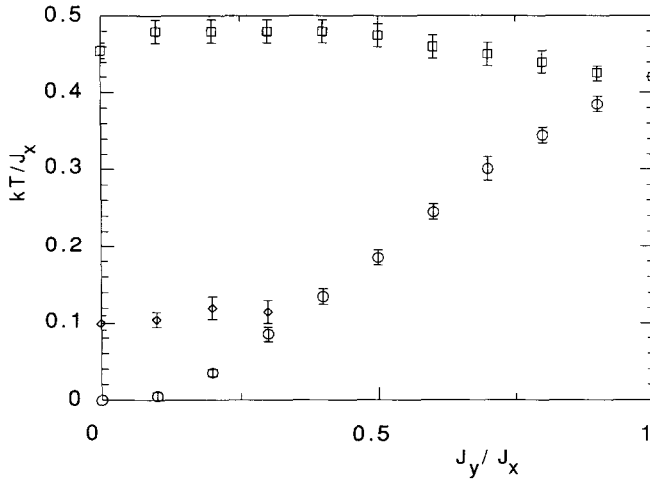


Fig. 9. The phase diagram. The abscissa is J_y/J_x and the ordinate is the temperature. The squares show T_x , the circles T_c and the diamonds T_0 . The error bars are estimated by fluctuations of the values of these temperatures obtained from several kind of quantities.

Now we may conclude that there is only one transition temperature for the system with isotropic XY-model of classical Heisenberg spins from the data shown in the phase diagram. Namely there are two phase transition temperatures T_c and T_x with $T_c < T_x$ in the anisotropic XY-model. There is a KT-type phase transition at T_x and the Ising-type phase transition at T_c (equal to T_y). These two transitions are merged into a single one of dominant Ising character in the isotropic XY-model. On the other hand, when γ goes to zero, T_c goes to zero but T_y remains non-zero. Hence we may conclude that the phase transition at T_x of the Ising model of infinite spins is a KT-type phase transition by the fact that the Ising model of infinite spins is equivalent to the case of $J_y = 0$ of the system investigated in the present paper.

4. Concluding remarks

In the present paper, we obtained the phase diagram of the system with the anisotropic antiferromagnetic XY-model of classical Heisenberg spins on the triangular lattice by using Monte Carlo simulations. We found that there are two phase transition temperatures T_c and T_x with $T_c < T_x$ in the anisotropic XY-model. There is a KT-type phase transition at T_x and the Ising-type phase transition at T_c . These two transitions are merged into a single one of dominant Ising character in the isotropic XY-model. In the case of $J_y = 0$, T_c goes to zero while T_x remains non-zero and then the nature of the phase

transition of Ising model of infinite spins is of the KT-type. However we need more detailed investigation including finite size analysis in order to clarify the nature of the phase transitions at T_x and T_c . This will be given elsewhere [28].

In the obtained phase diagram, there is a temperature T_0 at which the stability of the sublattices is changed. At the present state, we can not give a definite conclusion whether T_0 is a transition temperature or not. This is an open problem left for future investigation.

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