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MONTE CARLO STUDY OF AN ANTIFERROMAGNETIC TRIANGULAR LATTICE WITH THE SECOND NEIGHBOUR INTERACTION

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A Monte Carlo simulation is carried out on the triangular Ising system in which the antiferromagnetic nn interaction J and the ferromagnetic nnn interaction J' exist. The temperature dependences of sublattice quantities (magnetizations, energies, susceptibilities and specific heats) are calculated. Three singular temperatures are estimated for several values of the interaction ratio R = J'/J, and the phase diagram is obtained.

1. Introduction

Recently, the Ising model on the triangular lattice with the nearest neighbour (nn) and next nearest neighbour (nnn) interactions, J and J', has interested many people as a candidate of new type of ordered phase. The ground state of the system with the antiferromagnetic J (<0) and the ferromagnetic J' (>0) is known to be the two-sublattice ferrimagnetic (F_2) state [1]. Mekata [2] proposed a possibility that the partially disordered (PD) phase appears in the finite temperature region by the mean field approximation when J < 0, J' > 0 and R(=J'/J) > - 0.4. The PD phase is defined by the property that the one of the sublattices loses its averaged magnetization and the other two-sublattices magnetize in opposite directions. Mekata [2] also showed that the three-sublattice ferrimagnetic (F_3) state appears in the temperature region between F_2 and PD phases.

Mekata and Adachi [3] and Yoshizawa and Hirakawa [4] carried out magnetic studies on single crystals of Ising-like material $CsCoCl_3$. They observed the unusual temperature dependence of the magnetic reflection intensity by the neutron scattering above 13.5K, and it was interpreted as the appearance of the partially disordered phase in the temperature region (13.5K < T < 20.82K).

Kaburagi et al [5] carried out the cluster variation method of the system, and they showed that PD phase appears even when R < - 0.4. The feature that the critical value of R does not exist is different from that by the mean field approximation [2]. It is a question at this stage whether the mean field approximation or the cluster variation method derive an appropriate phase diagram and transition temperatures for the well frustrated system.

On the other hand, Wada et al [6] carried out the Monte Carlo (MC) simulation of the system for R = - 0.1, and claimed that the PD phase will not be realized as an equilibrium state, since the

interchanges of roles of sublattices occur frequently.

The purpose of the present paper is to clarify these problems by the Monte Carlo simulation, to estimate the singular temperatures which characterize the phase transitions among possible phases and to obtain the phase diagram of the well frustrated system.

2. Model and Method of Simulation

The Hamiltonian of the system is given by

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - J'\sum_{\langle k\ell\rangle}\sigma_k\sigma_\ell \qquad (1)$$

where J and J' are the nn and nnn interactions, and $\langle ij\rangle$ and $\langle k\ell\rangle$ denote nn and nnn pairs of spins, respectively. We denote J'/J by R, and we consider the case of J<0, J'>0.

We divide the lattice into three sublattices α, β, γ. At the first temperature we set the spin configuration to be the two-sublattice ferrimagnetic state as the initial state and we take the gradual heating and cooling method. We adopt the periodic boundary condition and carried out the simulation over the system size of N (total number of spins) = 24 x 24, 36 x 36, 48 x 48.

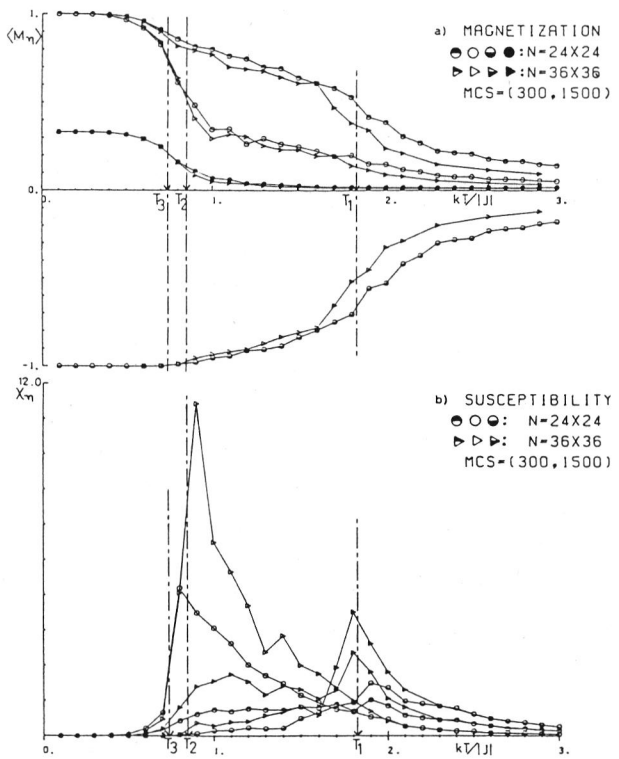

Fig. 1. A result of the present simulation when R(=J'/J) = - 0.2. ◓ and ◗ denote the α-sublattice, ○ and ▷ denote the β-sublattice, ◒ and ▶ denote the γ-sublattice, and ● and ▶ denote the total system. χ_{tot} is shown in Fig. 2. Each plotted values are obtained from the arithmetic means of the heating and cooling processes.

In the Monte Carlo simulation, we see that the roles of three sublattices interchange with finite time intervals. To evaluate thermal averages of sublattice quantities beyond the trivial interchanges of the roles of three sublattices in the finite system, we rename each sublattice so as to follow the spontaneous sublattice interchange (see details in [7]). We then calculate the thermal averages of the magnetizations and the energies of the three sublattices and of the total system over the Monte Carlo steps (MCS) = (300, 500) or (300, 1500) at each temperature, where MCS as the relaxation process is 300 (discarded) and MCS as the thermal equilibrium process is 500 or 1500. Susceptibilities and specific heats are calculated from fluctuations of magnetizations and energies,

respectively.

3. Results

Simulations are carried out for R(= J'/J) = 0, - 0.2, - 0.4, - 0.6, - 0.8, - 1.0. Figure 1 shows a result of the temperature dependence of sublattice magnetizations (a), and sublattice susceptibilities (b), when R = - 0.2 with MCS = (300, 1500). Figures 2 and 3 show the susceptibility and the specific heat of the total system for (a) R = - 0.2, (b) R = - 0.6, and (c) R = - 1.0, respectively. We see from these figures that the four states appear: the paramagnetic (P : $T > T_1$), partially disordered (Pd : $T_2 < T < T_1$), three-sublattice ferrimagnetic (F_3 : $T_3 < T < T_2$), and two-sublattice ferrimagnetic (F_2 : $T < T_3$) states.

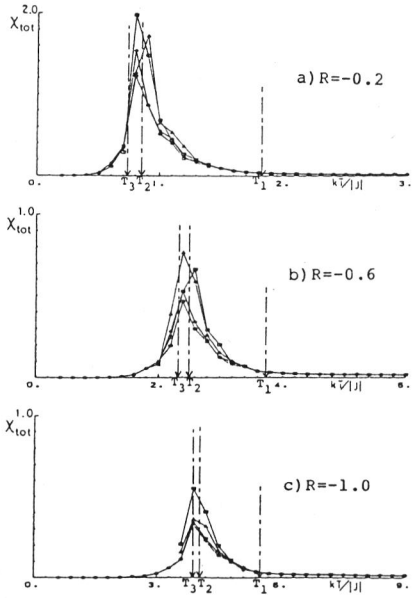

Fig. 2. The susceptibility of the total system χ_{tot}. χ_{tot} tends to diverges at T_2. ○, N = 24 x 24, heating process; ◇, N = 24 x 24, cooling process; △, N = 36 x 36, heating process; □, N = 36 x 36, cooling process.

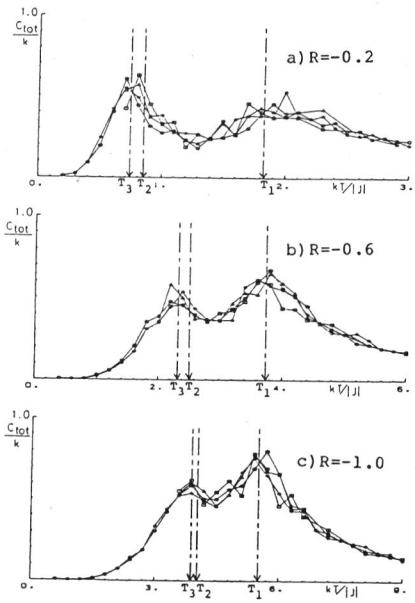

Fig. 3. The specific heat of the total system C_{tot}. C_{tot} is expected to diverge at T_3 and seems to have a cusp at T_1. The meanings of symbols are same as in Fig. 2.

We estimate the three singular temperatures T_1, T_2, T_3 for each value of R as follows. T_1 is estimated from the behaviour: $\langle M_\alpha \rangle$ and $\langle M_\gamma \rangle$ tend to vanish when the temperature increases; χ_α and χ_γ tend to diverge and C_{tot} seems to have a cusp at this temperature. T_2 is estimated from the behaviour: $\langle M_\beta \rangle$ and $\langle M_{tot} \rangle$ tend to vanish and $\langle E_\alpha \rangle$ and $\langle E_\gamma \rangle$ tend to become equal when the temperature increases; χ_β and χ_{tot}, and C_α, C_β, C_γ tend to diverge at this temperature. T_3 is estimated from the behaviour: $\langle M_\beta \rangle$ and $\langle E_\beta \rangle$ tend to have different values from those of $\langle M_\alpha \rangle$ and $\langle E_\alpha \rangle$, respectively, when the temperature increases; C_{tot} diverges at this temperature.

4. Conclusions and Discussion

From the estimation of singular temperatures T_1, T_2, T_3 for several values of R, we obtain the phase diagram shown in Fig. 4. In this figure the negative larger R we take, the narrower

partially disordered region ($T_2 < T < T_1$) is obtained. This feature is qualitatively in agreement with the results of the mean field approximation [2] and the cluster variation method [5]. The partially disordered (PD) state seems to be realized in the temperature region $T_2 < T < T_1$ even when the parameter R takes values of $R < -0.4$. The critical value of R at which PD phase vanish is not detected from the present simulation. This feature agrees better with the result of the cluster variation method [5] than that of the mean field approximation [2].

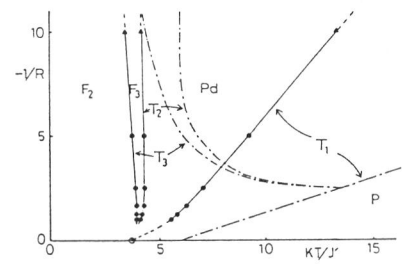

Fig. 4. Estimated temperatures T_1, T_2, T_3 v.s. inverse parameter $-1/R(=-J/J')$ and the phase diagram. Temperatures are estimated from the present simulation ●, and the simulation data of Wada et al [6] △. ⊙ is the exact transition temperature of the ferromagnetic ($J' > 0$) triangular lattice $kT_c/J' = 3.641$. Dash dotted lines are the result of the mean field approximation by Mekata [2]. P: paramagnetic, Pd: partially disordered, F_2: two-sublattice ferrimagnetic, and F_3: three-sublattice ferrimagnetic phases.

The present result of the susceptibility (Fig. 2(a) and the specific heat (Fig. 3(a)) of the total system, χ_{tot} and C_{tot}, in the case of $R = -0.2$ is qualitatively the same as that of the Monte Carlo simulation of $R = -0.1$ by Wada et al [6]. They, however, proposed that C_{tot} seems to have no singularity at T_1. They also claimed that the PD phase will not be realized as an equilibrium phase, because interchanges of roles of three sublattices frequently happen in PD phase region. Nevertheless we expect that the interchanges of roles of sublattices with some time interval will not happen at the thermodynamic limit. If the PD phase can not exist as an equilibrium phase, the breakdown of this phase should be brought out from domain-like local interchanges of roles of the three sublattices.

Very recently, we are noticed that this model belongs to the universality class of six-state clock model [8]. This model has a possibility that Kosterlitz-Thouless transition occurs at T_1.

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