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MONTE CARLO SIMULATIONS FOR DILUTE ANTIFERROMAGNETIC POTTS MODELS

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Monte Carlo simulations are carried out on dilute antiferromagnetic Potts models with q=3 and 4 on a simple cubic lattice and with q=3 on a triangular lattice. The transition temperature is shown to decrease monotonically with decreasing bond-concentration and its critical concentration to be dependent on the q-number in contrast to ferromagnetic cases.

1. Introduction

Recently phase transitions of q-state Potts model attract much attention of theoretical Physists. Pretty amounts of works are published on the ferromagnetic Potts model [1] and rigorous transition temperatures are known for the case of 2-dimensional lattice. On the other hand, there are not so many works [2-4] on antiferromagnetic (AF) Potts model. The ground state for AF Potts model with $q \geqq 3$ has highly degenerate spin arrangements on super cubic lattices. It should be expected that this causes the decrease of transition temperature and sometimes may destroy a spin ordering. These stuation would be somewhat similar to effects of zero-point entropy due to frustrations in some kind of spin-glasses.

In this paper we investigate the phase transitions of dilute AF Potts model by means of Monte Carlo simulations on simple cubic and triangular lattices.

2. Simple Cubic Lattices

The Hamiltonian for q-state Potts model may be written as

$$\mathcal{H} = - \sum_{<ij>} J_{ij} \, \delta(\sigma_i, \sigma_j), \qquad \sigma_i = 1, 2, \cdots, q \tag{1}$$

where $\delta(\sigma_i, \sigma_j)$ denotes the Kroneker's delta function, and sum $<i,j>$ is restricted to nearest neiboring pairs. We deal with the case of random bond dilution of AF Potts, where interaction J_{ij} is assumed to be either $-|J|$ or 0.

In the AF Potts model a spin ordering on the s.c. lattice is considered to break the lattice into two sublattices. For 2-state Potts, equivalent to Ising model, antiferromagnetic ordering is well known. For 3-state one we may assign the A-sublattice to the state-1, and the B to other states. Because there are no intra-sublattice interaction, any spin arrangements are allowed on the B-sublattice in the ground state, as far as the state-1 is excluded. Thus the zero-point entropy for q=3 AF Potts model becomes (N/2) log 2 which reaches about 32 percent of that of completely random spin arrangement, where N is the number of lattice sites.

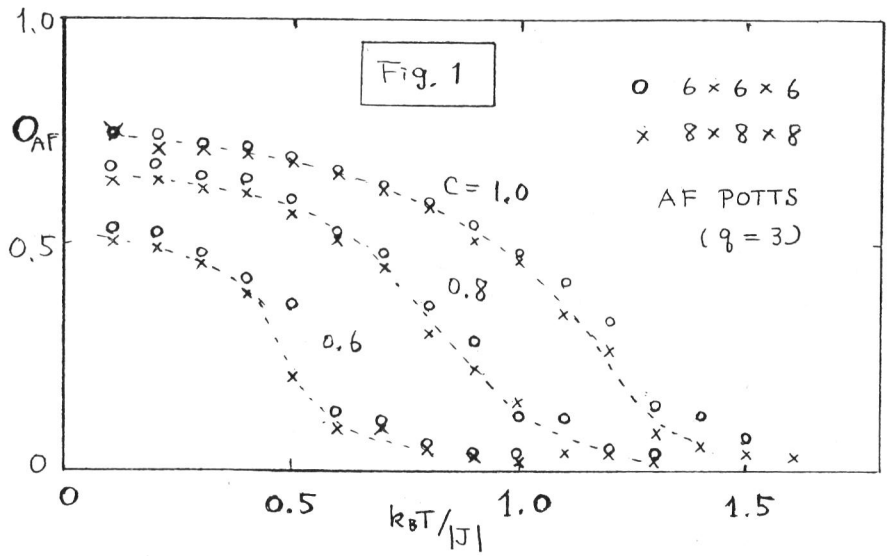
If the ordered phase is assumed to be uniaxial, a conventional order parameter is defined by

$$\xi = \frac{q}{q-1} <\delta(\sigma, 1) - \frac{1}{q}>_A \tag{2}$$

where $\langle \cdots \rangle_A$ represents the thermal average on the A-sublattice. We have found these order parameter is considerably scattered around the transition temperature. This would be partially because of sublattice switchings in M. C. sequences. So we adopt another order parameter defined by

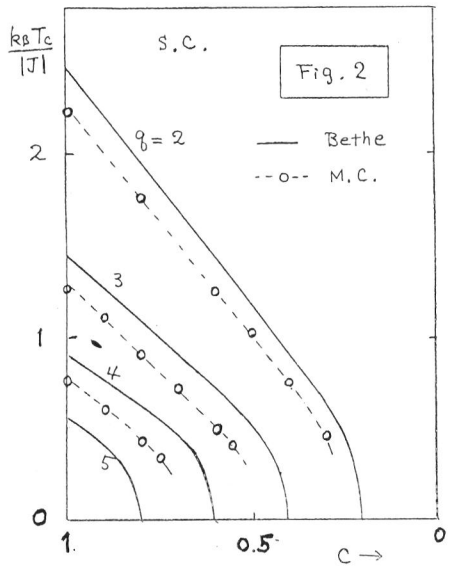
$$O_{AF} = \frac{1}{2}\left(\frac{2}{N}\right)^2 \Big\langle \sum_{i,i' \in A} \delta(\sigma_i \sigma_{i'}) + \sum_{j,j' \in B} \delta(\sigma_j \sigma_{j'}) - 2 \sum_{i \in A, j \in B} \delta(\sigma_i \sigma_j) \Big\rangle . \qquad (3)$$

The new order parameter consists of the sum of spin-spin correlation and is considered to be proportional to a staggered susceptibility times temperature or $k_B T \chi_S / N$ in the disordered phase. The above-mensioned sublattice ordering follows 3/4 of O_{AF} for q=3. In Fig. 1 we show the temperature dependence of O_{AF} obtained Monte Carlo simulations performed on 6×6×6 and 8×8×8 lattice. It would not be unreasonable that the transition temperature can be determined from the inflection point. Figure 2 shows the concentration dependence of transition temperatures for q=2, 3 and 4. Solid lines show the analytical results by Bethe approximations. The above two results are qualitatively agreement with each other. It should be noted that the critical concentrations are decreased with increasing q-number. These facts are contrast to dilute ferromagnetic Potts model [5].

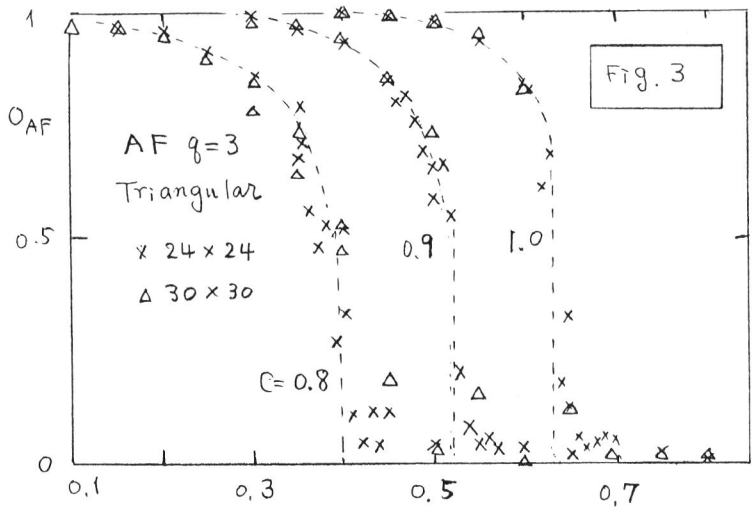


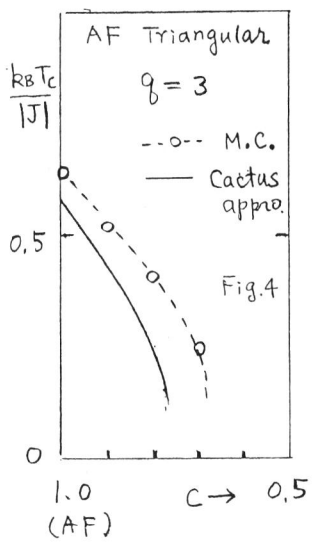
3. Triangular Lattices

The AF Ising model, equivalent to AF Potts model with q=2, exhibits no phase transition on a triangular lattice because of a highly frustrated ground state. On the other hand, an ordered phase for the 3-state AF Potts model is assumed to have three sublattices, where state-1, -2 or -3 are allotted to the A, B or c sublattice, respectively. This is free from frustration and not degenerate in the ground state. Monte Carlo simulations are performed on 24×24 and 30×30 periodic lattices. In Fig. 3, we plot the order parameter which is similar to (3) against temperatures. One can find the transition turns out to be 1st order. The estimated transition temperature $k_B T_c/|J|$ becomes around 0.64 for the pure AF Potts model. This value is in good agreement with the results by Grest [6] who found the discontinuety in the energy curve versus temperature by means of Monte Carlo methods. The results of the renormalization approaches by Schick and Griffith [2] led to the 2nd order phase transition, which is inconsistent with M. C. data. We have also analytically investigated these ordered phase by the triangular cactus approximation [7] and found this phase transition is to be 1st order at $k_B T_c/|J| = 0.57$. This value is about 10 percent lower than our M. C. data.



The concentration dependence of transition temperature is also shown in Fig. 4. Behaviors of transition temperatures are analogous to that for s.c. lattice. When $c \lesssim 0.8$ we could not clearly decided on the type of phase transition.





4. Conclusions

Preliminary Monte Carlo data are presented on the phase transitions of dilute AF Potts models on up to $8 \times 8 \times 8$ simple cubic and up to 30×30 triangular lattices. We have proposed the new order parameter which is found to have comparatively smooth variations against the temperatures even for fairly small lattice consisting of less than 1000 sites. The 2, 3 and 4-state AF Potts models on the s.c. lattice are shown to exhibit the 2nd order phase transition. The 3-state AF Potts on the triangular lattice, on the other hand, maintains the 1st order one at least until 80 percent of alived bonds. The AF bonds dilution follows a monotonical decrease in the transition temperature and the q-dependent critical concentrations in contrast to the q-independent values for the dilute ferro Potts models.

References

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