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LETTER TO THE EDITOR

Monte Carlo study of the antiferromagnetic Potts model on frustrated lattices

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Abstract. Results of computer simulations for the antiferromagnetic q-state Potts model on the triangle and FCC lattices are reported. For the triangle lattice, the three-state Potts model has a first-order phase transition at a temperature $T_c \simeq 0.63|J|$. For $q \geq 4$, the system is paramagnetic for all temperatures. For the FCC lattice, the transition is first order for $2 \leq q \leq 6$.

In systems which order ferromagnetically, it is known that the critical behaviour of the system near the critical temperature T_c is not affected by the nature of the underlying lattice. The critical behaviour depends only on the dimensionality d and number of the components of the order parameter n. However, when the interactions are antiferromagnetic (AF), the situation is often more interesting. The simplest example of this is the Ising model with only nearest-neighbour (NN) AF interactions. For the square, simple cubic and body-centre-cubic lattices, the system breaks into two well defined sublattices and the transition temperature and critical properties are the same as for the ferromagnetic Ising model. However, for the two-dimensional triangle lattice, the system is fully frustrated and remains paramagnetic down to $T = 0$. For the face-centre-cubic (FCC) lattice, the system is also frustrated, but not completely, and has a first-order transition to an infinitely degenerate AF ground state in which one third of the bonds are unsatisfied (Phani *et al* 1979, 1980, Grest and Gabl 1979). In the light of these results for the Ising model, it seems worthwhile to study other AF models on these two frustrated lattices to see if they show similar behaviour. In this Letter, I present results for the AF Potts models (Schick and Griffiths 1977, Banavar *et al* 1980, Grest and Banavar 1981) on the triangle and FCC lattices.

The AF Potts model is described by the Hamiltonian

$$-H = J \sum_{\langle ij \rangle} \delta_{S_i, S_j}, \qquad J < 0, \tag{1}$$

where $S_i = a, b, c, \ldots$ is one of the q-states, δ_{S_i,S_j} is the Kronecker delta and the sum is over nearest-neighbour pairs. For $q = 2$, one recovers the Ising model. The AF Potts models ($J<0$) on a hypercubic lattice have a highly degenerate ground state for $q \geq 3$. Following the one-parameter rescaling analysis of Berker and Kadanoff (1980), Monte Carlo (MC) simulations and ε-expansion techniques have been used to analyse the behaviour of the AF Potts model in three dimensions (Banavar *et al* 1980) and two

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dimensions (Grest and Banavar 1981). It was found that both $q = 3$ and $q = 4$ AF Potts models on a simple cubic lattice exhibit continuous transitions and are in the $n = 2$ and $n = 3$ universality classes respectively.

In this Letter, I report the results of a MC simulation for the AF Potts model on the triangle and FCC lattices. The MC results were obtained with finite-size lattices with periodic boundary conditions. A number of runs from different starting configurations were made and have confirmed the equilibrium nature of the final states.

Triangle lattice

For $q = 2$, the system is completely frustrated and does not order. However, for $q = 3$ the ground state is not frustrated and the system orders at a finite temperature. There are six possible ground states (Schick and Griffiths 1977), as the system breaks up into three-sublattices, with each of the three states occupying one of the sublattices. The ordering is perfect at $T = 0$, as each of the three states of the system is surrounded only by unlike states. A plot of the average energy $E(T)/|J|$ against $T/|J|$ is shown in figure 1 for the three-state Potts model on the triangle lattice. From this result and studies of the corresponding magnetisation against temperature, I find that the system has a first-order phase transition at $T_c \cong 0.63|J|$. This result disagrees with the position-space renormalisation group transformation of Schick and Griffiths (1977) who predicted a second-order phase transition. However, this should not be too surprising in the light of recent work on the F Potts model (Nienhuis *et al* 1979), which showed that the first-order transition predicted for $q > 4$ is not observed in the position-space renormalisation group calculations unless the disordered cells of spins are treated as vacancies. It would be of interest to apply these new real-space methods to the $q = 3$ AF Potts model to see if they can predict the first-order transition found here.

For $q \geqslant 4$, the system remains paramagnetic for all temperatures. Similar results were found for $q \geqslant 4$ for the two-dimensional square lattice (Grest and Banavar 1981).

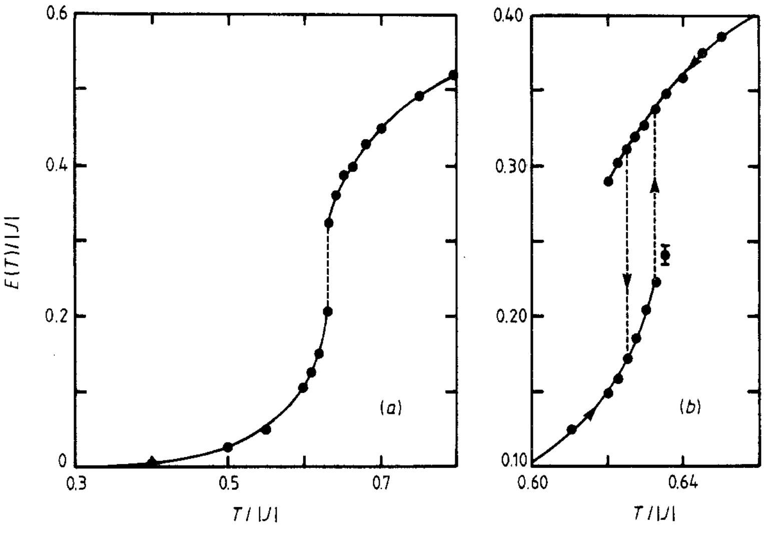

Figure 1. Average energy $E(T)/|J|$ against $T/|J|$ for the three-state AF Potts model on a triangle lattice for a 51×51 lattice. The transition is first order with $T_c \approx 0.63|J|$.

FCC lattice

For $q = 2$, the FCC differs from the triangle lattice, in that it orders via a first-order transition to an AF state. This state has an infinite ground-state degeneracy in which 4 of

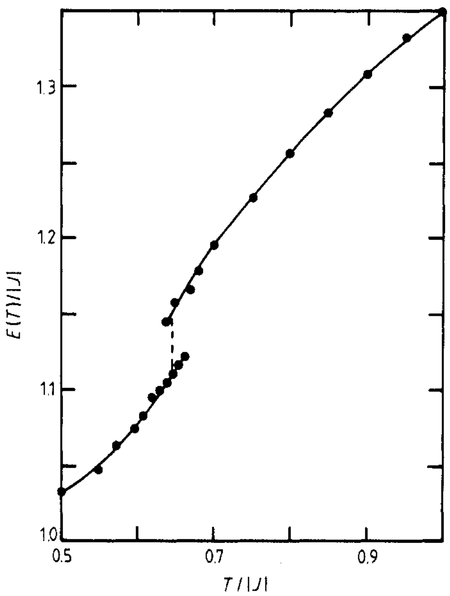

Figure 2. Average energy $E(T)/|J|$ against $T/|J|$ for the three-state AF Potts model on the FCC lattice with $N = 2048$ sites.

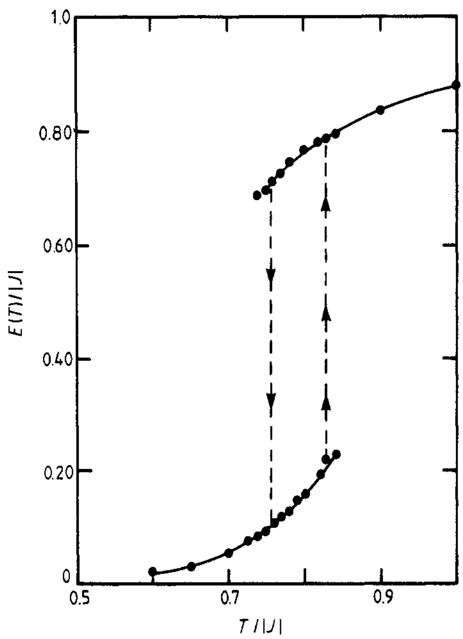

Figure 3. Average energy $E(T)/|J|$ against $T/|J|$ for the four-state AF Potts model on the FCC lattice with $N = 2048$ sites. The transition lies between the vertical broken lines.

the 12 NN bonds remain unsatisfied at $T=0$. For $q \geqslant 3$, the ground states are also infinitely degenerate. However, for $q=3$ on average only 2 of the 12 NN bonds remain unsatisfied at $T=0$, while no bonds are unsatisfied at $T=0$ for $q \geqslant 4$. In fact, the ground states were so highly degenerate that it was impossible to define a suitable order parameter to describe the low-temperature phase. Therefore, only the average energy $E(T)$ could be used to determine the order of the transition. The average energy $E(T)/|J|$ against $T/|J|$ is shown in figures 2–5 for $q=3$, 4, 5 and 6. All the transitions are first order. Table 1 gives the Monte Carlo estimates of the transition temperature $T_c/|J|$ and energy discontinuity $\Delta E/|J|$ at T_c. Note that T_c decreases with increasing q, except for $q=3$ for which T_c is lower than for $q=4$. Note also that ΔE is larger for $q=4$ and $q=5$ than for $q=2$ and 3. This is surely related to the fact that the ground states are partially frustrated for the two- and three-state AF Potts models, but not for $q \geqslant 4$.

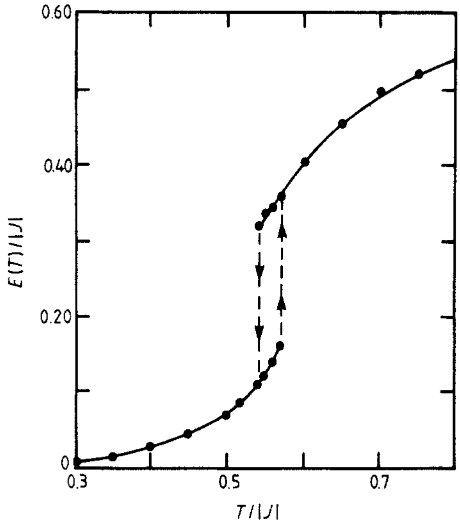

Figure 4. Average energy $E(T)/|J|$ against $T/|J|$ for the five-state AF Potts model on the FCC lattice with $N=2048$.

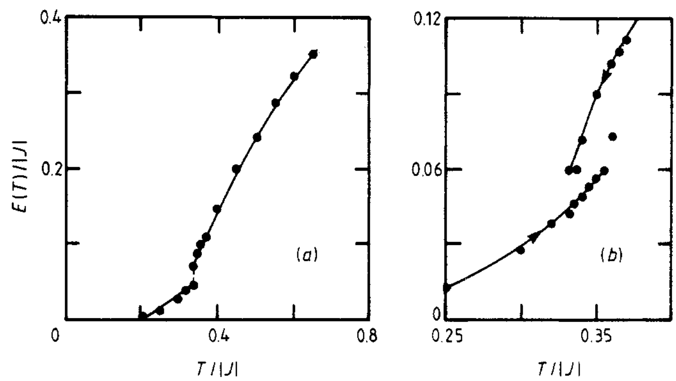

Figure 5. Average energy $E(T)/|J|$ against $T/|J|$ for the six-state AF Potts model on the FCC lattice with $N=2048$.

Table 1. Monte Carlo estimates of the transition temperature and energy discontinuities ΔE for the q-state AF Potts model on an FCC lattice.

q	$T_c/\|J\|$	$\Delta E/\|J\|$
2	0.883 ± 0.002[a]	0.1766 ± 0.004[a]
3	0.64 ± 0.02	0.04 ± 0.01
4	0.80 ± 0.02	0.60 ± 0.02
5	0.56 ± 0.02	0.20 ± 0.02
6	0.34 ± 0.01	0.02 ± 0.01

[a] Phani *et al* (1980).

In conclusion, I have observed first-order phase transitions for the $q = 3$ AF Potts model on the triangle lattice and for $2 \leq q \leq 6$ on the FCC lattice. The frustration in the AF Ising model ($q = 2$) on these lattices is removed for larger values of q. However, the large ground state degeneracy of the AF Potts model on the FCC lattice remains.

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