Monte Carlo Study of the Antiferromagnetic Potts Model in Two Dimensions

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(Received 9 February 1981)

Results of Monte Carlo studies of the q-state Potts model on a square lattice with antiferromagnetic nearest-neighbor coupling and ferromagnetic next-nearest-neighbor coupling are presented for $q \geqslant 3$. The three-state Potts model shows a variety of unusual transitions whereas for $q \geqslant 4$, we find two first-order phase transitions separated by a *broken sublattice symmetry* state.

PACS numbers: 64.60.Cr, 05.70.Jk, 61.40.Df

Recently, there has been considerable activity in the studies of phase transitions in ferromagnetic (F) q-state Potts models in two dimensions.[1] In this Letter, we present results of the first study of phase transitions in antiferromagnetic (AF) q-state Potts models on a square lattice. The Potts model is described by the Hamiltonian

$$-H = J_{\rm nn} \sum_{\langle ij \rangle} \delta_{S_i, S_j} + J_{\rm nnn} \sum_{\langle ij \rangle}{}' \delta_{S_i, S_j}, \qquad (1)$$

where $S_i = a, b, c, \dots$ is one of the q states and δ_{S_i, S_j} is the Kronecker δ function. The first sum is over pairs of nearest-neighbor (nn) spins and the second sum is over pairs of next-nearest-neighbor (nnn) spins. We restrict ourselves to AF nn exchange ($J_{\rm nn} < 0$) and F nnn exchange ($J_{\rm nnn} > 0$). AF Potts models on a hypercubic lattice, with $J_{\rm nnn} = 0$, have a highly degenerate ground state for $q \geqslant 3$. Following the one-parameter rescaling analysis of Berker and Kadanoff,[2] Monte Carlo (MC) simulations and ϵ-expansion techniques have been used to analyze the behavior of AF Potts models in three dimensions.[3] 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.[3]

In two dimensions, the AF Potts models, with $q \geqslant 4$ ($J_{\rm nnn} = 0$), are known to be paramagnetic at all temperatures. The $q = 3$ model, on the other hand, is in the XY universality class and may be expected to show rich and interesting behavior. At zero temperature, the $q = 3$ AF Potts model ($J_{\rm nnn} = 0$) is identical to the six-vertex problem and the three-coloring problem on a square lattice. Baxter[4] has solved a generalized hard-squares version of this problem in which one of the colors is regarded as a particle and the others form a background. Baxter[4] finds that the system undergoes a phase transition with infinite compressibility at the density of each color $\rho = \frac{1}{3}$. This suggests that the a-a, b-b, c-c correlations decay algebraically with distance at zero temperature.

Our MC results have been obtained with finite-size lattices (mostly 50×50) with periodic boundary conditions using both random and ordered searches and a single spin-flip sequence. Typically 500–1000 MC steps per spin were used except for the case $q = 3$, $J_{\rm nnn} = 0$ for which longer runs were made.

Our principal findings are summarized below:

(1) $q = 3$; $J_{\rm nnn} = 0$.—The three-state AF Potts model, with nn AF coupling only, in addition to the Baxter phase transition[4] at zero temperature, appears to undergo a continuous phase transition at a finite temperature. To describe this ordering it is convenient to divide the square lattice into two sublattices I and II such that spins on one sublattice have their nn's spins on the other sublattice. A simplified view of the ordering of the $q = 3$ AF Potts model[3] ($J_{\rm nnn} = 0$) in three dimensions is that one of the three states is on sublattice I and the other two states are distributed randomly on sublattice II, a state which we call the *broken–sublattice-symmetry* (BSS) state. However, even at zero temperature, the ordering is not perfect in that a given state occurs occasionally on the "wrong" sublattice. The ordering is similar, in principle, even in two dimensions. However, the exact results of Baxter[4] show that the three-state AF Potts model in $d = 2$ has an equal number of a's, b's, and c's. Further, the algebraic decay of correlations that occurs at zero temperature[4] is presumably a result of a very complex defect structure, one that is felt at all length scales. At low, nonzero tem-

peratures the system orders in one of six equivalent ways. The ordering is such that one of the three states is present almost entirely on one of sublattices while equal numbers of the other two states are found on each of the two sublattices. The order parameter M may be defined to be

$$M=\{|\sum_{i\subset \mathrm{I}}\delta_{s_i,a}-\sum_{i\subset \mathrm{II}}\delta_{s_i,a}|+|\sum_{i\subset \mathrm{I}}\delta_{s_i,b}-\sum_{i\subset \mathrm{II}}\delta_{s_i,b}|+|\sum_{i\subset \mathrm{I}}\delta_{s_i,c}-\sum_{i\subset \mathrm{II}}\delta_{s_i,c}|+\cdots\}/N, \tag{2}$$

where N is the total number of spins.

Figure 1 shows a plot of M as a function of the temperature for three $L\times L$ lattices and Fig. 2 a plot of the average energy. These results for $L=32$ and 50 were obtained with use of a random search by slow cooling or quenching from the paramagnetic phase and heating from the ordered phase at $T=0$. Results for $L=80$ were obtained by heating from $T=0$. For $L=32$ and 50, 1500–2000 MC steps per spin were used in the vicinity of the transition. Because of the defects in the order as described above, the value of the saturation magnetization is ≈ 0.64. M is found to vanish at a finite temperature T_c, with the specific heat showing a broad maximum at a temperature higher than T_c.

It is known that computer simulations in two dimensions are often difficult to interpret unambiguously for $n\geq 2$. Unfortunately, that appears to be the case here where there are at least three possible interpretations of the results shown in Figs. 1 and 2 which are not inconsistent with our present MC results. These are the following: (i) The low-temperature results in Fig. 1 are indicative of true long-range order below a nonzero transition temperature T_c. In fact, at temperatures $\lesssim \frac{1}{2}T_c$, the value of M averaged over 2000 passes through the lattice is equal to the corresponding quantity without the modulus in it. One may speculate that the behavior may then be analogous to that of an XY model with a sixfold-symmetry-breaking field.[5] Cardy[6] has recently argued that this may indeed be the case. (ii) There is no true long-range order in the system and the behavior is analogous to an XY model without any symmetry-breaking fields. One would then expect algebraically decaying correlation at all temperatures below T_c. The results of Fig. 1 could then be attributed to the finite size of the system and finite simulation times leading to an apparent nonzero M. (iii) There is no true long-range order in the system, with algebraic decay of correlations only at zero temperature.

It has been recently argued[7,8] that the three state AF Potts model has no long-range ordering but has algebraic decay of correlation at zero temperature, consistent with interpretation (ii) and (iii) above. While a naive analysis of the MC data would favor interpretation (i) over (ii) and (iii), the subtlety of the problem combined with the inadequacy of the MC technique does not permit us to arrive at any definitive conclusions.

(2) $q=3$; $J_{nnn}>0$.—With a weak F nnn coupling, the three state AF Potts model appears to undergo two transitions. At the lowest temperatures, the system is in an "AF" phase. The AF phase has a sixfold degeneracy with both sublattices

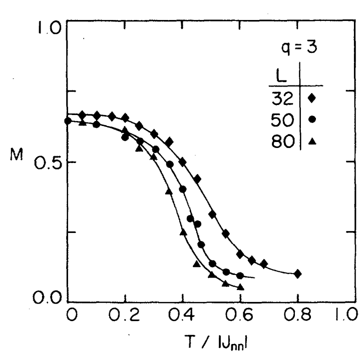

FIG. 1. Order parameter M of the three-state AF Potts model ($J_{nnn}=0$) vs temperature for three different $L\times L$ lattices.

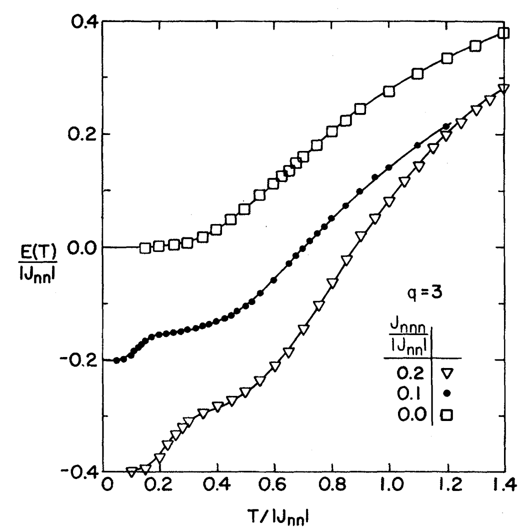

FIG. 2. Average energy of the three-state Potts model vs temperature for the values $J_{nnn}/|J_{nn}|$ shown for a 50×50 lattice.

ordered ferromagnetically, but antiferromagnetic with respect to each other. On heating to T_{c2}, the system has a phase transition to a BSS phase similar, in principle, to the ordering of the three-state AF Potts model with $J_{nnn}=0$ in two and three dimensions, but with an intermediate number of defects. M (as defined in the case with $J_{nnn}=0$) goes to zero continuously at a higher temperature T_{c1}. If case (i) or (ii) for $J_{nnn}=0$ is correct, then there are two transitions for $J_{nnn}>0$; however, if (iii) is correct, then there is only transition at T_{c2}. Figure 2 shows a plot of the average energy versus temperature for several values of J_{nnn}. Our results for $E(T)$ from Fig. 2 as well as results for larger values of J_{nnn} suggest a continuous transition at T_{c2}. However, a careful analysis of the MC sublattice magnetization data reveals that the lower transition at T_{c2} is probably first order characterized by a discontinuous jump in the magnetizations which describe these two states and a very small, unmeasurable latent heat. This transition occurs at a temperature above the maximum of the heat capacity associated with the sharp increase in internal energy as a function of temperature. For example, we estimate that, for $J_{nnn}/|J_{nn}|=0.1$, $T_{c2}/|J_{nn}|=0.155\pm0.01$, while the maximum in $dE(T)/dT$ occurs at $T/|J_{nn}|\simeq 0.12\pm0.01$. MC analysis cannot in this case unambiguously tell the difference between a first- and second-order phase transition.

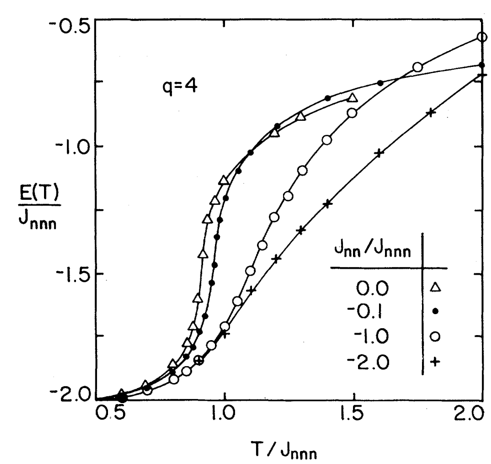

FIG. 3. Average energy of the four-state Potts model vs temperature for the values of J_{nn}/J_{nnn} shown for a 50×50 lattice. While these results suggest continuous transitions, a study of the sublattice magnetizations suggest two first-order phase transitions closely spaced.

As the strength of J_{nnn} increases, T_{c2} moves up closer to T_{c1}. For $J_{nnn}\geq|J_{nn}|$, we are unable to tell whether there are two transitions, or whether T_{c1} and T_{c2} have merged into a single T_c at a multicritical point. Finally, we note that in the absence of any J_{nn}, the model decouples into two F three-state Potts models, each of which is known to exhibit a continuous phase transition.[9]

(3) $q=4$; $J_{nnn}\geq 0$.—The $q=4$ AF Potts model with $J_{nnn}=0$ is known to be paramagnetic at all temperatures.[10] For any nonzero J_{nnn}, the system at $T=0$ orders into one of twelve degenerate states such that each sublattice is ordered ferromagnetically but antiferromagnetically with respect to each other. Figure 3 shows a plot of the average energy versus J_{nn}/J_{nnn}. These results suggest a continuous transition from the ordered state to the paramagnetic state. However, a careful analysis of the sublattice magnetizations suggest two first-order phase transitions. Between these two transitions is a *broken-sublattice-symmetry* state characterized by one sublattice being ordered ferromagnetically in one of the four states and the other sublattice randomly populated with the remaining three states. Note that for $J_{nn}=0$, the model reduces to two decoupled F Potts models. Since the F Potts models have a first-order transition for $q>4$, it should not be surprising that the addition of another relevant operator, J_{nn}, drives the transition first order, with a very small, unmeasurable latent heat.

(4) $q\geq 5$; $J_{nnn}\geq 0$.—$q\geq 5$ Potts models are paramagnetic at all temperatures for $J_{nn}<0$ and $J_{nnn}=0$ and reduce to two decoupled F Potts

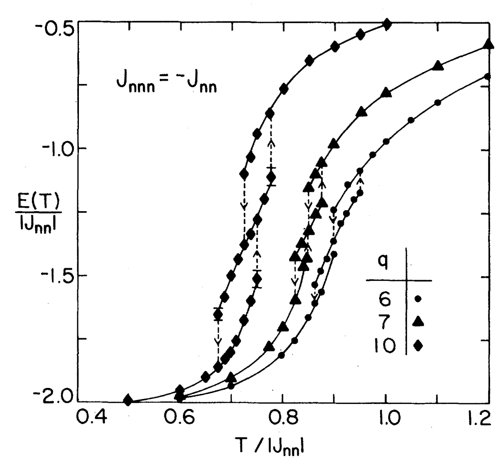

FIG. 4. Average energy of the q-state (q = 6, 7, and 10) Potts model vs temperature for $J_{nn}<0$ and $J_{nnn}/|J_{nn}|=1.0$ for a 50×50 lattice.

models for $J_{nn}=0$. For $J_{nnn}>0$, the system orders into one of $q(q-1)$ degenerate ground states with both sublattices ordered ferromagnetically but antiferromagnetically with respect to each other. Figure 4 shows the average energy versus the temperature for $J_{nnn}=-J_{nn}$ and three values of q. In all cases, the system disorders via two first-order transitions. Pronounced hystersis effects are observed especially for higher values of q. Between the two transition temperatures the system is found to be in a BSS state characterized by one of the sublattices being ordered ferromagnetically in one of the q states and the other sublattice populated randomly with the remaining $q-1$ states. This leads to a large gain in entropy with almost all the nn bonds satisfied and some of the nnn bonds being unsatisfied. The results for $q \geqslant 5$ differ from those discussed above for $q=4$ only in the magnitude of the associated latent heat. This BSS state has also been observed in three dimensions.

It is a pleasure to thank L. Kadanoff, M. den Nijs, D. Fisher, P. Hohenberg, J. Hirsch, S. Shenker, and C. Varma for many stimulating discussions and J. Cardy for communicating his results prior to publication. This work was supported in part by the National Science Foundation under Grants No. DMR-80-17758, No. DMR-79-07232, and No. DMR-78-24698.

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Phase Separation in Films of ^3He-^4He Mixtures

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(Received 9 January 1981)

We report detailed observations of the propagation of third sound in ^3He-^4He mixture films as a function of temperature and ^3He concentration. The data are consistent with a simple model for the film and we conclude that thin ^3He-^4He mixture films exhibit nearly complete phase separation.

PACS numbers: 67.60.-g, 67.40.Pm

The study of thin ^4He films[1,2] is at the forefront of the investigation into the physics of (quasi-) two-dimensional systems. In particular, the agreement achieved between experiment[1] and the Kosterlitz-Thouless-Nelson theory[3] of superfluid onset is a major triumph for that vortex-unbinding picture. It is expected that the addition of a ^3He component will, in analogy to the bulk, make this rich system even richer. There has already been some theoretical[4] and experimental[5,6] work concerned with the effects of the ^3He impurity on superfluid onset. The basic thrust of this paper, however, pertains to the phase-separation aspects of the equation of state. Below we shall present third-sound measurements in the mixture together with a hydrodynamic analysis which will lead us to conclude that the state of the film (for $T \lesssim 0.5$ K) is one of layered phase separation.

In the general situation we can picture the films as shown in Fig. 1. The lower film (l) will contain a (film-averaged) mass concentration, x_{3l} of ^3He, and in addition will contain *all* the superfluid. The upper film (u) will be considered to be