Antiferromagnetic Potts Models

Jian-Sheng Wang[a]
Department of Mathematics, Rutgers University, New Brunswick, New Jersey 08903

Robert H. Swendsen
Department of Physics, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213[b]
and Department of Mathematics, Rutgers University, New Brunswick, New Jersey 08903

Roman Kotecký
Department of Mathematical Physics, Charles University, V. Holešovičkách 2, 180 00 Praha 8, Czechoslovakia[b]
and Department of Mathematics, Rutgers University, New Brunswick, New Jersey 08903
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We present a study of the antiferromagnetic Potts model in two and three dimensions, using a new method of Monte Carlo simulations, which enables us to perform simulations with greatly improved efficiency. Illustrating the method for the three-state model, we have obtained new results for the entropy and critical exponents in two and three dimensions. The low-temperature phase in three dimensions is shown to have long-range order with a finite-size dependence similar to that of the XY model.

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Antiferromagnetic Potts models have been shown to possess interesting and unusual properties.[1-22] To begin with, the residual entropy at $T=0$ is bounded from below by $\frac{1}{2}\ln(q-1)$, where q is the number of states, so that it is nonvanishing for $q>2$. The $q=3$ model on a square lattice has a critical point at $T=0$.[1-6] In three dimensions, the evidence indicates the existence of phase transitions for the three- and four-state models,[7-13] although the nature of these transitions has been uncertain. Other studies have shown that the addition of second-neighbor interactions,[14-17] mixed anisotropic interactions,[18,19] or an external magnetic field[20] can produce new types of ordering and new phase transitions.

Monte Carlo (MC) simulations have played an important part in investigating antiferromagnetic Potts models, but they have been hampered by extremely long relaxation times at low temperatures (where things get interesting). The source of these long correlation times lies in the large number of degenerate states to be sampled and the restrictions on transitions between configurations at low temperatures due to the interactions, as exemplified by the slow diffusion of "vortex" excitations.[21,22]

In this Letter, we present a new method of MC simulation, based on the Swendsen-Wang (SW) algorithm[23] and an idea due to Wolff,[24,25] which enables us to simulate antiferromagnetic Potts models very efficiently. Using this new method, we simulated the critical point of the three-state model on a square lattice at $T=0$ and calculated the critical behavior. In three dimensions, we located the phase transition of the three-state model on a simple-cubic lattice, calculated the critical exponents, and showed that the order parameter does not vanish below T_c.

An essential part of this study was the use of a multiple-histogram analysis of the MC data.[26,27] This permitted us to accurately determine the location and height of the very narrow peaks associated with the transition, as well as to plot continuous scaling curves and calculate the residual entropy at $T=0$.

Potts models[28] are defined by the Hamiltonian

$$H=K\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j)\,, \tag{1}$$

where the spins take on the values $\sigma_i=1,2,\ldots,q$, and the sum is over nearest-neighbor pairs of sites on a lattice. K is a dimensionless coupling constant, in which we have absorbed the usual factor of $-1/k_BT$, so that the partition function is given by

$$Z=\mathrm{Tr}_\sigma e^H\,. \tag{2}$$

Antiferromagnetic Potts models are those for which K is negative, so that neighboring sites with different states are energetically favored.

The SW algorithm uses the Fortuin-Kasteleyn mapping of ferromagnetic Potts models onto percolation models.[29] Each interaction between pairs of like spins is transformed into a bond between the sites with probability $p=1-e^{-K}$. This procedure naturally runs into trouble when K is negative. Swendsen and Wang[23] pointed out that for $q=2$ (Ising model) the difficulty can be avoided by generalizing the Fortuin-Kasteleyn mapping. The resulting method used "antibonds," with probability $p=1-e^K$ between neighboring sites with opposite spin. They were not able to extend this approach to $q>2$, because of the ambiguity involved in having more than one "opposite" state.

The key observation that enables us to treat $q>2$ is

that we can embed an Ising model in an antiferromagnetic Potts model, in a manner closely related to Wolff's embedding of Ising reflection variables in $O(n)$ models.[24,25] We chose two states at random and restrict the MC update to sites containing these values, while sites containing other states remain frozen. This leaves us with a $q=2$ antiferromagnetic Potts model (taking on these two values) on a subset of the lattice sites.

Since the interactions between the chosen states and the frozen sites are unaffected, the reduced Hamiltonian can be updated with the SW algorithm.[23] If $q \geq 4$, two or more pairs of states can be updated simultaneously. Naturally, it is also possible to use Wolff's modification of the SW algorithm to pick a single site, and flip the cluster containing that site.[24]

In analyzing the behavior of antiferromagnetic Potts models, we consider a generalized staggered magnetization

$$M_a = 2\left[\sum_i^A \delta(\sigma_i,a) - \sum_i^B \delta(\sigma_i,a)\right], \tag{3}$$

where the sums are restricted to the A and B sublattices. An order parameter suggested by the possibility of "broken sublattice symmetry"[14] is

$$\langle M\rangle = \sum_{a=1}^{q} \langle |M_a| \rangle \tag{4}$$

and the susceptibility above T_c is given by

$$\chi = L^{-d} \sum_{a=1}^{q} \langle M_a^2 \rangle . \tag{5}$$

This can be either measured from the Potts configurations, or $\langle M_a^2\rangle$ can be rewritten in terms of the percolation clusters. If $N^A(\alpha)$ and $N^B(\alpha)$ denote the number of sites in the cluster α on the A and B sublattices, and $N(\alpha)=N^A(\alpha)+N^B(\alpha)$ is the total number of sites in the cluster, then

$$\chi = L^{-d}\left[\left\langle \sum_\alpha N^2(\alpha)\right\rangle + \left\langle \left[\sum_\alpha [N^A(\alpha)-N^B(\alpha)]\right]^2\right\rangle\right]. \tag{6}$$

For the $d=2$, $q=3$ Potts model, we first compared the new method with single-spin-flip Monte Carlo data for a simulation at $T=0$. For small lattices, the results of the two methods agreed, but the single-spin-flip Monte Carlo correlation times increased with lattice size approximately as $\tau = 0.3L^2$, so that the effective dynamical critical exponent was approximately $z=2$. The correlation time for the new algorithm was about seven from $L=4$ to 64. The effective value of z was too small to measure from our data.

The log-log plot of χ vs L was very nearly straight, giving $\gamma/\nu = 1.666 \pm 0.002$. Assuming scaling, this corresponds to $\eta = 0.334 \pm 0.002$. For $T>0$, we found that the susceptibility was proportional to $\exp(AT^{-\nu})$, where $\nu = 1.30$, in agreement with the results of Nightingale and Schick.[3]

To calculate the entropy of the ground state, which is known to be $S(\infty) = \frac{3}{2}\ln\frac{4}{3}$ (Ref. 30) in the thermodynamic limit, we used the multiple-histogram method.[27] Combining information from five simulations each for $L=4$ and 8, and nine simulations for $L=16$, we obtained[31] $S(4)=0.5000$, $S(8)=0.4484$, and $S(16)=0.4359$. These values fit extremely well to the equation $S(L)=S(\infty)+L^{-d}\ln 3$ (see note added). This equation is even in reasonable agreement for $L=2$, where it predicts 16.85 states, compared with the exact answer of 18.

For the $d=3$, $q=3$ model, the multiple-histogram method[27] was used to scan the entire temperature range. The entropy of the ground state showed a size dependence which we interpret to be similar to that in two dimensions. Although we only have values of the residual entropy[31] for $L=4$ and 8 [$S(4)=0.3953$ (10 histograms) and $S(8)=0.3708$ (16 histograms)], we note that they agree with the equation $S(L)=S(\infty)+L^{-d}\times\ln 6$, which would predict that $S(\infty)=0.3673$. This equation is also in reasonable agreement with the exact number of states for an $L=2$ lattice (113.3 vs 126).

We also examined the peaks in the specific heat at the critical point and found evidence for a divergence, as shown in Fig. 1. The approach to the asymptotic behav-

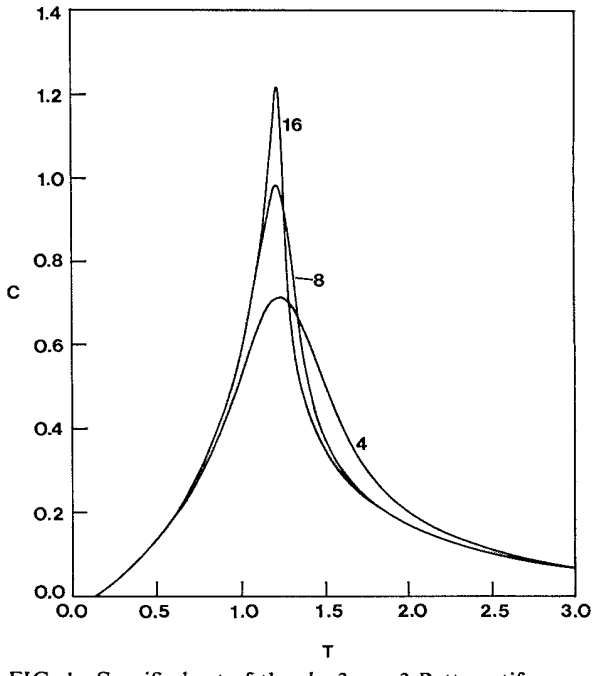

FIG. 1. Specific heat of the $d=3$, $q=3$ Potts antiferromagnet as a function of temperature for $L=4$, 8, and 16. The continuous functions in both figures were obtained from multiple-histogram analyses (Ref. 27). The run lengths in MC steps per site (and the number of runs used for the multiple-histogram analysis) are, respectively, 3×10^5 (10), 1.5×10^5 (14), and 10^5 (9).

ior seems to be rather slow, and the peak in the specific heat first moves toward lower temperatures as L increases ($T_{peak}=1.212$ at $L=8$), and then rises slightly for larger systems. Our best estimates for the transition temperature and the critical exponents comes from a scaling plot for the susceptibility, shown in Fig. 2. We find $T_c=1.225\pm0.005$, with $\gamma=1.27\pm0.05$ and $\nu=0.63\pm0.04$. These exponents are consistent with those of either the $d=3$ Ising- or XY-model values.

Below T_c, we found a strong dependence of the order parameter on the size of the system, in rough agreement with Ono.[12] However, we differ with Ono's conclusion that $\langle M\rangle(L=\infty)=0$ with a massless phase below T_c. Instead, we find that $\langle M\rangle$ approaches a nonzero value as $1/L$ below T_c. This is certainly more consistent with a finite value of ν than a line of fixed points would be. We also found that below T_c, the staggered susceptibility diverges proportional to L. Both behaviors are quite different from that of ferromagnetic Potts models, but are identical with the predictions of the spin-wave approximation for the XY model below T_c.

At the critical temperature, we observed the correlation time to grow approximately as $L^{0.5}$, while for the Metropolis MC simulation we found that it grows as L^2. However, below T_c, where the correlation time is usually size independent, even our algorithm shows a strong size dependence, as if the low-temperature phase exhibited critical fluctuations as suggested by Ono.[12]

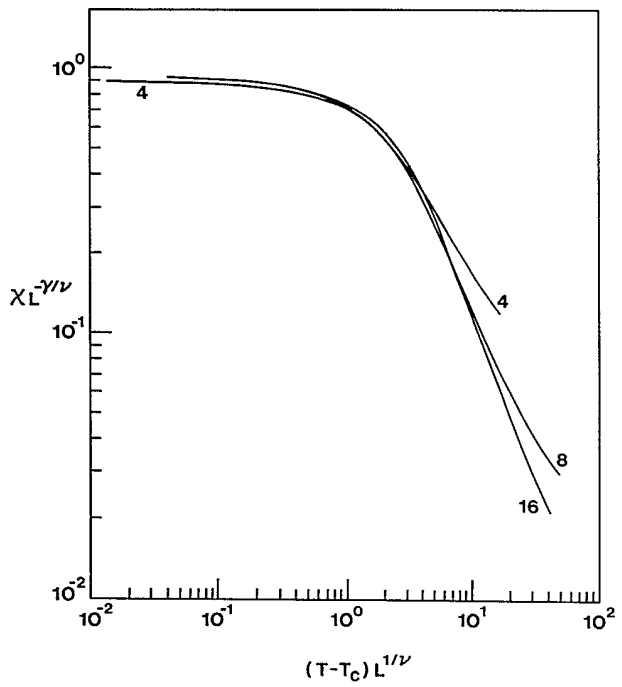

FIG. 2. Scaling plot for the $d=3$, $q=3$ Potts antiferromagnet of the susceptibility times $L^{\gamma/\nu}$ as a function of $(T-T_c)\times L^{-\nu}$, using $T_c=1.225$, $\gamma/\nu=2.02$, and $\nu=0.63$, for $L=4$, 8, and 16.

It is easy to see that if a "vortex," like that introduced by Kolafa,[21] appears in a two-dimensional slice of a three-dimensional configuration, it must actually be part of a closed vortex line. We suspect that such vortex lines play a role in mediating the phase transition.

Some further applications of our simulation method are already apparent. Two- and three-dimensional antiferromagnetic Potts models with $q\geq4$ are being simulated. The addition of second-neighbor ferromagnetic interactions gives a rich phase diagram, but presents no problems to the method, since it does not introduce any additional frustration. Simulations on other lattices (such as bcc) produce other types of transitions. It is also possible to study the antiferromagnetic Ising model on a triangular lattice with antiferromagnetic nearest-neighbor interactions and ferromagnetic next-nearest-neighbor interactions (both can be anisotropic), by updating the spins on two of the three sublattices.

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Note added.—Since we completed this work, Park and Widom[32] have calculated the exact value of $\gamma/\nu=5/3$ for the $d=2$ antiferromagnetic Potts model at $T=0$. This confirms our value of $\gamma/\nu=1.666(2)$. Park and Widom also determined the finite-size correction for $S(T=0)$ in two dimensions to be $L^{-2}\ln2.935\,779\,65\ldots$, correcting our suggestion that it might be $L^{-2}\ln3$. (The small difference is within the statistical errors.) On the other hand, for the three-dimensional case, where we suggested that the finite-size correction to $S(T=0)$ goes as $L^{-3}\times\ln6$, new work by Borgs and Imbrie[33] suggests that, below T_c, the coefficient is just the logarithm of the number of phases, which would mean that our speculation is indeed correct. Data taken since we submitted this paper have provided slightly more accurate estimates for the $d=3$, three-state Potts model: $T_c=1.2256\pm0.0005$, $\gamma/\nu=1.97\pm0.03$, and $\nu=0.66\pm0.03$. These exponents agree somewhat better with those of the XY model. Finally, we call attention to new related work by Ueno, Sun, and Ono[34] which describes MC simulations for $d=3$ and $q=3$–6. They used standard MC simulation methods with lower statistics than ours, and came to the conclusion that both $q=3$ and 4 are in new universality classes. This disagrees sharply with our results, which are most consistent with the $q=3$ model being in the XY universality class.

[a]Present address: Höchstleistungs Rechnungzenturm, Kernforschungsanlage Jülich, D-5170 Jülich, West Germany.

[b]Permanent address.
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