Monte Carlo renormalization-group analysis of the antiferromagnetic three-state Potts model on a square lattice

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Monte Carlo renormalization-group calculations have been performed on the three-state antiferromagnetic Potts model on a square lattice. The results are consistent with the conclusion that there is no transition as a function of temperature.

It is well known that the two-state antiferromagnetic Potts, i.e., Ising model on a square lattice has a second-order phase transition. It has a low-temperature phase with nonzero staggered magnetization and a high-temperature disordered phase. The situation for the three-state antiferromagnetic Potts model, on the other hand, is not well understood. The difficulty stems from the fact that the ground state is infinitely degenerate. This can be seen as follows: divide the square lattice into two sublattices; imagine all sites of one sublattice to be in state "1." Now a random arrangement of states "2" or "3" on the other sublattice yields a ground state. Thus, the system has a nonzero ground-state entropy. As pointed out by Berker and Kadanoff,[1] this fact combined with the complexity of the configurations (characterized by say an algebraic decay of correlations arising from defects) leads to the following situation: Any simple blocking rule (even those that put spins of the same sublattice in the same block) renormalizes zero temperature to a nonzero temperature. This observation led them to suggest that for dimension d less than some critical d_c there would be no phase transition. For $d \geq d_c$, they suggested a distinct low-temperature phase in which correlations decay algebraically with an infinite-order phase transition at d_c. Because their analysis was based on a one-parameter renormalization group they point out that their results are merely suggestive. On the other hand, for $d=2$, Cardy[2] has predicted two phase transitions separating a low-temperature phase of true long-range order from an intermediate phase of XY-like order which is separated from a disordered phase, as in a 2D XY model with a small sixfold anisotropy. His analysis is based on extrapolating the results of the XY model with a small anisotropy field to the case with an infinite field which corresponds to the antiferromagnetic Potts model. Finally, a recent Monte Carlo study[3] on the model came to the conclusion that they could not determine if there was any phase transition or not, nor could they determine the nature of the ordering (if any) at low temperatures. Despite this uncertainty in what happens there exists a simple technique for determining the existence of a phase transition, namely, Monte Carlo renormalization group (MCRG).[4] Using this technique we are able to locate the correct critical temperature for the Ising antiferromagnet and show that the three-state model has no phase transition. We note in passing that the antiferromagnetic Ising model on a triangular lattice which has nonzero ground-state entropy is disordered at all nonzero temperatures.[5]

The models considered here have the following Hamiltonian:

$$\frac{H}{k_B T} = -K \sum_{\langle ij \rangle} \delta_{S_i, S_j} \ , \tag{1}$$

where the spins take on the value 1 or 2 for the Ising model and 1, 2, or 3 for the three-state Potts model, and $\langle ij \rangle$ denotes near-neighbor pairs.

We now review the basic method of the MCRG. First we create a sequence of equilibrium spin configurations using standard Monte Carlo methods at a coupling $K = J/k_B T$. From these configurations we construct a sequence of block spin configurations, where each block spin is formed out of four spins from the same sublattice as shown in Fig. 1.[6] The value of the block spin is determined by the majority rule. In case of a tie a random assignment was made. From the block spin configurations we construct another sequence of block spins in the same way as above. This procedure is continued until we have reached a 2×2 lattice of "super" block spins. This method of blocking has the virtue of preserving the sublattice structure of the lattice. It has the disadvantage that on blocking the interactions between block spins are periodic with period 2. However, all

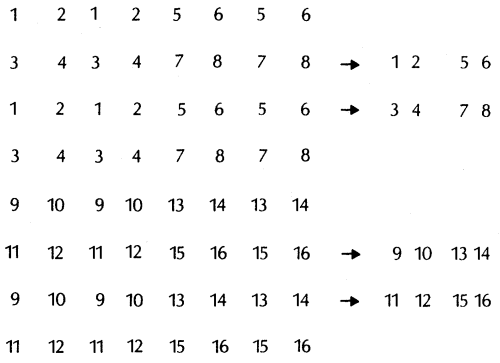

FIG. 1. Illustration of the blocking rule. Spins labeled by the same number are blocked together by the majority rule. As can be seen the lattice has periodicity 2.

further blockings are equivalent, and hence, this should only prevent us from matching averages over spin configurations with those of block spin configurations. How does one locate a critical temperature? At each blocking iteration all length scales are reduced by a factor of $b=2$. Thus, the correlation length ξ is reduced by a factor of 2. Any static average over the block spin system is an average of block spins weighted by the Boltzmann probability of the renormalized Hamiltonian. Thus, if the $l \times l$ block spins of two spin systems have the same static averages then the systems must have the same Hamiltonian and the same correlation length. Now imagine two lattices one with N spins and the other with Nb^d spins at the same temperature. Suppose further that to match static averages, we had to block the smaller lattice m times and the larger lattice $m+1$ times. Clearly, the first lattice has a correlation length of ξ/b^m and the second ξ/b^{m+1}. Since they must have the same correlation length (because static averages match) ξ must equal infinity and we are at the critical temperature.

In our simulation we have computed the nearest-neighbor and next-nearest-neighbor correlation of the spins and block spins as a function of temperature. In both the Ising and Potts models we found that the next-nearest-neighbor correlation for the block spins was virtually independent of temperature at low temperatures and thus not very useful for determining if the two Hamiltonians are the same. We used lattices of sizes 256 and 64 spins and ran each for about 12 000 passes at each coupling $K=J/k_BT$. Only the last 8000 passes were used to compute thermodynamic averages.

In Fig. 2 we show the results for the near-neighbor correlation functions for a 256 spin lattice after $m=2,3$ iterations and a 64 spin lattice after $m=1,2$ iterations, i.e., $C_{NN}(N=256,m=3)$, $C_{NN}(256,2)$, $C_{NN}(64,2)$, and $C_{NN}(64,1)$ for the Ising model.

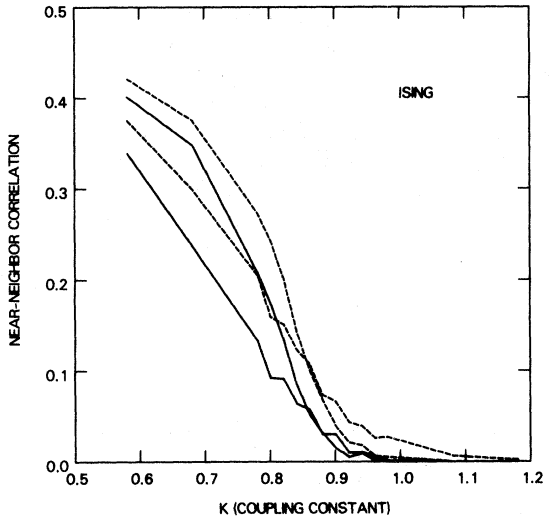

FIG. 2. Ising antiferromagnetic model block spin averages of the nearest-neighbor correlation as a function of K. The top dashed line is the 4×4 block spin lattice from the 256 spin original lattice, top solid line is 2×2 from $N=256$, bottom dashed line is 4×4 from $N=64$, and the bottom solid line is 2×2 from $N=64$. The transition occurs where both the 4×4 lines cross and the 2×2 lines cross.

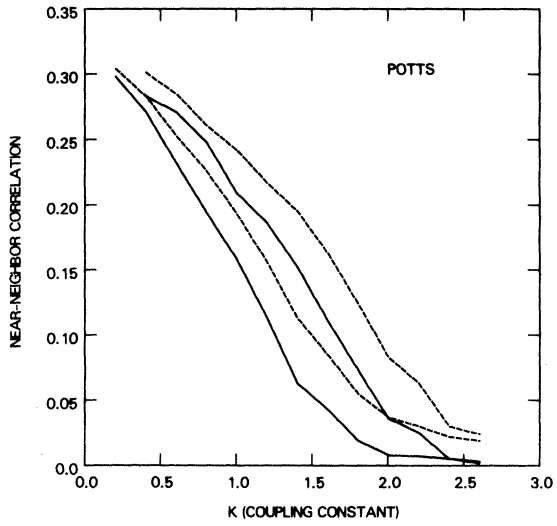

FIG. 3. Potts three-state antiferromagnetic model block spin averages for the nearest-neighbor correlation as a function of K. The top dashed line is the 4×4 block spin lattice from the 256 spin original lattice, top solid line is 2×2 from $N=256$, bottom dashed line is the 4×4 from $N=64$, and the bottom solid line is the 2×2 from $N=64$. There would be a phase transition if both the two 4×4 lines crossed and the two 2×2 lines crossed at the same value of K.

The results for the Potts model are shown in Fig. 3. If there were a phase transition then we would expect there to exist a K_c such that $C_{NN}(256,3) = C_{NN}(64,2)$ and $C_{NN}(256,2) = C_{NN}(64,1)$. From Fig. 2 it is clear that this occurs between $K_c = 0.85$ and 0.89, which is consistent with the exact $K_c = 0.88$ for the Ising model. For the Potts model there is no value of K where such a matching occurs at least up to $K = 2.5$. The bare thermodynamic quantities change relatively rapidly (e.g., the specific heat has a maximum) around $K = 1.0$, while above K around 2, the correlation functions are almost constant. One might hence expect a transition for K between 1 and 2. Since we find no matching up to $K = 2.5$, we conclude that there is no transition. The results for the next-near-neighbor correlation functions, although less reliable, are consistent with such a conclusion. We find this evidence convincing since the method has been used successfully to locate the infinite-order transition in a two-dimensional XY model and show the lack of any transition in the two-dimensional Heisenberg model.[4]

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[1]A. N. Berker and L. P. Kadanoff, J. Phys. A 13, L259 (1980).
[2]J. L. Cardy (unpublished).
[3]G. S. Grest and J. R. Banavar, Phys. Rev. Lett. 46, 1458 (1981).
[4]S. Shenker and J. Tobochnik, Phys. Rev. B 22, 4462 (1980).
[5]G. H. Wannier, Phys. Rev. 79, 357 (1950).
[6]See, for example, B. Nienhuis, thesis, 1978 (unpublished).