Cluster Monte Carlo study of the antiferromagnetic $Z(q)$ model

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(Received 14 October 2002; published 20 March 2003)

A cluster Monte Carlo (MC) updating algorithm is presented for the antiferromagnetic $Z(q)$ model, into which Ising variables are embedded. Using MC simulations combined with the histogram technique, we were able to study the q-state clock model, for $q=5$ and $q=7$, in $d=2$ and $d=3$ dimensions. The two-dimensional system exhibits a phase transition at temperature $T=0$ for both $q=5$ and $q=7$ system states. The critical exponents were derived as well as the ground state entropy for $T=0$. Our results for the $q=5$ and the $q=7$ three-dimensional systems show that they exhibit a phase transition at nonzero temperature.

DOI: 10.1103/PhysRevB.67.094415 PACS number(s): 75.10.−b, 05.10.Ln, 05.50.+q, 64.60.Cn

I. INTRODUCTION

The antiferromagnetic (AF) q-state Potts model, which is a special case of the $Z(q)$ model, has been intensively studied for $q=3$ and $q=4$. It has been shown that these models possess interesting and unusual properties since it is energetically favorable for two neighboring sites to be in distinct spin states. As a consequence, the residual entropy of the ground state at $T=0$ of the $q>2$ model on bipartite lattices does not vanish and is bounded from below by a nonvanishing value.[1] However following the argument given by Wannier,[2] one concludes that a transition to a phase with a long-range order will not arise. From rescaling arguments,[3] such systems may present a distinctive low-temperature phase, with an algebraic decay of correlations. Therefore this conclusion was criticized, suggesting that it is an artifact of the method.[4] Using different methods, it has been shown that the critical behavior of the three-state Potts model belongs to the universality class of the XY model in three dimensions and the four-state Potts model belongs to the universality class of the Heisenberg model, if the transitions are continuous.[1,5] The magnetization does not vanish, unlike the behavior suggested by Berker and Kadanoff.[3] Few results about the AF $Z(q)$ model, which is a generalization of a large class of models, are presented in the literature. Using a Migdal-Kadanoff renormalization group (MKRG) technique it was shown that the model exhibits a rich variety of phase diagrams for even values of q, while for odd values it does not exhibit a phase transition on a square lattice except at $T=0$.[6] This difference comes from the fact that for even values of q the $Z(q)$ group, which describes the different spin orientations, may be a subgroup of the $Z(2)$ group while for odd values it is not. Consequently, for even values of q the model possesses the symmetry of the Ising model, which exhibits a phase transition in two-dimensional bipartite lattices, whereas for odd values of q it does not. Since the AF $Z(q)$ models have q spin variables, many configurations are allowed[6] and a nonzero ground state entropy is obtained. In three dimensions, the AF $Z(q)$ model, for odd values of $q>5$, presents phase transitions between the disordered phase and AF phases or between the ordered phase and AF phases.

Monte Carlo (MC) simulations have played an important part in investigating the AF Potts model. The difficulty encountered in the Metropolis algorithm is the phenomenon of critical slowing down at a second-order phase transition.[7] It leads to a long relaxation time τ, which is related to the critical exponent z ($z\approx 2$ in the single-spin-flip algorithm) by $\tau \propto L^z$ at the critical temperature. Since then, a great deal of effort has been devoted to reduce considerably the dynamic critical exponent, developing cluster-flip-type algorithms[8,9] for the aim of improving the accuracy of MC data.

Since the MKRG method gives neither precise critical exponents nor the correct nature of phase diagrams, we developed a sophisticated numerical method. We performed a general cluster-flip algorithm for the AF $Z(q)$ model, which enables us to study its phase diagram and derive interesting results, especially for odd values of q, about the critical exponents and the nature of phase transitions. To this end, we elaborated on a MC cluster updating that generalizes the method used by Wang, Swendsen, and Kotecký.[1] Their algorithm was a generalization of the Swendsen-Wang procedure,[8] which was based on an idea of Wolff.[9] Embedded Ising variables were used in the three-state Potts model. Their algorithm consists of updating, in each step, two random Potts states in the usual Swendsen-Wang procedure by constructing clusters of sites connected by antibonds and flipping them with probability $\frac{1}{2}$, while sites containing spins of the other state remain frozen during the actual step. The process is repeated in the same way for the next step by taking two other states.

Nowadays considerable effort has been given to develop new alghorithms to reduce the relaxation time and then improve the MC simulation results. Recently, using the embedded cluster formalism, a probabilistic MC[10] changing alghorithm was extended in order to study the ferromagnetic XY and q-state clock model.[11] The Kosterlitz-Thouless transitions and the correlation decay exponent η were determined.

In this paper, we propose a generalization of the cluster-flip algorithm for the AF $Z(q)$ model for arbitrary values of the number of states q using the same idea of embedding Ising sign variables into the model. Using this method, we simulated the critical point of the q-state AF $Z(q)$ model for $q=5$ and 7 and calculated the associated critical quantities. We showed that the critical point of the model on a square lattice is located at $T=0$ while in three dimensions it is located at finite temperature. The critical exponents were also calculated for the two-dimensional system. In order to

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determine accurately the location and the height of very narrow peaks associated with the transition, as well as to plot continuous scaling curves and calculate the residual entropy at $T=0$, we used a multiple-histogram analysis.[12]

II. A CLUSTER UPDATING FOR AF $Z(q)$ MODELS

$Z(q)$ models are defined by the following Hamiltonian:

$$H=-\sum_{\langle ij\rangle}\sum_{\langle m=1\rangle}^{[q/2]} J_m\cos\left(\frac{2\pi}{q}m(\sigma_i-\sigma_j)\right), \tag{1}$$

where $\sigma_i=1,2,\ldots,q$. The first sum runs over all nearest neighbors and $[q/2]$ represents the integer part of $q/2$. In what follows, we use $u=2\pi/q$. The J_m are the nearest-neighbor coupling constants. If $J_m=0$ for every $m>1$, the $Z(q)$ model reduces to the clock model. The ground state of the AF $Z(q)$ model, whose J_m are negative, is characterized by a lattice where every two neighboring sites are in different states $\sigma_i\neq\sigma_j$ and the Hamiltonian (1) takes its minimum value.

Now, consider an arbitrary state n and accordingly, split the Hamiltonian (1) into two parts

$$H_1^{(n)}+H_2^{(n)}, \tag{2}$$

where

$$H_1^{(n)}=-\sum_{\langle ij\rangle}\sum_{\langle m=1\rangle}^{[q/2]} J_m\cos[u(m\sigma_i-n)]\cos[u(m\sigma_j-n)] \tag{3}$$

and

$$H_2^{(n)}=-\sum_{\langle ij\rangle}\sum_{\langle m=1\rangle}^{[q/2]} J_m\sin[u(m\sigma_i-n)]\sin[u(m\sigma_j-n)]. \tag{4}$$

Let us focus on the second part $H_2^{(n)}$ and set

$$\alpha_{i,m}^{(n)}=\mathrm{sgn}\{\sin[u(m\sigma_i-n)]\}. \tag{5}$$

Equation (4) can be rewritten as follows:

$$H_2^{(n)}=-\sum_{\langle ij\rangle} J_{ij}^{(n)}\alpha_{i,1}^{(n)}\alpha_{j,1}^{(n)} \tag{6}$$

with effective nearest-neighbor couplings

$$J_{ij}^{(n)}=J_1|\sin[u(\sigma_i-n)]\sin[u(\sigma_j-n)]| + \sum_{\langle m=2\rangle}^{[q/2]} J_m\frac{\sin[u(m\sigma_i-n)]\sin[u(m\sigma_j-n)]}{\alpha_{i,1}^{(n)}\alpha_{j,1}^{(n)}}. \tag{7}$$

The coupling $J_{ij}^{(n)}$ can be positive or negative depending on the sites it connects, and $\alpha_{i,m}^{(n)}=\pm1$ are Ising variables embedded into the state variables. The particular case of AF clock models ($J_m=0$ for all $m>1$) corresponds to negative values of $J_{i,j}^{(n)}$ and Eq. (6) becomes that of an effective AF Ising model. It is also possible to use other values of m in $\alpha_{i,m}^{(n)}$ for the purpose of Eq. (6). Note also that the $H_1^{(n)}$ part of the Hamiltonian is unchanged under the transformation $\alpha_{i,m}^{(n)}\rightarrow-\alpha_{i,m}^{(n)}$.

At this stage, we can give a typical cycle of our cluster updating procedure as follows:

(a) First, start with an arbitrary initial configuration.

(b) Randomly choose a state n from the set $\{1,2,\ldots,q\}$.

(c) Ignore all sites occupied by the state n and make bonds between neighboring sites occupied by states different from n with probability $p_{ij}^{(n)}=1-\exp(-2\beta|J_{ij}^{(n)}|)$. [For the $Z(q)$ models, the Ising variables on these sites do not need to be different as $J_{ij}^{(n)}$ can take any sign.] At the end of this step, the lattice is partitioned into Ising ''clusters'' that are, in fact, interconnected sites where the effective Ising variables $\alpha_{i,m}^{(n)}$ have the same sign for $J_{ij}^{(n)}$ positive and different signs otherwise. But, as it was noted before, only bonds between different states and compatible with the ground state energy are formed for the case of the clock model we have simulated here.

(d) The independent clusters are flipped with probability $\frac{1}{2}$. This operation corresponds to the transformation $\alpha_{i,m}^{(n)}\rightarrow-\alpha_{i,m}^{(n)}$, which is equivalent to $\sigma_i\rightarrow-\sigma_i+2n(\mathrm{mod}\,q)$ for the state variable [see Eq. (5)], for all sites of the clusters selected to be flipped.

(e) Generate a new configuration and repeat from step (b).

This completes one cluster updating of one updating cycle of our algorithm. It is straightforward to show that the procedure adopted by Wang *et al.*[1] for the AF three-state Potts model is rather a simple case of the actual more general algorithm. In addition, when Eq. (7) is applied to the case of the antiferromagnetic three-state Potts model, it gives only negative values for $J_{ij}^{(n)}$, and the updating reduces to that of a simple AF effective Ising model.

III. SIMULATION ANALYSIS AND RESULTS

Before analyzing the behavior of the AF $Z(q)$ model, let us give expressions for thermodynamic quantities of interest. Since the $Z(q)$ model possess $[q/2]$ order parameters that can define all the pure phases of the system, the staggered magnetizations, i.e., the order parameters, relative to the state l, where $l=1,2,\ldots,q$, are given for a d-dimensional lattice by

$$M_\delta(l)=\frac{2}{(L^d)}\left[\sum_i^A\cos[\delta u(\sigma_i-l)]-\sum_i^B\cos[\delta u(\sigma_i-l)]\right], \tag{8}$$

where $\delta=1,2,\ldots,[q/2]$. The first and the second summations are restricted to the A and B sublattices, respectively, such that the sites on the sublattice A have their nearest neighbors on the sublattice B and L is the linear lattice size. The order parameters that are expected to break sublattice symmetry are

$$\langle M_\delta\rangle=\frac{1}{q}\sum_{k=1}^{q}\langle|M_\delta(k)|\rangle. \tag{9}$$

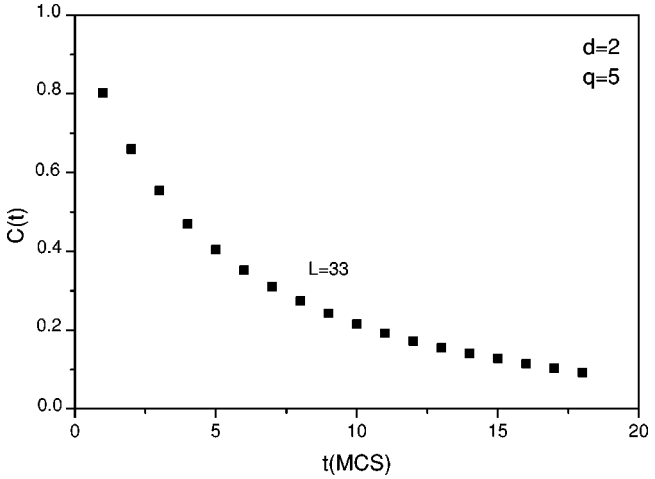

FIG. 1. Autocorrelation function $C(t)$ vs MC time [Monte Carlo steps (MCS)] for $d=2$, ,$q=5$ and $L=33$.

The susceptibility corresponding to each order parameter in the disordered phase can be given by

$$\chi_\delta = \frac{L^d}{q} \sum_{k=1}^{q} \langle |M_\delta^2(k)| \rangle. \tag{10}$$

Although the preceding algorithm is valid for general $Z(q)$ models, we will restrict ourselves, for the purpose of this work, to the clock model ($J_m=0$ for $m>1$). Then the order parameters reduce to those that characterize the pure phase of the system (for the clock model, $\delta=2$ and 3 for $q=5$ and 7, respectively). In order to compare the performance and the efficiency of our algorithm for the model, we plot, in Fig. 1, the variation of the magnetization autocorrelation function $C(t)=\langle M(t')M(t'+t)\rangle$ with the MC time t given in MC steps per spin for $q=5$ and $L=33$. The time dependence is, to a very good approximation, exponential: $C(t)\propto \exp(-t/\tau)$. The autocorrelation time τ is then determined from the log-log plot of $C(t)$ versus the time t. By fitting the dependence of the autocorrelation time, with respect to the linear size L, to the equation $\tau \sim L^z$, we obtain

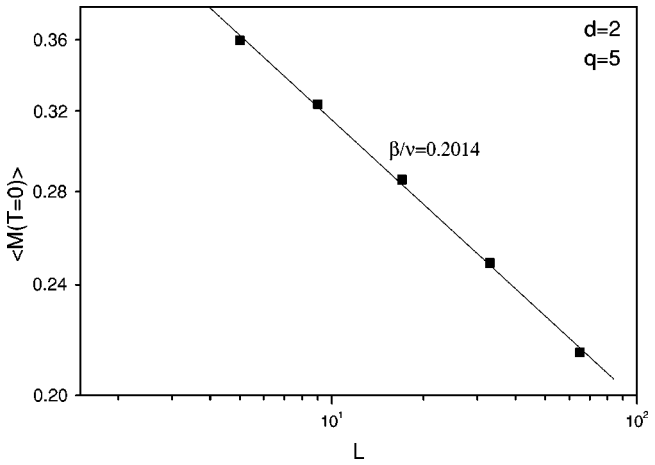

FIG. 2. Log-log plot of the zero-temperature magnetization $\langle M(T=0)\rangle$ as a function of lattice size L for $d=2$ and $q=5$.

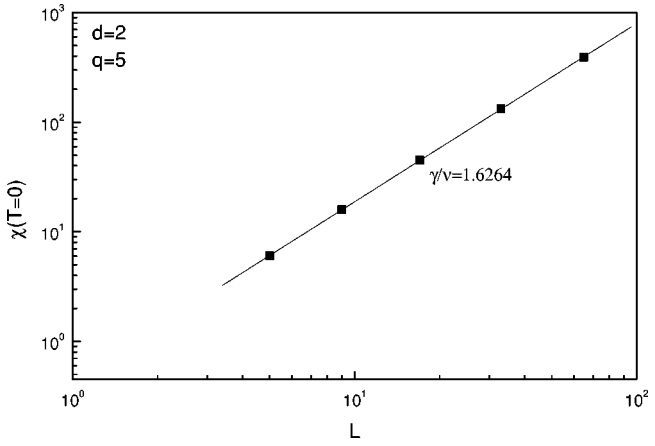

FIG. 3. Log-log plot of the zero-temperature susceptibility $\chi(T=0)$ as a function of lattice size L for $d=2$ and $q=5$.

the dynamic critical exponent z. While the standard Metropolis algorithm gives a value $z\approx 2$,[12] our algorithm reduces drastically the critical slowing down and leads to a correlation time value, $\tau\approx 9$ MC steps per spin for lattice sizes up to $L=64$. The effective value of z was too small to be measured from our data. This means that critical slowing down essentially disappears and much more accurate results can be obtained. Using this algorithm, we performed simulations at $T=0$ for five-state and seven-state clock models in $d=2$.

The log-log plot of the zero-temperature magnetization $\langle M\rangle$ and the susceptibility χ versus linear size L, for $d=2$ and $q=5$, are presented in Fig. 2 and Fig. 3, respectively. The two curves are practically straight, indicating a phase transition at $T=0$ as was suggested by the renormalization group method.[6]

We found, in one hand, that the $T=0$ critical exponents are $\beta/\nu=0.2014\pm 0.004$ and $\gamma/\nu=1.6264\pm 0.005$ for $q=5$ and, in the other hand, $\beta/\nu=0.1028\pm 0.003$ and $\gamma/\nu=1.7937\pm 0.001$ for $q=7$. Assuming scaling relations, this yields $\eta=2-\gamma/\nu=0.3736\pm 0.005$ and $\eta=0.2063\pm 0.001$ for $q=5$ and $q=7$, respectively. Note also that the hyperscaling relation $\gamma/\nu+2\beta/\nu=d$ is satisfied within statistical errors.

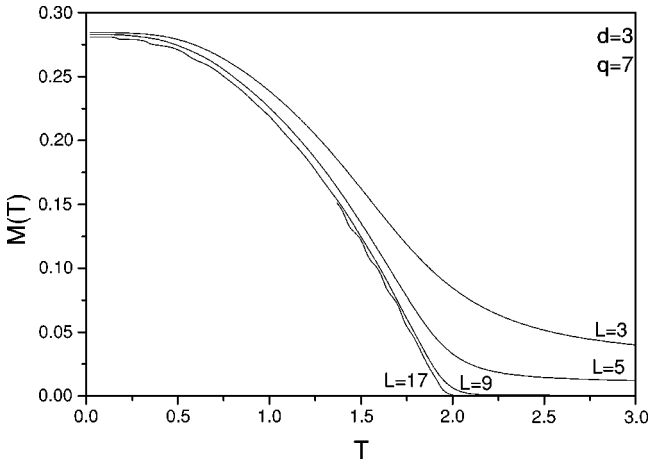

FIG. 4. Temperature variation of the magnetization $\langle M(T)\rangle$ of the $d=3$ system for different system sizes.

In addition, $Z(q)$ models present a highly degenerate ground state with a residual entropy at temperature $T=0$. We used the multiple histogram method[12] to derive the zero-temperature entropy for the $d=2$ system, using information combined from 10 simulations for $L=3$ and $L=9$ and 13 simulations for $L=9$ and $L=17$, each simulation has a length of 10^6 MC configurations. The results obtained are extended with the equation $S(L)=S(\infty)+bL^{-d}$ to derive the infinite size limit of the ground state entropy: $S(\infty)=0.4605$ for the five-state model and $S(\infty)=0.4584$ for the seven-state one. The coefficient b derived from our calculations is not compatible with the logarithm of the number of phases as stated by Borgs and Imbrie[13] for models with well-defined barriers between phases. These values are close to each other and slightly higher than those found for the three-state Potts model.[1]

Our preliminary results concerning the three-dimensional systems are compatible with a phase transition at a temperature different from zero. This is particularly evident when considering the temperature variation of the magnetization shown in Fig. 4 for $q=7$. Work is still in progress in this direction to derive more results.

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