Simulation of Potts models with real q and no critical slowing down

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A Monte Carlo algorithm is proposed to simulate the ferromagnetic q-state Potts model for any real $q>0$. A single update is a random sequence of disordering and deterministic moves, one for each link of the lattice. A disordering move attributes a random value to the link, regardless of the state of the system, while in a deterministic move this value is a state function. The relative frequency of these moves depends on the two parameters q and $\beta=1/kT$. The algorithm is not affected by critical slowing down and the dynamical critical exponent z is exactly vanishing. We simulate in this way a three-dimensional Potts model in the range $2<q<3$ for estimating the critical value q_c where the thermal transition changes from second order to first order, and find $q_c=2.620\pm0.005$.

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I. INTRODUCTION

The Q-state Potts model [1] is perhaps one of the simplest nontrivial models in statistical mechanics. A broad set of techniques has been brought to bear on it in a variety of disciplines and it has been the subject of considerable theoretical attention over the last two decades (for a review, see [2]).

This model is theoretically well defined for any real or complex value of q [3]. In particular, the limit $q\to1^+$ corresponds to the random percolation problem and the limit $q\to0^+$ has a fundamental role in enumerating the spanning trees of a graph [3]. Two-dimensional (2D) conformal field theory [4] suggests exact formulas for the critical indices and for other universal quantities as continuous functions of q in the range $0<q<4$. Another interesting problem involving noninteger q in three-dimensional Potts models is the determination of the universal value q_c for which the thermal transition changes from second order to first order. A variety of techniques have been used [5–9], which locate q_c in the range $2<q_c<3$. All these methods require extrapolations in q because the standard simulations work only at integer values of q. Reweighting techniques [10,11] and transfer matrix methods [12] allow one to estimate some thermodynamic functions [8] in a wider range of q; however, there is no way to evaluate correlation functions there.

In this paper we remove this limitation by constructing a Monte Carlo (MC) algorithm which works for any real $q>0$. Although the time required for a sweep through the system grows faster than its size because at some step of the algorithm nonlocal information is required, the simulations are not affected by a critical slowing down and the dynamical critical exponent z is exactly zero. We test the reliability of the method by comparison with some exact results for the 2D Potts model at criticality. We probe its effectiveness by performing large scale MC simulations of a three-dimensional Potts model for estimating the universal value q_c.

II. THE ALGORITHM

Starting with the Hamiltonian $H=-\Sigma_{\langle ij\rangle}\delta_{\sigma_i\sigma_j}$ where the site variable σ_i takes the values $\sigma_i=1,2,\ldots,q$, with $\langle ij\rangle$ ranging over the links of an arbitrary lattice or graph Λ, one can write the q-state Potts model partition function $Z=\Sigma_{\{\sigma\}}e^{-\beta H}$ in the Fortuin-Kasteleyn (FK) random cluster representation [3]

$$Z=\sum_{G\subseteq\Lambda}W(G)=\sum_{b,c}\Omega(b,c)v^b q^c, \tag{1}$$

where $v=e^\beta-1=p/(1-p)$, the summation is over all spanning subgraphs $G\subseteq\Lambda$, $W(G)=v^b q^c$ is their weight, expressed in terms of the number b of edges of G, called bonds, and the number c of connected components or FK clusters, and $\Omega(b,c)$ is the number of subgraphs with b bonds and c clusters. This representation now defines a model for any real or complex q.

In principle, one could directly use Eq. (1) to define a Metropolis algorithm working for positive noninteger q [13], but this is a difficult problem to simulate because, for each proposed change of a link, the number c of FK clusters, a nonlocal property, must be determined. Large lattices require a huge amount of CPU time. As a matter of fact, such a method has been applied only to two-dimensional systems, where special topological relations can be used [13].

Our strategy is different. We start by considering a useful identity that can be derived using the methods described in Ref. [14].

Let l be any link of Λ. Denote by $\{G_l^+\}$ the set of spanning subgraphs where l is a bond and by $\{G_l^-\}$ those in which this bond is missing. We have $Z=Z_l^++Z_l^-$, with $Z_l^\pm=\Sigma_{G_l^\pm}W(G_l^\pm)$. Introducing a bond variable α_l equal to 1 when l is a bond and 0 otherwise yields

$$\langle\alpha_l\rangle=\frac{Z_l^+}{Z}. \tag{2}$$

The same quantity can be evaluated in a different way by addition of a bond to each graph of type G_l^-. There are two kinds of missing bonds. Those joining two different clusters, called potential bridges, are picked out by a variable β_l which takes the value 1 only on them and is zero otherwise; their addition lowers the number c of FK clusters. We have

$$\beta_l = 1 \Rightarrow W(G_l^-)\frac{v}{q} = W(G_l^+). \tag{3}$$

The remaining missing bonds, described by a similar variable γ_l, join two sites of the same cluster; their addition keeps c invariant, and thus

$$\gamma_l = 1 \Rightarrow W(G_l^-)v = W(G_l^+). \tag{4}$$

Combining Eqs. (2), (3), and (4) yields $\langle \alpha_l \rangle = (v/q)\langle \beta_l \rangle + v\langle \gamma_l \rangle$ which is the wanted identity. Since of course $\alpha_l + \beta_l + \gamma_l = 1$, we can rewrite it as

$$\langle \alpha_l \rangle = p\langle \alpha_l \rangle + \frac{p}{q}\langle \beta_l \rangle + p\langle \gamma_l \rangle, \tag{5}$$

where the weighting factors can now be interpreted in terms of probabilities. The idea is now to regard this identity as the limit of a recursion relation of the type

$$\pi_l^{(n+1)} = p\,\alpha_l^{(n)} + \frac{p}{q}\beta_l^{(n)} + p\,\gamma_l^{(n)}, \tag{6}$$

where $\pi_l^{(n+1)}$ is the probability of having a bond on the link l in the configuration $G^{(n+1)}$. It is expressed as a state function (α_l, β_l, or γ_l) of the same link in the $G^{(n)}$ configuration. This generates a Markov process $\cdots \to G^{(n)} \to G^{(n+1)} \to \cdots$ where the equilibrium distribution yields Eq. (5). This stochastic chain fulfills two important conditions: (i) there is a nonzero probability of going from any configuration to any configuration in a single sweep through Λ, and (ii) the equilibrium distribution maps to itself as Eq. (5) is kept invariant by the process. One can then argue that detailed balance is satisfied.

To see it directly, assume, for instance, that in the nth configuration l is a potential bridge ($\beta_l^{(n)} = 1, \quad G^{(n)} = G_l^-$) which is promoted to a bond in the $(n+1)$th configuration ($\alpha_l^{(n+1)} = 1, \quad G^{(n+1)} = G_l^+$). The transition rate is $P(G_l^- \to G_l^+) = p/q$. Conversely, Eq. (6) yields $P(G_l^+ \to G_l^-) = 1 - p$. Then, according to Eqs. (1) and (4),

$$\frac{P(G_l^- \to G_l^+)}{P(G_l^+ \to G_l^-)} = \frac{W(G_l^+)}{W(G_l^-)} \tag{7}$$

as detailed balance requires. The same conclusion can be reached in all the other cases.

A straightforward, preliminary, implementation of the recursion relation (6) is the following. (i) Go over each link $l \in \Lambda$ of the configuration $G^{(n)}$ and generate a pseudorandom number X_l uniformly distributed from 0 to 1. (ii) Create a bond on l only in the following two cases: (a) $X_l < p$ *and* l is a bond ($\alpha_l = 1$) or a missing bond joining two sites of the same FK cluster ($\gamma_l = 1$); (b) $X_l < p/q$ *and* l is a potential bridge ($\beta_l = 1$). This generates uniquely the configuration $G^{(n+1)}$.

Let $q > 1$ for definiteness. It is worth noting that when $X_l < p/q$ the algorithm adds a bond to l regardless of which configuration $G^{(n)}$ we are dealing with. Similarly, when $X_l > p$ no bond is added. In the remaining cases ($p/q \leqslant X_l \leqslant p$), the value attributed to l (bond or no bond) is unambiguously determined by $G^{(n)}$.

Inspecting all the cases leads to the following better implementation of the algorithm.

Step 1. Pick a link $l \in \Lambda$ and generate a pseudorandom number $0 \leqslant X_l \leqslant 1$.

Step 2. Update the link according to the following scheme:

Move		Current state	New state
(a)	$X_l < \frac{p}{q}$	any	bond
(b)	$X_l > p$	any	no bond
(c)	$\frac{p}{q} \leqslant X_l \leqslant p$	$\alpha_l = 1$	bond
		$\beta_l = 1$	no bond
		$\gamma_l = 1$	bond

Step 3. Return to step 1.

The first two moves do not need any information on the state of the system: they just disorder it. The last one is a purely deterministic move; its only effect is to put a bond whenever a link joins two sites of the same cluster. It requires distinguishing between the two kinds of missing bonds ($\beta_l = 1$ or $\gamma_l = 1$). One can infer this nonlocal property by identifying the connected components of the configuration, as in the Swendsen-Wang (SW) algorithm [15]. This cluster reconstruction is time demanding; however, it gives complete information on the state of the missing bonds of the whole lattice. As the update proceeds through the lattice this amount of information is progressively lost because of disordering moves [the deterministic moves never change (c)]. We may partly keep track of the cluster structure by relabeling the cluster indices whenever a disordering move creates a bond between two of them. Cluster reconstruction is truly necessary only when a deterministic move touches a missing bond of a putative single cluster where some bond has been erased by previous disordering moves.

Because of nonlocality, the number of operations involved every MC step is proportional to N^α, where N is the number of links and $1 < \alpha \leqslant 2$. The efficiency of the algorithm depends crucially on the actual number of cluster reconstructions per sweep. In our 3D simulations reported below the fraction of links requiring cluster reconstruction was about 3% with a decreasing trend for larger lattices.

III. CORRELATION TIMES

An unusual feature of the described algorithm is the presence of randomly distributed disordering moves. The mean number of links subjected to disordering moves in a single sweep is Np_r with $p_r = 1 + p/q - p$. For instance, in the Ising model ($q = 2$) at criticality more than 70% of the links are disordered every sweep. It is now easy to find an upper bound for the mean number τ of MC steps needed to generate effectively independent configurations. After n sweeps the mean number of links which have not yet undergone a disordering move is $N(1-p_r)^n$. When this number is of the

TABLE I. The decorrelation time τ of the algorithm described here for the critical 2D Ising model for different linear lattice sizes L is compared with the same quantity from the SW algorithm τ_{SW} and with the upper bound τ_0. The definitions of τ and the τ_{SW} data are taken from Ref. [16].

L	τ	τ_{SW}	τ_o
8	2.65(3)	5.17696(32)	3.3869
16	3.16(5)	6.5165(12)	4.5158
32	3.69(6)	8.0610(18)	5.6448
64	4.3(1)	9.794(4)	6.7737

order of 1 all the links have been touched by a disordering move and the upper bound $\tau_0 \geqslant \tau$ is given by the obvious relation $N(1-p_r)^{\tau_0} \sim 1$, i.e., $\tau_0 = -\ln N/\ln(1-p_r)$. Thus the dynamical exponent z is 0, as critical slowing down manifests itself by the power law $\tau \propto N^z$ at the critical temperature where a second-order phase transition occurs [16]. A numerical estimate of the decorrelation time of the dynamics of this algorithm for the critical Ising model on a square lattice is reported in Table. I. Note that the actual value of τ does not saturate the upper bound and is much smaller than the analogous quantity of the SW algorithm.

Our algorithm also proves useful in combating another dynamical problem that one deals with in the case of first-order transitions, namely, the exponentially fast suppression of the tunneling between metastable states with increasing lattice size.

To reduce this type of slowing down the multicanonical MC algorithm has been proposed [17]; also the method of simulated tempering [18] proves useful [19]. In a few numerical tests for two-dimensional models with $q=7$ and $20 \geqslant L \geqslant 100$ we found that the tunnelling time of the canonical algorithm described in the present paper grows with the system size V as $\tau_t \propto V^{\alpha}$ with $\alpha = 1.03 \pm 0.03$, as in an optimal variant [20] of the multicanonical method, but with a smaller proportionality factor.

The reason for this performance is that the random moves accelerate the tunneling between order and disorder. The drawback is that our algorithm is nonlocal, so the CPU time grows as V^b with $b>1$; for instance, in the present case we found $b \sim 1.85$. Thus this algorithm certainly cannot be recommended for integer q, although at a first-order transition it performs much better than any local canonical algorithm.

IV. SIMULATIONS

As a first, simple, application of our algorithm we tested the reliability of our code by checking a percolation property of the Potts model on a square lattice which is supposed to be exact in the range $0<q<4$, namely, that the mean frequency of active bonds $\langle \alpha_l \rangle$ at criticality [corresponding to $v=\sqrt{q}$ in Eq. (1)] should coincide, in the thermodynamic limit, with the random percolation value, i.e., $\langle \alpha_l \rangle = \frac{1}{2}$, irrespective of the value of q [2]. We simulated critical Potts models on a 128×128 square lattice with q ranging from 1.5 to 3.5. In all the cases the mean number of bonds was compatible with the exact result. The finite size effects of this

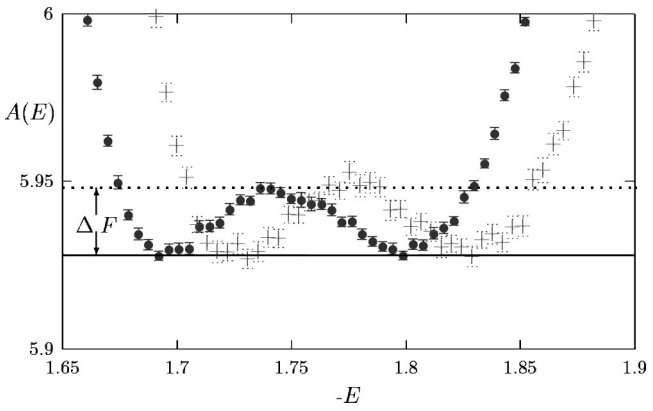

FIG. 1. Plot of $A(E,L)$ resulting from a simulation of a 3D Potts model at $q=2.75$ with 3.3×10^7 Monte Carlo Steps (MCS) for $L=14$ (full circles) compared with the extrapolation at the same value of q of an actual SW simulation of 4.1×10^7 MCS at $q=3$ (crosses). The latter data are shifted to the right for clarity.

observable, which are visible on smaller lattices, allow us to evaluate the critical thermal exponent ν as a function of q. This could be used to check a conjectural formula suggested by the 2D conformal field theory [4]. We plan to study this problem in a future publication.

This algorithm allows us to deal with an important issue of the three-dimensional Potts model, namely, the estimate of the tricritical point q_c in the range $2<q_c<3$, where the thermal transition changes from second order for $q \leqslant q_c$ to first order for $q>q_c$. Many different techniques have been used to locate this point [5–9]. We applied a method very similar to that described by Lee and Kosterlitz [8] by computing the double histogram $N(b,c)$ of bond and cluster number distribution in a cubic lattice of volume L^3 at a given β and q and then extrapolating the data to nearby values. Using Eq. (1) we can write

$$N(b,c;\beta,q,L) = \mathcal{N}\Omega(b,c)\frac{v^b q^c}{Z}, \tag{8}$$

where $\mathcal{N}$ is the number of MC sweeps. We can trade the number of bonds b for the energy per site E using the relation $E=-b(v+1)/v\,L^3$. Near a first-order transition the histogram $P(E)=\Sigma_c N(b,c)/\mathcal{N}$ has a characteristic double peak structure corresponding to the ordered and the disordered phases. A suitable reweighting through Eq. (8) of the energy distribution yields the value $\beta_c(L,q)$ where the two peaks at $E_1(\beta,L)$ and $E_2(\beta,L)$ are of equal height. A typical plot of the quantity $A(E,q;\beta_c,L) = -\Sigma_c \ln[N(b,c)/\mathcal{N}]$ is shown in Fig. 1. A useful estimator of the interface free energy between the ordered and the disordered phases [21] is given by

$$\Delta F(q,L) = A(E_m,q;\beta_c,L) - A(E_1,q;\beta_c,L), \tag{9}$$

where E_m is the local maximum that separates the two dips at E_1 and E_2 (see Fig. 1). At a first-order transition $\Delta F(L)$ increases monotonically with L and is expected to vanish at the tricritical point. By extrapolating the numerical data in both β and q one may locate this point. The region of reliable extrapolation [11] is $O(1/L^3)$ for both β and q. This

TABLE II. The simulations were performed on cubic lattices of side L at the values of q and β listed below. MCS is the number of Monte Carlo steps considered.

L	q	β	MCS
12	2.70	0.52270	3.0×10^7
13	2.70	0.52270	3.0×10^7
14	2.75	0.52721	3.3×10^7

does not cause a problem for β, since it can be adjusted continuously, but q cannot in standard simulations, being by necessity an integer value. Actually Lee and Kosterlitz performed their simulations at $q=3$ and found that the extrapolated data become too noisy for $|\delta q|>0.3$ [22]. In our case we can directly evaluate the range of reliable extrapolations. Indeed, the main advantage of the algorithm described in this paper is that now also q can be adjusted continuously.

Our simulations were performed on three different lattices as listed in Table II. The statistics is good since in all the cases the mean flipping time between coexisting states was no larger than 30 MC steps. The errors were calculated by gathering the histogram $N(b,c)$ every 10^6 MC steps and then performing a standard analysis.

In all the cases the energy histogram showed a double peak structure, providing a direct evidence of the first-order nature of the transition for these values of q (see Fig. 2). This yields the upper bound $q_c<2.7$. In shorter simulations at $q=2.6$ we found no trace of a double peak structure. This suggests $q_c>2.6$. Using the reweighting method we estimated the values $\beta_c(L,q)$ where the two peaks are of equal height for each L and for few values of q near $q=2.7$ and the corresponding values of ΔF. The results are reported in Fig. 3.

A further reweighting up to $q=3$ allowed us to compare the extrapolated data with those coming from a similar extrapolation of standard SW simulations at $q=3$. This comparison showed that the range of reliable extrapolations is $|\delta q|<0.25$. It has to be noted that we could not use for this comparison the high precision data of Ref. [25], because the energy distribution in terms of spin variables used there does not coincide with that expressed in terms of bond variables

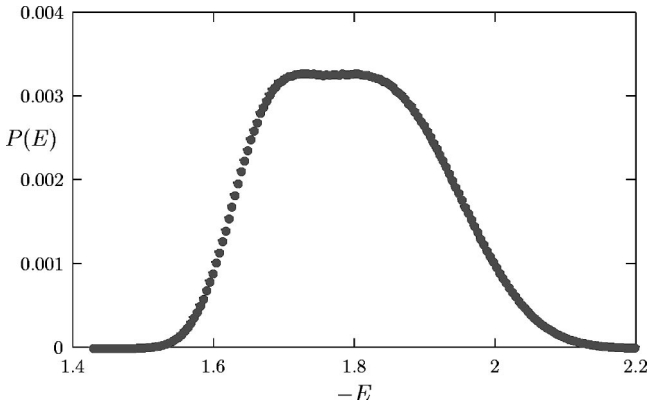

FIG. 2. Energy histogram at $\beta_c(L,q)$ obtained by a simulation at $q=2.7$ and $L=13$.

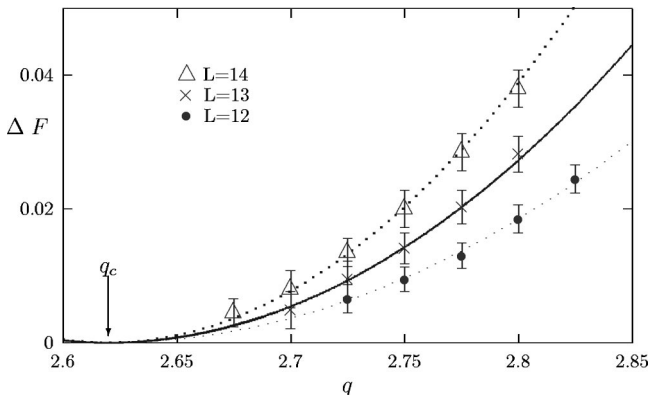

FIG. 3. Plot of $\Delta F(q,L)$ near $q=2.7$.

used by necessity in the present approach. In particular, the $\beta_c(L,q)$'s are shifted and our $\Delta F(q,L)$ is always smaller.

Simple finite size scaling considerations suggest [8] that near q_c the interface free energy has the simple form $\Delta F(q,L)\sim(q-q_c)^2L^a$ which fits our data very well (see Fig. 3). To within our numerical accuracy $a=4.8\pm0.1$ and $q_c=2.620\pm0.005$. This agrees with the value $q_c=2.55\pm0.12$ obtained in the large q expansion of the latent heat [6]. Lee and Kosterlitz [8] extrapolating $q=3$ data found a smaller value, $q_c=2.45\pm0.10$. The difference could be due to the fact that extrapolations with $|\delta q|>0.25$ give an overestimate of ΔF (this is already visible in Fig. 1). Other approximate methods give even smaller values: real space renormalization group methods [5] yield $q_c\sim2.2$ while an Ornstein-Zernike approximation [9] gives $q_c\sim2.15$.

V. CONCLUSIONS

This work provides a MC algorithm to simulate the ferromagnetic q-state Potts model which has two very unusual features: it works for any real $q>0$ and does not suffer any critical slowing down. The former property is an obvious consequence of the fact that it is based on the Fortuin-Kasteleyn random cluster representation, where q acts as a continuous parameter. The latter is more tricky and is due to the implementation of the algorithm with a random sequence of disordering moves, randomly distributed over the lattice. There is no reason to believe that this disordering mechanism is specific to the Potts model and it would be very interesting to try to implement it in other, more general MC methods. A drawback of the algorithm is that it is nonlocal, so the CPU time of a single sweep grows with the volume V as V^b with $1<b<2$; thus it is not recommended for integer q, where the SW algorithm works with $b=1$. Actually, at a first-order transition our algorithm performs better than the SW method, but there the multicanonical MC algorithms are more suitable.

It is straightforward to extend the algorithm in order to take into account quenched bond randomness, provided that all the couplings are ferromagnetic. On the contrary, generalizing to systems with frustrations seems a rather difficult

task, because it is not obvious how to define in this case the FK clusters for noninteger q [14].

We used such an algorithm to study the region $2<q<3$ of a three-dimensional Potts model in order to estimate the critical value q_c for which the thermal transition changes from second to first order. We obtain a rather precise estimate compared to other methods, [5–9], the reason being that all the other methods are based on extrapolations from integer values of q, while the algorithm described here simulates the system at nearby values of q_c.

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