Graphical representations and cluster algorithms for critical points with fields

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Abstract

A two-replica graphical representation and associated cluster algorithm is described that is applicable to ferromagnetic Ising systems with arbitrary fields. Critical points are associated with the percolation threshold of the graphical representation. Results from numerical simulations of the Ising model in a staggered field are presented. For this case, the dynamic exponent for the algorithm is measured to be less than 0.5.

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Monte Carlo simulations of equilibrium critical points have been revolutionized by cluster methods [1–4]. These methods effectively reduce critical slowing for a broad class of spin models. However, cluster methods developed thus far are efficient only for systems with a high degree of internal or translational symmetry. In this paper we show how to construct graphical representations and associated cluster algorithms appropriate for ferromagnetic Ising systems in the presence of fields. We demonstrate the method for the Ising system in a staggered field.

The Swendsen-Wang (SW) cluster algorithm [2] as applied to the Ising model updates both spin variables and bond variables. Starting from a spin configuration, satisfied bonds are occupied with probability $p = 1 - e^{-2\beta}$ where β is the inverse temperature. A bond is *satisfied* if the spins at its two ends agree. Clusters of spins connected by occupied bonds are identified. Each cluster is randomly assigned a new spin value and each spin in the cluster takes that value. This constitutes one Monte Carlo step. The efficiency of the method is associated with the fact that the critical point of the Ising model coincides with the percolation point of the graphical model described by the bond variables [5,6]. Thus, at criticality, spin-clusters are coherently updated on all length-scales.

A fundamental problem is encountered in applying the Swendsen-Wang method when fields are present. Clusters can be defined in the usual way but then the fields must accounted for in determining the probability of flipping clusters. Fields may be introduced directly via a Boltzmann factor [7] or via ghost bonds. In either case, large clusters will tend to be 'frozen' in the sense that they almost always take one spin value. Because large clusters are frozen, equilibration occurs slowly on large length scales. In addition, the percolation transition of the graphical representation typically occurs in the disordered phase so that at criticality there are large clusters that are dynamically frozen. As a result, the qualitative gains expected from cluster methods (characterized by a small value of the dynamic exponent) are not realized. Nonetheless, limited quantitative success has been achieved for the random field Ising model by ad hoc methods that restrict the cluster size [8].

In this paper we present a graphical representation and associated cluster algorithm with the property that the percolation transition in the graphical representation coincides with the ordering transition in the spin-system. Furthermore, at criticality, the large-scale clusters are free to flip. We achieve this by using a replica method related to the replica Monte Carlo approaches that have been applied with some success to spin glasses [9–11]. We also note a related cluster method [12–14], in which the system is "folded" on itself and pairs of sites are used to make clusters.

The idea of our algorithm is as follows. Two independent replicas of the system in the same field are simulated simultaneously. Each site of the lattice is therefore associated with two spins, one from each replica, and can be in one of four spin states, $(++)$, $(--)$, $(+-)$ and $(-+)$. Sites where the replicas disagree, $(+-)$ and $(-+)$, are called *active* sites. Clusters of active sites are constructed and flipped. Allowed cluster flips interchange $(+-)$ with $(-+)$. Additional updating is applied independently to each replica to insure ergodicity. Since there is no net field on active clusters these flip freely. It turns out that percolation of active clusters signals the onset of long range order.

The plan for the remainder of the paper is as follows. First we construct a joint distribution of the Edwards-Sokal [15] type whose spin marginal is two independent Ising models. Next we indicate why percolation of the associated graphical representation coincides with the onset of magnetic ordering in the spin–system. We then describe a cluster algorithm which simulates this joint distribution and present numerical results for the Ising model in a staggered field. Finally, we discuss generalizations of the method.

The Hamiltonian for the Ising model is

$$\mathcal{H}[\sigma] = -\sum_{<i,j>} \sigma_i \sigma_j - \sum_i H_i \sigma_i \tag{1}$$

where the spin variables, σ_i take the values ± 1. The first summation is over the bonds of the lattice (or more generally, an arbitrary graph). The second summation is over the sites of the lattice and the fields H_i are arbitrary. The Ising model on a square lattice in a staggered field (equivalently, the Ising antiferromagnet in a uniform field) is obtained by setting $H_i = +H$ if i is in the even sublattice and $H_i = -H$ if i is in the odd sublattice.

We now define a joint distribution of two sets of Ising spin variables, $\{\sigma_i\}$ and $\{\tau_i\}$, and a bond variable $\{\eta_{ij}\}$. The bond variable is defined for each bond $<i,j>$ and takes values 0 and 1. We say that $<i,j>$ is *occupied* if $\eta_{ij} = 1$. The statistical weight $X(\sigma,\tau,\eta)$ for the joint distribution is

$$X(\sigma,\tau,\eta) = e^{-\beta \sum_{<i,j>} \sigma_i \tau_i \sigma_j \tau_j + \beta \sum_i H_i(\sigma_i + \tau_i)} \Delta(\sigma,\tau,\eta) B_p(\eta). \tag{2}$$

B is the standard Bernoulli factor,

$$B_p(\eta) = p^{|\eta|}(1-p)^{N_b - |\eta|}, \tag{3}$$

$|\eta| = \#\{< i,j > \mid \eta_{ij} = 1\}$ is the number of occupied bonds and N_b is the total number of bonds of the lattice. The Δ factor enforces the rule that only satisfied bonds are occupied: if for every bond $<i,j>$ such that $\eta_{ij} = 1$ the spins agree in both replicas ($\sigma_i = \sigma_j$ and $\tau_i = \tau_j$) then $\Delta(\sigma,\tau,\eta) = 1$; otherwise $\Delta(\sigma,\tau,\eta) = 0$. Equation (2) is closely related to the "red-blue" graphical representation of the Ashkin-Teller model given in [16]. It is straightforward to verify that integrating $X(\sigma,\tau,\eta)$ over η yields the statistical weight for two independent Ising models in the same field,

$$e^{-\beta\mathcal{H}[\sigma] - \beta\mathcal{H}[\tau]} = \text{const} \sum_{\{\eta\}} X(\sigma,\tau,\eta) \tag{4}$$

if the identification is made that $p = 1 - e^{-4\beta}$.

Consider a two-replica spin system in which the σ-replica has $(+)$ boundary conditions and the τ-replica has $(-)$ boundary conditions. The local order parameter is the difference between the magnetization of the two replicas, $m_i = (<\sigma_i> - <\tau_i>)/2$. Observe that magnetization in a single Ising model in a field is not generally the correct order parameter because the field induces local magnetization even in the disordered phase. By taking the difference between the magnetization of the two replicas with opposite boundary conditions, this contribution is canceled leaving only the spontaneous magnetization induced by the boundary conditions.

Given a bond configuration η we can ask for the conditional probabilities for the spins. Due to the Δ factor in the statistical weight, $\sigma_i = +1$ and $\tau_i = -1$ if i is connected to the boundary by occupied bonds. On the other hand, due to the symmetry of the exponential factor in the statistical weight a site that is not connected to the boundary is equally likely to be $(+-)$ or $(-+)$. Finally, $(++)$ and $(--)$ spin states do not contribute to m_i. Thus m_i is *exactly* equal to the probability that i is connected to the boundary and the onset of long range order coincides with percolation. For a more detailed argument, see [17].

Our replica cluster algorithm simulates two independent Ising models, σ and τ, on the same lattice and in the same field. Sites i at which $\sigma_i \neq \tau_i$ are called *active* sites. Bonds $<i,j>$ connecting like spins in both replicas ($\sigma_i = \sigma_j$ and $\tau_i = \tau_j$) are called *satisfied* bonds.

- Step 1: Satisfied bonds connecting active sites are occupied with probability $p = 1 - e^{-4\beta}$.

- Step 2: Clusters of active sites connected by occupied bonds (including single active sites) are identified. The k^{th} cluster is independently assigned a spin value, $s_k = \pm 1$ with probability 1/2. If site i is in cluster k then the new spin values are $\sigma_i = s_k$ and $\tau_i = -s_k$. In this way all active sites are updated.

- Step 3: Each replica is independently updated in a way that preserves detailed balance and insures ergodicity. This completes one Monte Carlo step.

Without Step 3, the algorithm is not ergodic since the product $\sigma_i \tau_i$ is locally conserved. Step 3 can be implemented in many ways. For example, each replica can be separately updated using the Metropolis algorithm. For the staggered field model in periodic boundary conditions we can effect further mixing by translating the τ replica by a random amount relative to the σ replica. If the translation is an odd vector, all τ spins are flipped. Since the Hamiltonian is invariant with respect to even translations and odd translations plus spin flips it is clear that the translation part of the algorithm satisfies detailed balance. (Note that Metropolis sweeps are required even with random translations because the net staggered magnetization, $s = [\sum_{i\,\varepsilon\,\text{odd}} - \sum_{i\,\varepsilon\,\text{even}}](\sigma_i + \tau_i)$ is otherwise a conserved quantity.) The simulations reported here implement Step 3 with both a Metropolis sweep and a random translation.

The validity of the algorithm is proved by showing that it is ergodic and that the joint distribution, $X(\sigma, \tau, \eta)$, defined in Eq. (2) is the stationary distribution of the algorithm. Ergodicity follows immediately from Step 3. To prove stationarity we observe, following [15], that the Steps 1 and 2 of the algorithm correspond to conditional probabilities associated with $X(\sigma, \tau, \eta)$. Step 1 is the conditional probability of a bond configuration given a spin configuration. Note that the bonds connecting inactive sites are not actually specified in the algorithm but since bonds are independently occupied this is of no consequence. Step 2 is the conditional probability of the spin configuration on the active sites given a bond configuration, a set of active sites and the spin configuration on the inactive sites.

We simulated the square lattice, staggered field Ising model in periodic boundary conditions using the two-replica cluster algorithm described above. Data was collected for $\beta H = 0$, 2 and 4 and for size L in the range 16 to 256. Each L and βH was simulated for 50,000 Monte Carlo steps, dropping the first 5,000. Figure 1 shows the probability that there is a spanning cluster $\mathcal{S}$ as a function of temperature T for several system sizes and $\beta H = 2$. Spanning is defined as wrapping around the torus in either direction. The vertical line is the high precision value of T_c given in [18]. Figure 2 is a plot of $\mathcal{S}$ versus $c(\beta H)[T - T_c(\beta H)]L$ of the data for all values of βH and L. Data collapse is achieved using $T_c(\beta H)$ from [18],

$c(0) = 1$, $c(2) = 2.64$ and $c(4) = 7.30$. This figure illustrates that the model is in the Ising universality class independent of βH. The fact that $\mathcal{S} \rightarrow 1/2$ for large systems and $T < T_c$ is due to periodic boundary conditions. For half of the Monte Carlo steps, replicas are magnetized in the same direction preventing active clusters from spanning. These results provide a clear numerical verification that percolation in the two-replica representation is coincident with the critical point.

The Table shows the integrated autocorrelation time for the absolute value of the magnetization of one replica, τ_m and the net staggered magnetization τ_s versus system size. The integrated autocorrelation time is 1/2 plus the sum of the normalized autocorrelation function from time 1 through 200. The system size dependence of τ_s and τ_m can be reasonably fit either as AL^z or as $A + B\log(L)$. For the whole range of L, logarithmic growth gives a better fit visually. Fitting a power law for system sizes greater than 40, we find dynamic exponents, $z_m = 0.19 \pm .09$ and $z_s = 0.33 \pm .09$ for $\beta H = 4$ with nearly identical results for the other two field values. The quoted error is the statistical part and does not include systematic errors due to finite system size and finite cut-off in summing the autocorrelation function. A conservative conclusion is that $0(\log) \leq z < 0.5$. It is clear that the algorithm achieves considerable acceleration over local dynamics, where $z \geq 2$. This is perhaps surprising in view of the fact that the algorithm uses local dynamic to break conservation of staggered magnetization. The autocorrelation times for the present algorithm and the ordinary Ising model ($\beta H = 0$) are roughly a factor of five larger than for the Swendsen-Wang algorithm however, further study is needed to determine whether the two algorithms share the same z. On the other hand, in the presence of a staggered field, autocorrelation times for both the Swendsen-Wang algorithm and the two-replica algorithm without translations are much larger than the values obtained here. Rough estimates of exponential autocorrelation times for the present algorithm show that they are about twice the corresponding integrated autocorrelation time.

In the case of a staggered field, we have made use of the symmetries of the problem to incorporate as much mixing as possible into Step 3 of the algorithm. For systems such as the random field Ising model which do not enjoy translational symmetries, local dynamics are all that is available to equilibrate the average magnetization at each site. Thus, the two replica algorithm may not be a qualitative improvement over local dynamics alone. However, significant acceleration may be achieved by using many replicas. Suppose we have $2K$ replicas, $\{\sigma^{(l)} | l = 1, \ldots, K\}$ all in the same field $\{H_i\}$. In each Monte Carlo step, the replicas are randomly paired and the two replica cluster procedure is applied to each pair. Each replica is also updated independently by some local ergodic algorithm. The replica summed magnetization at each site, $\sum_{l=1}^{2K} \sigma_i^{(l)}$, is conserved except by the local dynamics and so may relax slowly to equilibrium. This implies that the average magnetization at any site may reach equilibrium slowly resulting in a large exponential autocorrelation time. However, once the equilibrium values of the magnetization are reached, the fluctuations of the replica summed magnetization are small for large K and thus couple weakly to the observables of individual replicas. This may yield rapid decorrelation and small values of integrated autocorrelation times. Note that in the two replica simulations, we observed τ_{exp} to be about twice τ_{int}.

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TABLES

TABLE I. Integrated autocorrelation times for the absolute value of the magnetization of a single replica τ_m and the net staggered magnetization of both replicas τ_s. For each entry, the one standard deviation error is 13%.

	$\beta H = 0$	$\beta H = 2$		$\beta H = 4$	
L	τ_m	τ_m	τ_s	τ_m	τ_s
16	9.3	10.7	8.1	17.1	15.0
24	14.5	14.8	12.6	22.2	19.9
32	17.5	20.4	15.6	28.2	23.6
40	22.1	27.2	23.9	22.4	21.0
48	28.2	31.3	26.6	31.5	29.4
56	29.6	27.8	22.6	36.1	34.3
64	28.6	34.0	30.6	30.4	27.3
80	32.5	34.9	35.6	30.2	29.8
96	35.5	36.2	31.0	36.2	37.2
112	29.6	38.6	36.4	38.8	43.0
128	30.0	35.9	35.9	36.7	40.1
144	35.9	37.4	37.5	37.7	43.0
160	35.3	37.5	35.0	40.9	47.6
192	42.6	37.0	36.7	42.9	46.3
256	37.8	44.4	48.4	40.1	46.9

FIGURES

FIG. 1. The spanning probability vs. T for various system sizes and $\beta H = 2$.

FIG. 2. The spanning probability $\mathcal{S}$ vs. $c(\beta H)[T - T_c(\beta H)]L$ for all system sizes and the three values of βH.