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Comparison of Different Boundary Conditions for Monte Carlo Simulations of Ising Models

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The effects of various boundary conditions on the Monte Carlo method have been studied through an analysis of the two-dimensional Ising model using a 30×30 system. The following boundary conditions were used: mean field, free edges, periodic, and correlated. The results confirm the reliablility of periodic boundary conditions but the correlated boundary conditions are comparable and in some instances yield results (the critical temperature, for example) that are in better agreement with the exact values.

KEY WORDS: Monte Carlo; critical phenomena; boundary conditions.

1. INTRODUCTION

The Monte Carlo (MC) method is a very powerful tool in the study of phase transitions and critical phenomena.[1] Phase diagrams have been obtained with reasonable accuracy but until the recent consideration of large systems[2] it was impossible to determine the critical properties with the same degree of accuracy. There may be several reasons for this; to observe the singularities of critical phenomena it is necessary to take the thermodynamic limit, i.e., to let the size of the system tend to ∞. We are constrained to study finite systems and from these results extrapolate the properties of the infinite system. In addition, finite systems, unlike infinite systems, necessitate special considerations of the boundary. The most popular form of boundary conditions used are periodic[3] (pbc) and these

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are expected to be reliable for ξ, the correlation length, much less than $N/2$ (N being the linear length of the system). However, other boundary conditions have been considered; free edges[4,5] (fe) and mean-field boundary conditions (mf).[6]

In this work we investigate the influence of various boundary conditions on the Monte Carlo method through the analysis of the two-dimensional Ising model. In addition to the above boundary conditions we consider a correlated mean field (cmf) and correlated boundary conditions,[7] which will be explained below. We shall also introduce a novel technique for expediting the sampling of independent configurations in the critical region. Of course, the two-dimensional Ising model is well studied and many of its properties are known exactly. The aim of the present work is not to learn something new about the model but to use it as a test for the results obtained with competing boundary conditions. In the next section we briefly describe the MC method and the modification to expedite sampling in the critical region. We next describe the boundary conditions and then the results are presented and compared with each other and with exact values.

2. MONTE CARLO METHOD

We apply the standard MC method to a 30×30 Ising lattice. Each spin is visitied in a nonsequential manner and flipped or not dependent on the comparison of a random number with $\exp(-\Delta E/kT)$, where ΔE is the energy change, k the Boltzman constant, and T the temperature of the system. Near T_c (the exact critical temperature which, in units for which J, the interaction parameter, and k are equal to unity, is 2.2692) the relaxation time of the order parameter is large, the phenomenon referred to as critical slowing down. From the point of view of a MC calculation this means that we sample a small region of the "important" phase space. Thus for a given amount of computing time there would be inadequate sampling near T_c.

We have minimized this effect by periodically perturbing a portion of the lattice. This size is the same as an average droplet, which is determined from inspection of equilibrium configurations. The system is allowed to attain thermal equilibrium and "important" configurations generated. This approach is equivalent to but more efficient than one using several different starting configurations.

3. BOUNDARY CONDITIONS

We present a brief description of the boundary conditions.

(i) Periodic (pbc). The external nearest neighbors (nn) of the spin at an edge are the spins at the opposite side.

(ii) Free Edges (fe). The external nearest neighbor spins do not exist. These are the conditions pertinent to the surface of the crystal.

(iii) Mean Field (mf). The states of spins external to the edge are replaced by the average magnetization of the system. In order to enhance fluctuations we select a value for the surface magnetization from the range $M_A \pm \Delta M$, where ΔM is equal to $(\langle M^2 \rangle - \langle M \rangle^2)^{1/2}$.

(iv) Correlated mean field (cmf). The states of the spins external to an edge are replaced by the average magnetization but now the sign of this magnetization is correlated through the nearest-neighbor correlation function to the edge spin.

The energy of such a boundary spin, S_i, is calculated by

$$E_i = S_i \left(\sum_{j=1}^{3} S_j + \epsilon |M| \right) J \tag{1}$$

where S_j are the nearest neighbors of S_i and ϵ taken as $+1$ or -1 with probabilities such that $\langle S_i \epsilon \rangle = \langle S_k S_1 \rangle$ (the average nearest-neighbor correlation of the interior). M is the average interior magnetization and J is the nearest-neighbor interaction energy.

(v) Correlated boundary conditions (cbc). The boundary conditions employed above focus on the complete system. This statement is self-evident for pbc and fe, whereas for mf the average magnetization used for the external layer replaces the external portion of the system. cbc is based on a different point of view: properties of the infinite system may be obtained by observing a finite portion of the system over a sufficiently long period. In the case of the Ising model in contact with a heat reservoir, for example, we may determine the average magnetization of the infinite system from the time-averaged magnetization of a single spin of the infinite lattice. In order to determine the properties of the section of interest we need to know the states of the first layer of external spins. The states of the spins external to an edge are determined with a probability such that the nearest-neighbor correlation function is satisfied between these and nearest-neighbor edge spins.

In this instance the energy of a boundary spin S_i is

$$E_i = S_i \left(\sum_{j=1}^{3} S_j + \epsilon \right) J, \qquad \epsilon = \pm 1 \tag{2}$$

where S_j are the neighbors of S_i and ϵ taken as $+1$ or -1 with probabilities such that $\langle \epsilon S_i \rangle = \langle S_k S_1 \rangle$, the average nearest-neighbor correlation of the interior. This approach is close to cmf described above but in that case the average magnetization instead of ± 1 is used for the states of the external spins.

4. RESULTS

We have calculated various thermodynamic properties (correlation functions, specific heat, energy, magnetization, and susceptibility) as functions of temperature.

These averages were computed from approximately 6000 Monte Carlo steps per spin for temperatures away from T_c, the critical temperature, and from a maximum of 18,000 Monte Carlo steps per spin for temperatures close to T_c. The following features are observed. The nearest-neighbor, second-nearest-neighbor, and third-nearest-neighbor correlation functions show good agreement for all boundary conditions for T greater than 2.30. For T of the order of T_c there is a small disagreement between pbc and fe as compared with cbc and mf. This disappeared at low T for pbc but the

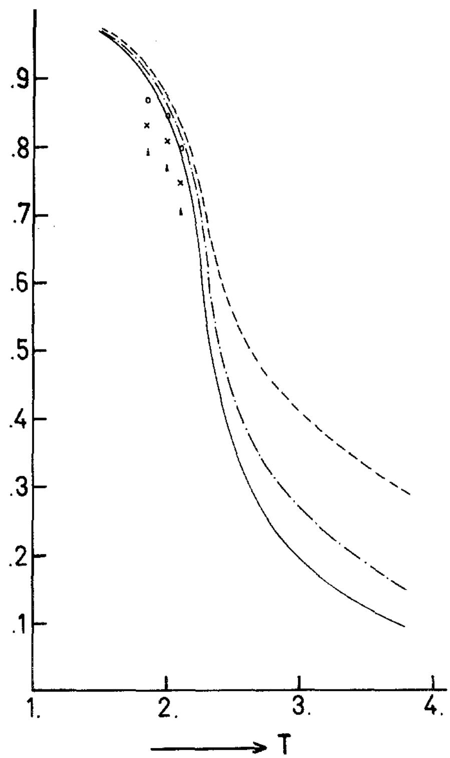

Fig. 1. The nearest-neighbor (- -), next-nearest-neighbor (- ·), and third-nearest-neighbor (——) correlation functions versus temperature. The various boundary conditions all agree for T greater than 2.50. The values obtained with periodic boundary conditions are less than those shown only in the region 2.1 to 2.5. Free edges values show increasing deviation from the other results at low temperatures where these correlation functions are shown by ○ (nn), X (nnn), and △ (third nn).

discrepancy between fe and the others increased. The correlation functions are shown in Fig. 1.

For temperatures greater than 2.30 the magnetization obtained from the various boundary conditions reflects finite size effects. cbc, however, shows a sharp transition at approximately 2.325. Below T_c all the boundary conditions apart from fe agree with the exact results, although it seems that the magnetization for pbc is slightly less than the exact values for T less than 2.20. In the critical region mf and cbc are slightly greater than the exact values. The magnetizations obtained with pbc, fe, and cbc are shown in Fig. 2. The specific heat and susceptibility show some general features. cbc, fe, and pbc give larger values than mf for T less than 2.30 whilst for T

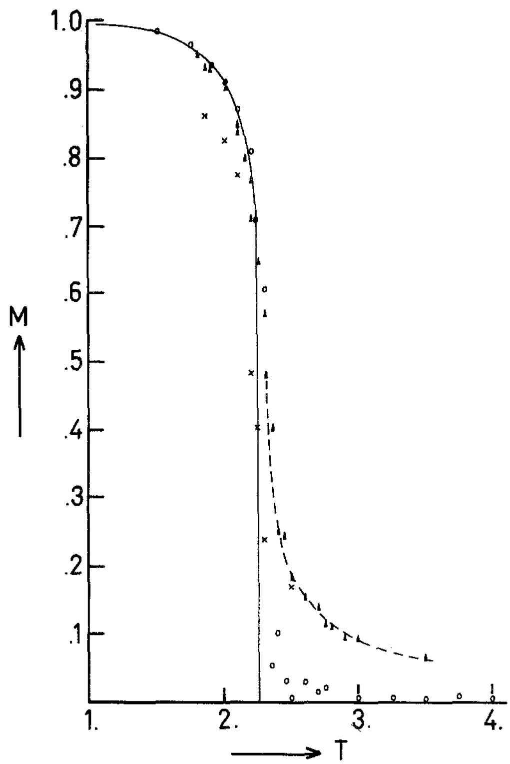

Fig. 2. The magnetization as a function of temperature. The exact result is shown by the solid line. Mean field and correlated boundary conditions (O) agree for T less than 2.1 but above this temperature the mean field values converge to the free edges (×) becoming identical at 2.50. The values of this magnetization obtained with free edges are much less than those obtained with other conditions for low temperatures. Periodic boundary conditions are indicated by △. The correlated boundary magnetization above 2.30 are in some cases negative and give the most precise estimate for T_c. We have shown the absolute values.

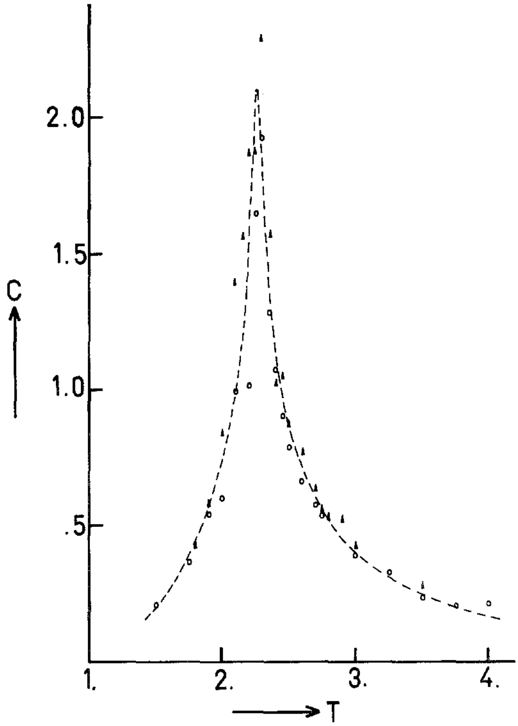

Fig. 3. Specific heat obtained with periodic boundary conditions (△) and correlated boundary conditions (○). These boundary conditions show good agreement with the exact values (- - -) for T greater than 2.30. The agreement is not as good in the range 2.0 to 2.25 where periodic boundary conditions yield values above and correlated boundary conditions less than the exact results. The peak in the specific heat is not as pronounced for free edges and mean field (not shown) and the free edges peak is noticeably shifted to a lower temperature.

greater than 2.30 the various methods agree. We have compared in Fig. 3 the specific heat of the cbc and pbc with the exact values and both show the same degree of accuracy over the complete temperature range. The energy per spin as a function of temperature is shown in Fig. 4. For clarity we have excluded the results of the fe and mf. Note that cbc shows good agreement with the exact values over the complete temperature range whereas pbc values are greater than the exact results and the difference increases with temperature.

5. CONCLUSION

We have compared the results obtained with MC and various boundary conditions with the exact values. Binder[1] notes that the two-dimensional Ising system is one of the most challenging models to simulate

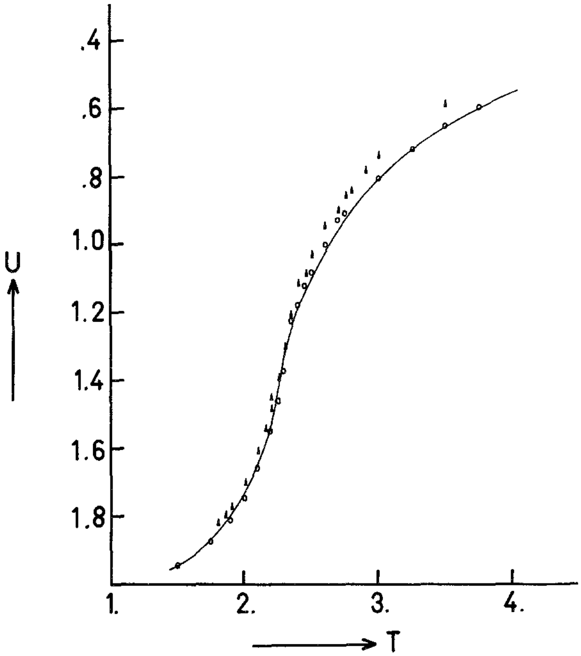

Fig. 4. The energy as a function of temperature for periodic boundary conditions (△) and correlated boundary conditions (○). There is good agreement between correlated boundary conditions and the exact results which is shown by the solid line. For T less than 2.3 mean field and correlated boundary conditions are almost identical whereas free edges values are less than periodic boundary conditions. For T greater than 2.3 free edges and mean field agree and their values lie between the results of correlated boundary conditions and periodic boundary conditions.

(the slow decay of the correlation functions). It is also one of the few systems for which exact results exist and thus allows for an independent estimate of the accuracy of the method.

Free edges produce the greatest discrepancy with the other conditions and also with the known results. This effect is also seen from Landau's[4] work but unlike that observed for bond percolation.[5] The two mean field conditions did not produce any noticeble differences and we may conclude that the effects of the average field are stronger than those of correlations. mf reduced to fe for T greater than T_c. A possible generalization of the mf, therefore, is to randomly select the states of the layer of external spins such that the average magnetization of this layer is equal to the average magnetization of the internal section. As expected, the values of the fluctuating quantities, e.g., specific heat and susceptibility are smaller for mf than with the other boundary conditions.

cbc and pbc are superior to the other conditions when we apply MC to critical phenomena. On the whole, cbc shows better agreement with the exact values, e.g., the magnetization and the energy, but there is little difference when we compare quantities involving fluctuations. This attractive feature of pbc is due to the enhancement of the growth of droplets and was also noted by Landau.[4] This may also explain why the specific heat results with pbc are greater than the exact values for T less than T_c. Another feature worth noting is the CPU time required to determine the boundary states. pbc and fe took the least CPU time whilst mf took the longest by a factor of 1.5. A drawback with pbc, however, is that the correlation functions will not show the proper variation with distance, especially in the critical region. The choice of the "best" boundary conditions thus depends on the quantities one wants to calculate, but cbc has sufficient attractive features to encourage future investigation.

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