Efficient search method for obtaining critical properties

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Abstract

A method for obtaining critical properties is presented. Based on self-organized criticality, it drives the system spontaneously to the critical point, providing an efficient way to estimate critical properties. The method is illustrated for Ising spin systems, and despite the small lattice sizes used, it yields critical temperatures and $\beta$ exponents in good agreement with those available in the literature. © 2000 Elsevier Science B.V. All rights reserved.

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Statistical mechanics has become one of the most successful physical theories nowadays; through simple models, it has been able to describe, reasonably well, a wide diversity of experimental observations. Among the most interesting models of statistical mechanics are those exhibiting critical phenomena [1]. Such models, although simple to define, usually are not easy to be solved exactly [2]; most of them are treated through approximation methods. Due to a significant improvement in computer technology, computer simulations [3] represent, at the present time, powerful tools for studying physical systems. Among all types of numerical simulations, the Monte Carlo (MC) method [4–7] is probably the most used technique, being applied extensively in a wide variety of problems. In a standard MC simulation each dynamical variable (which may be defined on sites of regular lattices) is visited either at random or in well-defined sequences, to be afterwards updated according to certain dynamical rules;

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the main drawback of such a technique is the large computational effort required for obtaining reliable results. The MC method has been improved frequently, in a permanent search for better efficiency, always balancing the accuracy of results with computational efforts. Histogram techniques have been combined with MC methods, providing a significant optimization of the data analysis: the information about the equilibrium probability associated with a given set of external parameters may be used to estimate thermodynamic averages at neighboring values of the external parameters [8–10].

The use of cluster algorithms [11–13], in which all dynamical variables in previously defined clusters are updated at once, has considerably decreased the relaxation times near critical points. The algorithm of Machta et al. [13], known as invaded cluster algorithm, correlates a modified type of percolation (used to define the clusters) with configurations of dynamical variables. After the identification of clusters, each cluster is updated with probability \( \frac{1}{2} \) (like in the Swendsen–Wang algorithm [11]), taking the system to a new configuration, from which new clusters are defined.

An important step in the theory of critical phenomena occurred through the concept of self-organized criticality (SOC) [14], according to which certain dynamical systems evolve spontaneously towards the critical state, i.e., the critical state is an attractor of the dynamics. The recent algorithm of Machta et al. makes use of such a concept, and due to the fact that invasion percolation is a self-organized critical phenomenon, after a long time, the system reaches the critical point.

A conceptual framework for SOC was proposed by Sornette et al. [15], based on the idea that a control rule, designed to keep the order parameter close to a small positive value, pushes the system automatically to the vicinity of the critical point. As an example, for a ferromagnetic system, instead of controlling the temperature \( T \), one may reach criticality by taking the magnetization \( m \rightarrow 0^+ \), which is equivalent to approaching the critical temperature, \( T \rightarrow T_c^- \). Herein, we shall present a method, based on a recursive relation, in such a way as to implement operationally the proposal of Sornette et al. Once the order parameter is properly chosen, the recursion drives physical systems spontaneously to the value of the control parameter associated with such a choice; in particular, if the order parameter is set to a small value, the system will be driven towards the critical point. Let us consider the relation [16–18]

\[
X_{n+1} = X_n - \alpha(Y_n - Y^*)
\]

involving two dimensionless variables \( (X_n, Y_n) \), related to two relevant parameters of a given physical system (e.g. for a magnetic system, such quantities may be related to the temperature and magnetization, respectively). The variables \( (X_n, Y_n) \) will change at each iteration step \( n \), in such a way that after a sufficient number of steps, \( X_n \) will converge to a stationary value \( X^* \), compatible with the stationary value \( Y^* \equiv Y(X^*) \), assumed by \( Y_n \). The desired stationary state \( (X^*, Y^*) \) may be previously selected by an appropriate choice of the quantity \( Y^* \); the rate of convergence to the stationary state is controlled by the parameter \( \alpha \) (which plays a similar role as the spring constant of a harmonic oscillator). The method works as follows:
(a) One previously defines $x$ and $Y^*$, which will control, respectively, the rate of convergence and the stationary state to be accessed.

(b) At the first iteration, one chooses the initial value $X_0$. This will define the range of parameters to be investigated [$X_0$, $Y_0$] will vary from $(X_0, Y_0)$ to $(X^*, Y^*)$.

(c) A particular initial configuration is assigned to the dynamical variables and the system is let to evolve dynamically according to a given MC prescription. After equilibration is attained ($t_0$ MC steps) one may calculate thermodynamic averages (associated with the particular choice of $X_0$) over $t_1$ MC steps. To improve the statistics, this procedure is repeated over $N_s$ samples. The average value $Y_0$ is computed, and from Eq. (1) one obtains $X_1$.

(d) Step (c) is now performed for parameter $X_1$, and so on, in such a way that one gets, iteratively, $(X_0, Y_0) \rightarrow (X_1, Y_1) \rightarrow (X_2, Y_2) \cdots$.

(e) The process stops when $Y_n$ and $X_n$ present small oscillations around the values $Y^*$ [defined in step (a)] and $X^*$ (the desired stationary value of the parameter $X$), respectively.

(f) After the stationary regime is attained, one may consider a number $\Delta n$ of oscillations around $(X^*, Y^*)$, in order to get a statistics for the parameter $X^*$.

The method described above has been applied successfully for the determination of critical frontiers in nonmagnetic systems, like branched polymers [16], in which case $X \equiv b$ (branching probability) and $Y \equiv N$ (number of alive tips), as well as percolation [17], with $X \equiv p$ (occupation probability associated with sites or bonds) and $Y \equiv N$ (number of active sites or bonds). The present method has also determined, within a good accuracy, the critical temperatures of Ising ferromagnets on a linear chain, square and cubic lattices [18].

In this paper we show that the method described above is appropriate not only for obtaining critical frontiers, but also for the critical exponents, i.e., the system is driven to criticality through the correct thermodynamic path.

Let us illustrate this for the ferromagnetic Ising model, defined through the Hamiltonian,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j \quad (J > 0; \; S_i = \pm 1),$$

where the sum $\sum_{\langle ij \rangle}$ is restricted to nearest-neighbor pairs or spins on a given $d$-dimensional Bravais lattice of linear size $L$ (with a total number of spins $N = L^d$). In this case, the recursive relation (1) becomes

$$K_{n+1} = K_n - \alpha(m_n - m^*) ,$$

where $K = J/k_B T$ and $m$ is the magnetization per spin (herein properly defined, in such a way as to be a dimensionless quantity, $m = N^{-1} \sum_i \langle S_i \rangle$, where $\langle \cdots \rangle$ stands for a thermodynamic average).

For a finite system of linear size $L$, the magnetization per spin is finite at the critical point, decreasing for increasing values of $L$ [3]: since the correlation length becomes comparable to the lattice size, i.e., $\xi \sim L$, if one considers the correlation
length and magnetization power-law behaviors, one gets that \( m \sim L^{-\beta/\nu} \) at criticality. Therefore, the choice of \( m^* \), so as to drive the system towards the critical point, must satisfy \( 0 < m^* < L^{-\beta/\nu} \). If \( m^* \) is taken outside such a range, the system is driven through a different thermodynamic path and never converges to the critical point, e.g. by considering \( m^* \sim O(1) \), the recursion yields a convergence to a low temperature, compatible with the value of \( m^* \) \[18\]. Of course, the exponents \( \beta \) and \( \nu \) are unknown quantities, to be determined. The present method provides, in advance, a rough estimate of the ratio \( \beta/\nu \), through the observation of the convergence of the magnetization after many iterations. Hence, in order to approach the critical point, in the present work we choose a small value for \( m^* \) (e.g. \( m^* = 10^{-2} \)).

In principle, for a given finite size \( L \), the stationary temperature \( T^* \) also depends on the choice of the parameter \( \varkappa \). By considering several choices of decreasing values of \( \varkappa \), we verified that there is an optimal \( \varkappa \), below which \( T^* \) does not alter within the error bars. In all cases studied herein, such a value is \( \varkappa = 10^{-2} \). However, in order to obtain reasonable data for estimating the critical exponents, we consider a smaller value for \( \varkappa \) \((\varkappa = 10^{-3})\); as mentioned, such a choice does not alter, within the error bars, the stationary temperature (compared with the one estimated for \( \varkappa = 10^{-2} \)), but yields closely spaced temperatures near the critical point. We suspect that the independence of the results on the particular choice of the parameter \( \varkappa \), whenever \( \varkappa \) is smaller than a certain value, is a general property of the method; this has been verified in all other applications considered so far \[16–18\].

At each iteration \( n \), the MC prescription used, as mentioned at item (c) above, was a single spin-flip updating, following the Glauber dynamics \[19\], according to which

\[
S_i(t + 1) = \begin{cases} 
1 & \text{if } z_i(t) \leq p_i(t) \\
-1 & \text{if } z_i(t) > p_i(t)
\end{cases} 
\]

and

\[
S_i(t + 1) = \begin{cases} 
-1 & \text{if } z_i(t) \leq 1 - p_i(t) \\
1 & \text{if } z_i(t) > 1 - p_i(t)
\end{cases} 
\]

In the above equations, \( z_i(t) \) is a uniform random number in the interval \([0,1]\) and \( p_i(t) \) is the probability

\[
p_i(t) = \left(1 + \exp[-2h_i(t)]\right)^{-1},
\]

where

\[
h_i(t) = K \sum_j S_j(t)
\]
is the local field acting on site \( i \), at time \( t \), and \( K = K_n \); \( K_n = J/k_BT_n \) is the parameter related to the temperature \( T_n \) at iteration step \( n \).

We have applied the above method for the ferromagnetic Ising model on several two-dimensional lattices (square, triangular and honeycomb) of linear size \( L = 40 \) and
Table 1
The dimensionless stationary temperatures \((k_B T^*/J)\) and the corresponding magnetization critical exponents for the ferromagnetic Ising model on several Bravais lattices are compared with critical temperatures \((k_B T_c/J)\) and exponents \(\beta\) available in the literature. For the two-dimensional lattices \(k_B T_c/J\) and \(\beta\) are known exactly \([2]\) (\(\beta = \frac{1}{2}\) in all cases, due to universality), whereas for the cubic lattice, we have used the approximate values of Ref. \([20]\). In each case, the relative discrepancy of \(T^*\) with respect to the critical temperature \((|T^* - T_c|/T_c)\) is given (up to three decimal digits)

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Square lattice</th>
<th>Triangular lattice</th>
<th>Honeycomb lattice</th>
<th>Cubic lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>(k_B T^*/J)</td>
<td>2.385 ± 0.002</td>
<td>3.671 ± 0.005</td>
<td>1.553 ± 0.001</td>
<td>4.487 ± 0.002</td>
</tr>
<tr>
<td>(k_B T_c/J)</td>
<td>2.269185…</td>
<td>3.640956…</td>
<td>1.518651…</td>
<td>4.51142 ± 0.00005</td>
</tr>
<tr>
<td>(</td>
<td>T^* - T_c</td>
<td>/T_c)</td>
<td>0.051</td>
<td>0.008</td>
</tr>
<tr>
<td>(\beta) (Present work)</td>
<td>0.127 ± 0.002</td>
<td>0.125 ± 0.003</td>
<td>0.124 ± 0.002</td>
<td>0.311 ± 0.010</td>
</tr>
<tr>
<td>(\beta) (From literature)</td>
<td>1/8</td>
<td>1/8</td>
<td>1/8</td>
<td>0.3258 ± 0.0044</td>
</tr>
</tbody>
</table>

for the cubic lattice with \(L=10\). At each iteration \(n\), our simulations always started with a completely ordered configuration (all spins up) and a time \(t_0 = N/2\) MC steps was required for attaining equilibrium. After that, we have computed the thermodynamic average for the magnetization per spin over \(t_1 = N\) MC steps. In order to improve the statistics, the whole procedure was repeated over \(N_s=200\) samples (different sequences of random numbers). The magnetization per spin may be obtained from

\[
m = \frac{1}{N t_1 N_s} \sum_{y=1}^{N_s} \sum_{t=1}^{t_1} \sum_{i=1}^{N} S_i(t).
\]

After the stationary state was achieved, we let the system oscillate for \(\Delta n = 100\) iteration steps; from this data we have estimated the average value \(K^* = J/k_B T^*\) and its respective error bars.

Our results are summarized in Table 1. In each case, the value of the stationary temperature \(T^*\) is very close to the well-known critical temperature \(T_c\) (the largest discrepancy occurs for the square lattice, where \(|T^* - T_c|/T_c \approx 0.05\)). From the set of data points of the magnetization per spin versus temperature (in Fig. 1 we present, as a typical example, such a set for the triangular lattice), one may compute the magnetization critical exponent \(\beta\) of each lattice, as shown in Fig. 2. In spite of the small lattice sizes used, our critical exponent estimates agree, within the error bars, with those available in the literature. For the two-dimensional lattices (square, triangular and honeycomb), our results are universal, as expected, recovering the well-known exact value, \(\beta = \frac{1}{2}\) \([2]\).

It is important to compare some of our results with those found from standard MC approaches. The present estimates of \(\beta\) and \(T_c\) for a cubic lattice of linear size \(L=10\) are in good agreement with the values obtained from scaling of MC simulation data of lattice sizes \(8 \leq L \leq 96\) \([20]\), as shown in Table 1. For the square lattice, recent finite-size scaling analysis on data from conventional MC simulations for several lattice sizes \((10 \leq L \leq 200)\) yields \(k_B T_c/J = 2.27 ± 0.01\), as well as the magnetic susceptibility and correlation-length critical exponents, \(\gamma = 1.76 ± 0.01\), \(\nu = 1.00 ± 0.05\) \([21]\); using
Fig. 1. The set of data points of the magnetization per spin versus temperature [in units of the corresponding exact value of $T_c$ (see Table 1)] obtained from the recursive relation [Eq. (3)], for the ferromagnetic Ising model on a triangular lattice of linear size $L = 40$. The iteration started at $T_0/T_c = 0.60$ and the parameters used were $m^* = 10^{-2}$ and $s = 10^{-3}$. The temperature range used for the estimation of the critical exponent $\beta$ is indicated; such a range is inside the scaling region.

Fig. 2. Log-log plot of the fits for the estimates of the critical exponents $\beta$. In each case, the abscissa is written in terms of the corresponding stationary temperature value ($T^*$) in Table 1.
scaling relations, one gets from such results, $\beta = 0.12 \pm 0.05$, which is comparable to the values displayed in Table 1, obtained for two-dimensional lattices of size $L = 40$. It is amazing how the present method can yield such good estimates for very small lattice sizes; it should be pointed out that the results presented in Table 1 may be improved further by increasing the lattice sizes.

To conclude, we have presented a procedure capable of following iteratively the way to any desired stationary state, based on a recursive relation for the order parameter of the system; if the order parameter is set to a small positive value, the corresponding control parameter converges to its critical value. It is important to mention that the power of the method has already been illustrated in obtaining accurate critical-temperature estimates of the ferromagnetic Ising model on both square and cubic lattices [18]. Herein, the robustness of the procedure is confirmed through several new results, not considered in the previous work, as we describe below.

(i) A better statistics for obtaining the stationary temperatures (and their corresponding error bars) was carried, by considering a large number of fluctuations around the stationary state. Considering the same lattice sizes, the present stationary temperature estimates, for the square and cubic lattices, are slightly closer to the well-known critical temperatures than those of Ref. [18].

(ii) Two additional ferromagnetic Ising models were also considered herein, namely, those on the triangular and honeycomb lattices. The relative discrepancies of the stationary temperatures with respect to the corresponding exact critical temperatures are even better than the one obtained for the square lattice.

(iii) The method’s capability for providing critical exponents has been attested herein. For all systems investigated, the magnetization of critical exponents agree, within the error bars, with the well-known values of the literature; in particular, the universality property for two-dimensional Ising ferromagnets was verified. The right critical exponents ensure that the system is driven to criticality throughout the correct thermodynamic path. The evaluation of critical exponents in our opinion, represents, a substantial improvement with respect to the previous work, providing a strong support to the method.

The present recursive procedure may also be used in problems with several attractors, where the desired basins of attraction may be reached through convenient choices of the order parameter. For ferromagnetic models, as the ones considered herein, by setting the magnetization per spin to a small value, the recursion drives the system spontaneously from any temperature to the critical temperature; however, if the magnetization is set to a large value, the recursion converges to a low-temperature state, compatible with the corresponding magnetization. Other recursion relations may also be constructed, and in particular, for thermodynamic quantities which diverge at the critical point (e.g. by considering the inverse of such quantities); the results are expected to be similar to the ones presented above. The efficiency of the method may be improved further if, at each iteration step, one uses more sophisticated Monte Carlo prescriptions (e.g. cluster updatings), instead of the conventional single spin-flip procedure employed herein. The present scheme may become a useful tool for studying critical properties
in more complicated models of statistical mechanics, for which no exact treatments are available, with only a few conclusive (approximate) results. In particular, new insights on problems characterized by disorder, or frustration (or both ingredients), may be achieved.

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