Damage-spreading simulations through exact relations for the two-dimensional Potts ferromagnet

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A powerful computational method for dealing with correlation functions in magnetic systems, based on damage-spreading simulations, is reviewed and tested, by investigating the q-state Potts ferromagnet, on a square lattice, at criticality. Exact relations involving special kinds of damage and the spin-spin correlation function, as well as the magnetization, are used. The efficiency of the method arises with a significant reduction of the finite-size effects, with respect to conventional Monte Carlo simulations. Correlation functions, which represent usually a hard task within this latter procedure, appear to be much more easily estimated through the present damage-spreading simulations. The effectiveness of the technique is illustrated by an accurate estimate of the exponent η, of the spin-spin correlation function, for $q=2$, 3, and 4, with rather small lattice sizes. In the cases $q \geqslant 5$, an analysis of the magnetization is consistent with the well-known first-order phase transition.

I. INTRODUCTION

Statistical mechanics has become one of the most successful physical theories nowadays, with applications in a wide diversity of problems, which have overcome the frontiers of theoretical physics. In principle, any system composed of a large number of interacting subunits may be suitable to be analyzed through statistical mechanics. An important step consists in the definition of simple models, which should take into account the most significant characteristics of the system under investigation. The big triumph of this theory stands in the fact that such models have been able to describe, reasonably well, a wide variety of empirical observations. Among the most investigated models of statistical mechanics are those exhibiting critical phenomena [1,2]. Such models, although simple to define, usually are not easy to be solved exactly [3]; most of them are treated through approximation methods. Due to a significant improvement in computer technology, computer simulations [4] represent, at the present time, powerful tools for studying physical systems. Among all types of numerical simulations, the Monte Carlo (MC) method [5,6] is probably the most used technique, being applied successfully to many systems. In a standard MC simulation, one deals with a single copy of the system, where each dynamical variable (which may be defined on sites of regular lattices) is visited either at random or in well-defined sequences, to be afterward updated according to certain dynamical rules. Since one is always impelled to simulate finite systems, dealing with the finite-size effects represents a hard task when one tries to extrapolate to the desired thermodynamic limit; therefore, the main drawback of such a procedure turns out to be the large computational effort required for obtaining reliable results.

Another type of MC simulation that has proven to be very effective in the study of the dynamics of statistical models is the so-called "damage-spreading" (DS) technique [7,8]. Essentially, it consists in following the time evolution of the Hamming distance between two (originally identical) copies of a given system, subjected to the same thermal noise, given that a perturbation (or damage) is introduced in one of them at the initial time. The DS method was applied successfully to many magnetic models like the Ising [7–14], Potts [15–19], Ashkin-Teller [15], and discrete N-vector [20] models, among others. Usually, more than one regime is found, depending on the external parameters (e.g., the temperature) or on the initial conditions (e.g., initial damage). In the case of the Ising ferromagnet, on lattices of dimension equal to or greater than 2, one finds a chaotic regime, for which the initial damage spreads through the system, and a frozen one, where the initial damage is suppressed. For more complicated systems, like the two-dimensional Potts ferromagnet [17], or Ising spin glasses [8], apart from these two regimes, one may also find another one characterized by memory effects (i.e., a dependence on memory effects). Surprisingly, the location of such regimes may depend on the kind of dynamical procedure employed: for the Ising ferromagnet (in lattices of dimension equal to or greater than 2), one finds suppression at low and propagation at high temperatures, in both Glauber and Metropolis dynamics; in the case of a heat-bath algorithm, these regions are reversed [12].

An important question concerns the possible connections between DS features and equilibrium thermodynamic properties. Exact relations involving quantities like magnetization, magnetic susceptibility, as well as two-spin correlation functions, with differences of certain types of damage were found, for translationally invariant Ising models [13], and have been extended for more complicated models, like Potts [15], Ashkin-Teller [15], and discrete N-vector [20] models. These relations hold for any ergodic dynamical procedure, and their possible use in simulations was illustrated for the case of the two-dimensional Ising ferromagnet, where thermodynamic properties were obtained, through DS simulations, with a significant reduction of finite-size effects [13].

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To our knowledge, this technique has not been much explored in the literature.

In the present work we make use of the exact relations, valid for translationally invariant Potts models, in order to compute the magnetization and two-spin correlation function of the q-state Potts ferromagnet on a square lattice, through DS simulations. The power and reliability of the method is confirmed herein. In particular, the two-spin correlation function, which is usually a hard quantity to estimate through standard MC simulations, due to large fluctuations, is computed, accurately, within the present DS numerical procedure. In spite of relatively small lattice sizes, the exponent η, associated with the power-law decay of the two-spin correlation function at the critical point, is estimated in some cases, up to a four-digit agreement with the well-known exact values. For $q \geq 5$, our results for the exponent β of the magnetization are consistent with the expected first-order phase transition. In the next section, we define the numerical procedure and in Sec. III we present and discuss our results.

II. THE MODEL AND THE NUMERICAL PROCEDURE

Let us consider the q-state Potts ferromagnet on a square lattice of linear dimension L ($N = L^2$ is the total number of spins), defined through the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j) \quad (\sigma_i = 1, 2, \ldots, q), \quad (1)$$

where $J > 0$, the summation $\sum_{\langle ij \rangle}$ applies to nearest-neighbor pairs of spins only, and $\delta(\sigma_i, \sigma_j)$ represents a Kronecker delta function.

The DS technique consists in the investigation of the time evolution of two configurations of the system, for a given temperature T ($\{\sigma_i^A\}$ and $\{\sigma_i^B\}$), subjected to the same thermal noise and same set of random numbers. For each configuration, the simulation is performed by visiting all sites of the lattice in a sequential way, and each spin $\sigma_i^\mu(t)$ ($\mu = A, B$), at time t, is updated according to the following rules [16].

(i) A possible new state $\sigma_i^\mu(t+1)$ is chosen at random, with $\sigma_i^\mu(t+1) \neq \sigma_i^\mu(t)$, from which one calculates the change in energy $\Delta \mathcal{H}^\mu = \mathcal{H}^\mu(t+1) - \mathcal{H}^\mu(t)$.

(ii) Then one can define the probability

$$p_i^\mu(t) = \frac{1}{1 + \exp(\beta \Delta \mathcal{H}^\mu)} \quad [\beta = 1/(k_B T)]. \quad (2)$$

(iii) By introducing a random number $z_i(t)$, uniformly distributed in the interval $[0, 1]$, one performs the change if $z_i(t) < p_i^\mu(t)$; otherwise, the spin $\sigma_i^\mu(t)$ is not updated.

A complete sweep of the lattice defines our unit of time (currently denominated 1 MC step). First of all, we let one configuration (e.g., $\{\sigma_i^A\}$), evolve for $t_{\rm eq}$ MC steps toward equilibrium; this is checked by verifying small fluctuations in time on thermodynamic quantities, like magnetization and energy. Then, one defines time $t=0$, and a copy of system A is made, which will correspond to the second configuration ($\{\sigma_i^B\}$). In the standard DS procedure [7,8], a fraction of spins of the copy B is chosen, in order to change their states,

introducing the initial damage, which is defined as the Hamming distance between the two configurations. Then both copies are submitted to a new thermalization process, where the damaged copy is taken to equilibrium, and after that, one starts measuring the Hamming distance between the two copies.

In the present approach, we follow a slightly different procedure: we introduce a "source of damage," only at the central site of the lattice, by imposing constraints on its associated spin at all times $t \geq 0$. Such constraints can be set to one of the copies (A or B), or to both of them; all remaining spins of the lattice, on both copies, are allowed to evolve freely following the previously defined dynamical procedure. In this case, at $t=0$, copies A and B differ only at the central site; therefore, there is no need for a second thermalization process. Then, one starts computing averages over time (i.e., thermal averages), for a time interval $t_{\rm av}$. In order to reduce the possible effects of correlations in time, we only consider, in our time averages, data at each time interval of 5 MC steps. Therefore, each time average consists in an average over $t_{\rm av/5}$ measurements. It is important to recall that the two copies should always evolve under the same dynamics and random numbers, so as to ensure that any possible difference between them, for $t \geq 0$, should be a consequence only of this source of damage. Each simulation is then repeated for M samples (i.e., M sets of random numbers), providing averages over samples, to reduce the effects on the sequences of random numbers.

In order to explore the exact relations of Ref. [15], two types of evolution should be considered.

(a) We impose $\sigma_0^B(t) \neq 1$ (the choice of state 1 is arbitrary), for all $t \geq 0$, whereas all other spins on both copies are left free to evolve under the above dynamical procedure. Within this kind of time evolution, the following exact relation holds [21]:

$$\Gamma_{0i} = \frac{C_{0i}}{1 - \xi}, \quad (3)$$

where

$$\Gamma_{0i} = \langle \delta(\sigma_i^A, 1) \rangle_t - \langle \delta(\sigma_i^B, 1) \rangle_t, \quad (4a)$$

$$C_{0i} = \langle \delta(\sigma_i, 1) \delta(\sigma_0, 1) \rangle_T - \langle \delta(\sigma_i, 1) \rangle_T \langle \delta(\sigma_0, 1) \rangle_T, \quad (4b)$$

$$\xi = \langle \delta(\sigma_0, 1) \rangle_T. \quad (4c)$$

In the equations above, $\langle \cdots \rangle_t$ represent time averages over trajectories in phase space, whereas $\langle \cdots \rangle_T$ stand for thermal averages.

(b) We impose $\sigma_0^A(t) = 1$ and $\sigma_0^B(t) \neq 1$ (again, the choice of state 1 is arbitrary), for all $t \geq 0$; all remaining spins on both copies should evolve under the above dynamical procedure. For this kind of time evolution, one has the following exact relation [21];

$$\Gamma_{0i}' = \frac{C_{0i}}{\xi(1 - \xi)}, \quad (5)$$

where Γ_{0i}' is given by the same expression as Eq. (4a), but it should computed within a different evolution process.

TABLE I. The critical exponents β and η for the two-dimensional ferromagnetic Potts model, obtained from the present numerical approach, are compared with the corresponding exact values (from Ref. [2]).

	$q=2$	$q=3$	$q=4$
β (exact)	$1/8=0.125$	$1/9=0.1111\ldots$	$1/12=0.0833\ldots$
β (present work)	0.1223 ± 0.0032	0.1115 ± 0.0040	0.0840 ± 0.0009
η (exact)	$1/4=0.25$	$4/15=0.2666\ldots$	$1/4=0.25$
η (present work)	0.2501 ± 0.0014	0.2667 ± 0.0023	0.2518 ± 0.0023

Therefore, after the equilibration process of copy A (time $t=0$), this configuration is stored as a new copy A_0 that will remain untouched; then, the time evolution described in (a) is continued for copies A and B, in such a way that one obtains, after t_{av} MC steps, Γ_{0i}. Now, recovering configuration A_0, which will become configuration A for the second time evolution, one performs such an evolution, in order to get Γ'_{0i}. From these two quantities, using Eqs. (3) and (5), one obtains C_{0i} and ξ.

The quantity C_{0i} in Eq. (4b) represents the two-spin correlation function of the spin at the central site of the lattice, σ_0, and a spin at an arbitrary site i, σ_i, a distance r apart. It is important to notice that on a square lattice, in most cases, there are four spins σ_i with the same distance r from the central site. In fact, there are a few exceptions to this statement, for which more than four spins present the same distance from σ_0; as examples, if one assumes a unit lattice spacing, one has eight spins whose distance to σ_0 is $\sqrt{5}$, and 12 spins whose distance to σ_0 is 5. However, it is always possible to define the correlation function $C(r)$ as an average value,

$$C(r) = \frac{1}{4}\sum_{i(r)} C_{0i}, \qquad (6)$$

where $\sum_{i(r)}$ corresponds to a summation over four sites with the same distance r from the central site; in the exceptional cases where there are more than four sites with the same distance r from the central site, the remaining spins are not be taken into account in the average of Eq. (6).

The parameter ξ in Eq. (4c) is directly related to the magnetization per spin of the system. Notice that $\xi=1$ at zero temperature, but for high temperatures, where all states are equally probable, one gets $\xi=1/q$. Let us then define the magnetization per spin as

$$m = \frac{1}{q-1}(q\xi-1) = \frac{1}{q-1}[q\langle\delta(\sigma_0,1)\rangle_T - 1]. \qquad (7)$$

In the next section we present and discuss the results obtained for the magnetization per spin m and the correlation function $C(r)$, for several values of q.

III. RESULTS AND DISCUSSION

We studied the q-state Potts ferromagnet on a square lattice of linear size $L=100$, through the DS numerical procedure explained above. Periodic boundary conditions were always used and the correlation function $C(r)$ was measured with respect to the central site, located at coordinates $(L/2, L/2)$. We have always started copy A with all spins of the lattice in the state $\sigma_i^A=1$ ($\forall$ i); after that, the system evolved toward equilibrium, for an equilibration time $t_{eq}=10^4$ MC steps. The thermal averages were carried over $t_{av}=2.5\times10^5$ MC steps, with measurements taken at each time interval of 5 MC steps, which yields a total of 5×10^4 measurements for each time average. Besides that, each simulation was repeated for $M=50$ different samples, in order to improve the statistics, as well as to reduce possible dependence on sequences of random numbers. All simulations were carried out within these figures, otherwise specified. It is important to recall that the critical temperature of this model is known exactly, for an arbitrary value of q [3], $k_B T_c(q)/J = 1/[\ln(1+\sqrt{q})]$, whereas the critical exponents associated with the continuous phase transition (cases $q=2$, 3, and 4) are known exactly (see Table I). For $q>4$, this model exhibits a first-order phase transition; one usually defines a critical number of states $q_c=4$, above which the first-order phase transition takes place.

In Fig. 1 we exhibit the correlation function $C(r)$ versus r for three different temperatures near criticality, in the case $q=3$; temperatures are rescaled by the exact critical temperature mentioned above. Our criterion for locating the "critical temperature" (associated with the finite size of the system considered) consists in searching for the temperature at which the function $C(r)$ presents the slowest decay with r. From Fig. 1, one notices that, in spite of the relatively small lattice size used, the slower decay occurs for a temperature that coincides with the exact critical temperature. We consid-
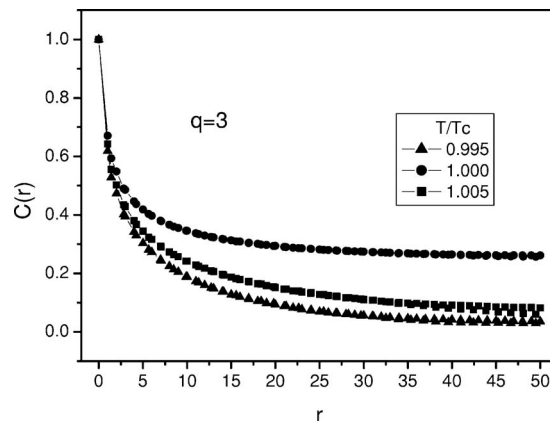

FIG. 1. The correlation function $C(r)$ versus r, in the case $q=3$, for different temperatures (scaled by the corresponding exact critical temperature) near criticality.
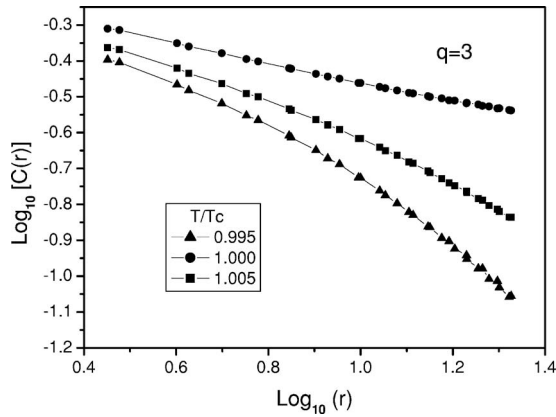
FIG. 2. Log-log plots of the correlation functions exhibited in Fig. 1.

ered temperature increments (scaled by the corresponding exact critical temperature) of 0.001 around criticality, although, for the sake of clearness, in Fig. 1 we exhibited data from only three typical temperatures. The log-log plots of the data in Fig. 1 are presented in Fig. 2, where one verifies that the best power-law behavior,

$$C(r) \sim r^{-\eta} \quad (r \to \infty), \tag{8}$$

is obtained for $T=T_c$ [recall that, for a d-dimensional lattice, one should have $C(r) \sim r^{-(d-2+\eta)}$, at $T=T_c$ [1,2]]. The resulting critical exponent η, from Fig. 2, is given in Table I.

The behavior exhibited in Figs. 1 and 2 was verified for all values of q investigated, namely, $q=2$, 3, 4, 5, and 6. In all cases, the critical temperature estimated coincides with the exact values, up to a relative accuracy of 0.001, i.e., the slowest decay in the correlation function $C(r)$ was obtained for a temperature

$$\frac{k_B T_c^{(L)}(q)}{J} = \frac{1}{\ln(1 + \sqrt{q})} \pm 0.001, \tag{9}$$

where $T_c^{(L)}(q)$ stands for the "critical temperature" for the finite size L. It is important to recall that the power-law behavior of Fig. 2 is not expected for $q=5$ and 6, in the thermodynamic limit, where a well-known first-order phase transition takes place. We attribute such conflicting results to finite-size effects, although up the maximum lattice sizes investigated ($L=200$), we have found no significant changes in this behavior.

In Fig. 3 we exhibit the magnetization per spin as a function of the temperature (scaled in units of the corresponding exact critical temperature), as obtained by the above-mentioned numerical procedure, for the case $q=3$. In spite of the small lattice size considered, one observes a whole smooth curve—even near criticality—with weak finite-size effects; this represents one of the greatest advantages of the present DS simulations. A simple plot of $\log_{10} m$ versus $\log_{10}(1-T/T_c)$ yields the critical exponent β (cf. Table I). Similar plots were found for other values of q, namely, $q=2$, 4, 5, and 6. As expected for a first-order phase transition, one should have $\beta=0$, for $q \geqslant 5$, signaling a discontinuity in the order parameter. We have found, in the cases $q \geqslant 5$, a
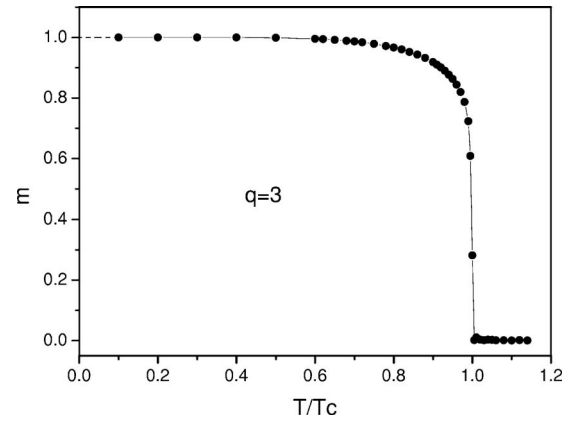

FIG. 3. The magnetization per spin versus temperature (in units of the corresponding exact critical temperature), in the case $q=3$. The full line is just a guide to the eye, whereas the dashed line, at low temperatures, corresponds to an extrapolation to zero temperature.

critical exponent β that approaches zero, very slowly, for increasing lattice sizes. This is exhibited in Fig. 4, where three different lattice sizes were considered in the analysis of the exponent β, for $q=5$; in this case, we obtained $\beta=0.0725\pm0.0013$ ($L=50$), $\beta=0.0679\pm0.0009$ ($L=100$), and $\beta=0.0649\pm0.0010$ ($L=200$). Such a slow convergence to the thermodynamic limit reflects the smooth crossover, in the thermodynamic properties, that occurs near $q_c=4$, when one goes from the continuous to the first-order phase transition [3]. Even though the estimates of the exponent β for the case $q=5$ (empty symbols in Fig. 4) are far from the exact value (full circle), the other estimates of β in Fig. 4 ($q=2$, 3, and 4) appear essentially superposed on the corresponding exact values.

In Table I we list our quantitative results for the critical exponents β and η, for $q=2$, 3, and 4, compared with the corresponding exact values. The values obtained are remarkable, considering the lattice size used ($L=100$). In all cases of Table I, one has an agreement (within the error bars) up to four decimal places with the exact values.
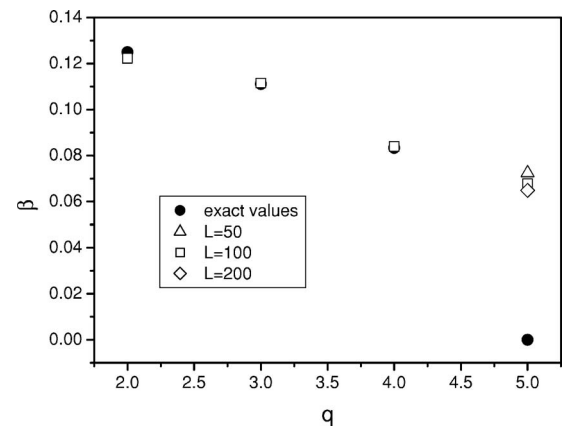

FIG. 4. The critical exponents β, obtained from the present approach (empty symbols), are compared with the exact values (full circles) for different values of q. In the case $q=5$, three different lattice sizes were used, whereas in the other cases, the results of our simulations correspond to a lattice size $L=100$.

To conclude, we have tested an important computational method for evaluating correlation functions in magnetic systems, based on DS simulations, by investigating the q-state Potts ferromagnet on a square lattice. The two-spin correlation function, which is usually a hard quantity to estimate through standard MC simulations, due to large fluctuations, has been computed accurately for this model. We have used exact thermodynamic relations, involving measurable quantities within DS simulations and the two-spin correlation function, as well as the magnetization per spin. Although this method was introduced several years ago for the Ising model (with a rough check of its validity) [13], it has not been fully explored in the literature. We have shown its effectiveness herein, where, in spite of the small lattice sizes considered, the results for the Potts model are very impressive. The present analysis gives reliability to the method, which may now be applied to more complicated open problems in the literature, like Ashkin-Teller and discrete N-vector models, for which the necessary theoretical backgound has been fully developed.

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[21] There are misprints in Eqs. (9) and (12) of Ref. [15]; the corresponding correct equations have been written in Ref. [20].