Alternative boundary conditions for Monte Carlo simulations based on self-consistent correlations: Application to the two- and three-dimensional Ising models

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An alternative to periodic boundary conditions is developed and tested in Monte Carlo simulations of the two- and three-dimensional Ising models. The boundary conditions are based on a mean-field approach that incorporates consistency constraints for the magnetization and correlations between nearest neighbors by means of an effective field and an extra coupling between nearest neighbors at the boundary of the simulation box. During the simulation the self-consistent equations are solved, and statistics are accumulated to obtain thermodynamic averages. In comparison with the standard periodic boundary conditions the method gives a more accurate estimation of nonuniversal magnitudes, such as the transition temperature and the behavior of the magnetization, but it cannot compete with the accuracy of other strategies such as finite-size scaling theory or Monte Carlo renormalization group to obtain critical exponents.

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I. INTRODUCTION

The most extended choice for the boundary conditions in Monte Carlo or molecular-dynamics simulations of infinite periodic systems corresponds to periodic boundary conditions. They work well far from a phase transition, but close to a continuous phase transition the correlation length grows without limit and all the singularities associated to the transition are rounded. Approximation methods, such as the mean-field approach, constitute an alternative to simulations: the periodic infinite system is reduced to a single unit and the effect of the rest of the crystal is taken into account by replacing the interactions with its neighbors by effective fields that fulfill a self-consistency condition.

Both approaches, simulations and mean-field approximations, can be combined by considering, instead of a single site, a collection of sites and applying self-consistent fields at the boundary of the system. For large systems only simulation methods can be used to obtain statistical information of the system and the resulting technique can be considered as a simulation with self-consistent boundary conditions. This kind of calculations has been already applied to Monte Carlo simulations [1–4]; there is not rounding at the transition and the critical point can be calculated unambiguously. Unfortunately, the simulated systems correspond to the mean-field universality class and more sophisticated techniques such as finite-size scaling (FSS) [5] or coherent anomaly method (CAM) [6] must be used to extract accurate estimates of the critical temperature and critical exponents by performing several simulations with different system sizes.

More elaborate versions of the mean-field approach that extends the self-consistencies to correlations between different sites have been developed for two-dimensional Ising models in Refs. [7,8]. Unfortunately, their application is restricted to systems of small size, the number of self-consistent equations to be solved increases prohibitively with the size of the system, the prioritization of the dominant couplings is not clear and, as a consequence, the generalization to large systems and/or three dimensions is not feasible. We propose a method that gives a simple way to handle any system size and any dimension and that, in combination with the Monte Carlo method, opens a simple way to explore accurately the statistical properties of simple Hamiltonians. The effective parameters correspond to a single effective field and a single coupling between nearest neighbors at the boundary. During a sequence of Monte Carlo simulations two objectives are achieved: a system of two self-consistent nonlinear equations is solved and statistics are accumulated to obtain thermodynamic averages. Although this work is focused on the Ising model in two and three dimensions, the method can be, in principle, generalized to more complex Hamiltonians.

II. EFFECTIVE FIELDS AND COUPLINGS WITHIN MEAN-FIELD APPROXIMATION

The Hamiltonian of the Ising model in the presence of an external field h can be described as

$$H = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i.$$

Within the mean-field approximation the most basic theoretical treatment of such a model corresponds to the Weiss [9] or Bragg-Williams [10] theory. A single spin (*reference spin*) must be chosen, and the influence of the neighboring spins is taken into account by considering an effective field h_{eff}. The value of this field at a given temperature is obtained by imposing the consistency between the thermal average value of the reference spin and the applied effective field ($h_{\text{eff}}=\langle s\rangle$). The generalization of this approach to larger systems is straightforward. Instead of a single spin one can select a collection of spins and replace the interactions with the

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spins outside the system by an effective field. There are several alternatives to choose the reference spins: a single spin, the whole system or any set of spins inside the system. In general, if Λ_0 is the set of n_0 reference spins, the value of the effective field is obtained from the following self-consistent condition:

$$\langle \sigma_0 \rangle = \frac{1}{n_0} \sum_{s_i \in \Lambda_0} \langle s_i \rangle = h_{\text{eff}}. \tag{1}$$

The Bethe approximation [11] handles more correctly the local fluctuations and represents an improvement of the previous scheme. The minimal system consists of one spin (reference spin) and all its first neighbors at the boundary of the system (*test spins*), and the effective field that replace the missing bonds of the boundary spins is tuned to give the same mean value for the reference and test spins. For larger systems not all the spins at the boundary are equivalent, and their mean values must be averaged to obtain the effective field from a self-consistent equation.

Nevertheless, there is no reason to choose the test spins at the boundary of the system; they can be selected from any region of the system and the choice of the boundary spins may not be the best alternative, as we will see in the next section. As in the generalization of the Weiss approximation above, there is no restriction to choose the reference spins. Thus, if Λ_0 is the set of n_0 reference spins and Λ corresponds to n test spins, the self-consistent equation to be solved can be expressed as

$$\langle \sigma_0 \rangle = \frac{1}{n_0} \sum_{s_i \in \Lambda_0} \langle s_i \rangle = \frac{1}{n} \sum_{s_i \in \Lambda} \langle s_i \rangle = \langle \sigma \rangle. \tag{2}$$

Both methods provide a certain level of uniformity for the average values of the spins over the whole system but due to the missing bonds of the boundary, correlations ($\langle \gamma \rangle = \langle s_i s_j \rangle$) between adjacent spins are very different for spins at the central region of the system and those that are close to the boundary. A much more homogeneous distribution of the correlations can be achieved if, following the spirit of the mean-field approach, an effective coupling term of the form:

$$H_K = -K \sum_{\langle i,j \rangle \in \Lambda_B} s_i s_j \tag{3}$$

is added between pairs of nearest neighbors at the boundary of the system (Λ_B).

The value of the effective coupling can be obtained again from a self-consistent equation that relates m_0 reference correlations ($\gamma \in \Omega_0$) and m test correlations ($\gamma \in \Omega$) for different sets of spins:

$$\langle \Gamma_0 \rangle = \frac{1}{m_0} \sum_{\gamma_i \in \Omega_0} \langle \gamma_i \rangle = \frac{1}{m} \sum_{\gamma_i \in \Omega} \langle \gamma_i \rangle = \langle \Gamma \rangle. \tag{4}$$

Under the conditions of Eqs. (2) and (4) the statistical behavior of a finite collection of spins should resemble more the infinite periodic system under study, and although there are some exceptions [12], for closed form approximations [13] the general trend is that increasing the system size results in an improvement of the estimation of the critical temperature.

One of the advantages of the mean-field approaches is that an estimation of the transition temperature can be directly obtained as the solution of nonlinear equations. The Hamiltonian of a collection of Ising spins in an external field h can be written in mean-field (Weiss) approximation as [6,7]

$$H = H_0 - hS - h_{\text{eff}}\Sigma,$$

with

$$H_0 = -J \sum_{\langle i,j \rangle} s_i s_j,$$

$$S = \sum_i s_i,$$

and

$$\Sigma = \sum_{i \in \Lambda_B} z_i s_i,$$

where z_i is the number of missing bonds of the s_i spin at the boundary. For a small applied field h the mean value of a spin may be expressed as

$$\langle s_i \rangle \approx \langle s_i \rangle_0 + \beta h(\langle s_i S \rangle_0 - \langle s_i \rangle_0 \langle S \rangle_0) + \beta h_{\text{eff}}(\langle s_i \Sigma \rangle_0 - \langle s_i \rangle_0 \langle \Sigma \rangle_0),$$

where the symbol $\langle\ \rangle_0$ represents the average value calculated with H_0. At the critical temperature T_c, $\langle s_i \rangle_0 = 0$, and close to the critical point we have

$$\langle s_i \rangle \approx \beta(h\langle s_i S \rangle_0 + h_{\text{eff}} \langle s_i \Sigma \rangle_0).$$

According to the Weiss approach, the average mean value of the reference spins must be equal to the effective field [Eq. (1)]:

$$\langle \sigma_0 \rangle \approx \beta(h\langle \sigma_0 S \rangle_0 + h_{\text{eff}} \langle \sigma_0 \Sigma \rangle_0) = h_{\text{eff}}, \tag{5}$$

and at the transition temperature the susceptibility must show a divergence:

$$\frac{dh_{\text{eff}}}{dh} = \frac{\beta_c \langle \sigma_0 S \rangle_0}{1 - \beta_c \langle \sigma_0 \Sigma \rangle_0} = \infty.$$

Thus, the critical temperature can be obtained from the following equation:

$$\beta_c = \frac{1}{\langle \sigma_0 \Sigma \rangle_0}. \tag{6}$$

For the Bethe-like approximation the constraint of Eq. (5) is replaced by imposing the same mean value on the reference and test spins [Eq. (2)]:

$$h\langle (\sigma_0 - \sigma) S \rangle_0 + h_{\text{eff}} \langle (\sigma_0 - \sigma) \Sigma \rangle_0 = 0, \tag{7}$$

and the singularity of the susceptibility at the critical point gives the relation to obtain the critical temperature:

$$\langle (\sigma_0 - \sigma) \Sigma \rangle_0 = 0. \tag{8}$$

As stated above, the inclusion of self-consistencies among correlations at different regions of the system can be

achieved by adding effective couplings between nearest neighbors at the boundary [Eq. (3)], and the Hamiltonian of the system becomes

$$H = H^* - hS - h_{\text{eff}}\Sigma,$$

with

$$H^* = H_0 + H_K = -J\sum_{\langle i,j\rangle} s_i s_j - K \sum_{\langle i,j\rangle \in \Lambda_B} s_i s_j.$$

In this case, the statistical averages must be performed with respect to $H^*=H_0+H_K$. The critical temperature and the effective coupling can be obtained by solving a system of two nonlinear self-consistent equations analogous to Eqs. (4) and (8) [7]:

$$\langle(\sigma_0 - \sigma)\Sigma\rangle^* = 0, \tag{9a}$$

$$\langle\Gamma_0\rangle^* - \langle\Gamma\rangle^* = 0, \tag{9b}$$

where $\langle\ \rangle^*$ represents the average value calculated with H^*. The first equation gives the condition for the divergence of the susceptibility at the critical point and the second one improves the homogeneity of the correlations at different regions of the system.

III. PRELIMINARY CALCULATIONS WITH SMALL SYSTEMS

We have done an initial test to compare the efficiency of the different schemes using a small system of 6×6 spins. The nonlinear equations have been solved using the MATHEMATICA software, which gives any desired accuracy for such a small sets of spins. The test and reference spins and correlations can be chosen almost arbitrarily at any region of the system. Obviously, the influence of the missing bonds is much stronger at the boundary of the system than at the central region, and the statistical behavior of the internal spins should resemble more faithfully the real behavior of a spin embedded in an infinite periodic system. In consequence, we have chosen the reference spins and reference correlations at the center of the system, as shown schematically in Fig. 1. The critical temperatures given in Table I have been calculated according to three different schemes of self-consistency: the Weiss (W) approximation [Eq. (6)], the standard Bethe (B) approximation for different test spins [Eq. (8)] and the Bethe approximation with constraints that include correlations (C) for different sets of test spins and test correlations [Eq. (9)] as explained in Fig. 1.

As can be seen in Table I the Weiss approximation gives a modest estimation of the critical temperature for such a small sizes as compared with the Bethe approximation that can reach a relative error of 9–10 % when the test spins that are not located at the boundary of the system. The improvement due to the inclusion of the self-consistency in the C between adjacent spins is remarkable, the overestimation of the transition temperature is lowered by a factor of two approximately with respect to the Bethe approximation. The best results (C-3c and C-5e) correspond to the test spins and correlations that are closest to the symmetry axes shown in Fig. 1.

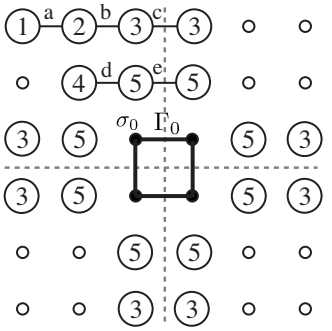

FIG. 1. Test and reference spins and correlations for a system with 6×6 spins. σ_0 and Γ_0 are the reference spin and correlation close to the center of the system. The rest of labels corresponds to test spins (numbers) and test correlations (letters). Except for the three and five spins, we have only drawn a single representative of all the symmetry equivalent test spins and test correlations. The dashed lines are the symmetry axes perpendicular to the boundaries.

IV. SOLVING THE SELF-CONSISTENT EQUATIONS BY MONTE CARLO SIMULATIONS

Larger systems cannot be solved using any analytical method, but all the magnitudes and derivatives required to find a solution to the constraint equations can be expressed in terms of statistical averages. Therefore, the self-consistency constraints can be solved by combining Monte Carlo simulations and an algorithm to solve systems of nonlinear equations—the Newton-Raphson method in this work. The derivatives of the nonlinear equations with respect to $\beta = 1/k_B T$ and K (effective coupling between spins at the boundary) that must be obtained to solve the self-consistent Eqs. (9) can be expressed in terms of statistical averages that

TABLE I. Transition temperatures for the combinations of Fig. 1. In the first column W stands for the Weiss approximation, B for the Bethe approximations, and C for the present method that incorporates constraints in the correlations. Figure 1 shows the labels of the test spins and correlations. For instance, C-2b indicates that spin 2 and correlation "b" (between spins 2 and 3) have been used respectively as test spin and test correlation in the self-consistent equations. The third column corresponds to the percentage of overestimation in the transition temperatures with respect to the exact value $k_B T_c^*/J \approx 2.2692$ [14].

6×6	$k_B T_c/J$	$T_c - T_c^*/T_c^* \times 100$
W	2.7953	23.2
B-1	2.5188	11.0
B-2	2.5011	10.2
B-3	2.4994	10.1
B-4	2.4751	9.1
B-5	2.4688	8.8
C-1a	2.4964	10.0
C-2b	2.4296	7.1
C-3c	2.3853	5.1
C-4d	2.4131	6.3
C-5e	2.3765	4.7

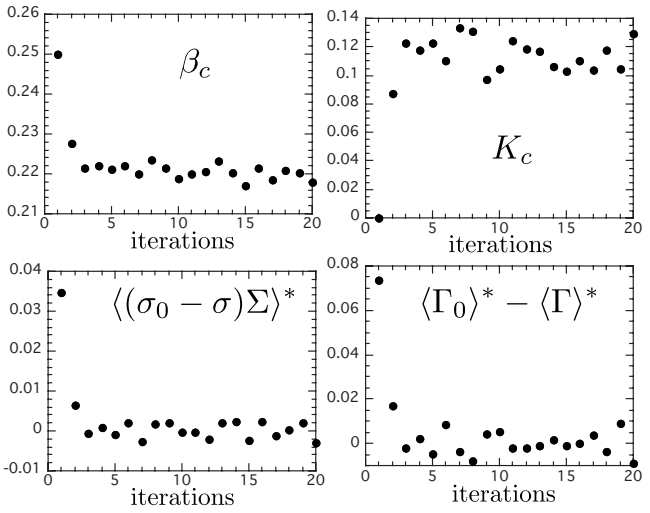

FIG. 2. Evolution of the convergence of the critical temperature (β_c), effective coupling (K_c), and the values of $\langle f_1\rangle=\langle(\sigma_0-\sigma)\Sigma\rangle^*$ and $\langle f_2\rangle=\langle\Gamma_0\rangle^*-\langle\Gamma\rangle^*$ during 20 iteration of the Newton-Raphson algorithm. The size of the system is $6\times6\times6$ and for each iteration 10^5 Monte Carlo steps have been performed.

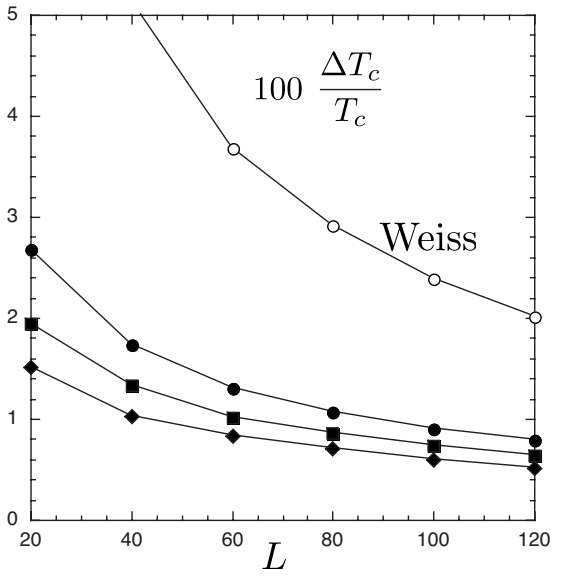

FIG. 3. Percentage of the overestimation in the transition temperatures with respect to the exact value $k_BT^*/J\approx2.2692$ [14] for several two-dimensional square systems and different approximation schemes: Weiss (open circles) and the present method for depth 0 (closed circles), depth 1 (squares), and depth 2 (diamonds).

are available during a standard Monte Carlo run. If $f_1=(\sigma_0-\sigma)\Sigma$ and $f_2=\Gamma_0-\Gamma$ we have for $i=1,2$:

$$\frac{\partial\langle f_i\rangle^*}{\partial\beta}=\langle H^*\rangle^*\langle f_i\rangle^*-\langle H^*f_i\rangle^*, \tag{10a}$$

$$\frac{\partial\langle f_i\rangle^*}{\partial K}=\frac{\beta}{K}\langle H_K\rangle^*\langle f_i\rangle^*-\langle H_Kf_i\rangle^*. \tag{10b}$$

The main drawback of the Monte Carlo method is the uncertainty associated to the estimation of the statistical magnitudes. The derivatives of Eq. (10) correspond to correlations among four spins and their accuracy must be well controlled in order to obtain a minimal convergence of the Newton-Raphson method. When the errors are small enough, the application of successive iterations gives a series of values of β and K that are scattered around the solution and can be used to obtain an estimation of the critical temperature and its standard error. Figure 2 shows the typical evolution of the first 20 iterations of the Newton-Raphson procedure. For each iteration a Monte Carlo simulation with 10^5 steps have been performed. The convergence is achieved after three iterations and the rest of the points may be used to estimate the desired statistical properties. However, a minimum accuracy in the estimation of the derivatives is needed; for this system we have found that for Monte Carlo simulations with less that 10^4 steps the method fails to converge.

In consequence, during a sequence of Monte Carlo simulations two goals are achieved, the nonlinear equations [Eq. (9)] are solved approximately and the physical quantities of interest are calculated as in standard Monte Carlo runs.

V. RESULTS

We have applied the method to several square and cubic systems of dimension L^d for $d=2,3$ and even L. This systems are analogous to the previously studied 6×6 case. The value of the reference spin is obtained from the average of four (or eight in three dimensions) symmetry-equivalent spins at the center of the system as in Fig. 1. For the test spins, we have considered three sets of average values and correlations. The first set (depth 0) corresponds to the eight (24 in three dimensions) equivalent spins at the center of the sides (faces) in the boundary of the system and the four (24 in three dimensions) correlations between first neighbors. Figure 1 can be used to illustrate the two dimensional case; the eight test spins are the analogous in a larger system of the sites labeled by "3," and the four test correlations are calculated between the pairs 3–3 of adjacent spins ("c" correlations). The second set (depth 1) is composed by a similar choice, but one lattice spacing deeper into the system. In Fig. 1 they correspond to the eight spins labeled by "5" and the four correlations of type "e." The third set (depth 2) is similar to the previous ones as we go one lattice spacing deeper into the system and it cannot be defined in Fig. 1 due to the small size of the system shown.

Transition temperatures and effective couplings have been obtained by solving the Eq. (9) by the combination of Monte Carlo calculation and the Newton-Raphson algorithm, and the discrepancies in the estimation of the critical temperature are shown in Figs. 3 and 4 for two and three-dimensional cases, respectively. As in the test with small systems, increasing the depth of the test spins and correlations gives more accurate estimations of the transition temperatures. For the two-dimensional system it is enough to set $L=60$ (depth 2) to obtain a relative error close to 1%. The results of the three-dimensional cases are even more remarkable: for $L=6$ the relative error is less than 1% and the estimation of the critical temperature is much better than the obtained with the Weiss approximation ($\sim$6%) for the same system size (out of the scale of Fig. 4).

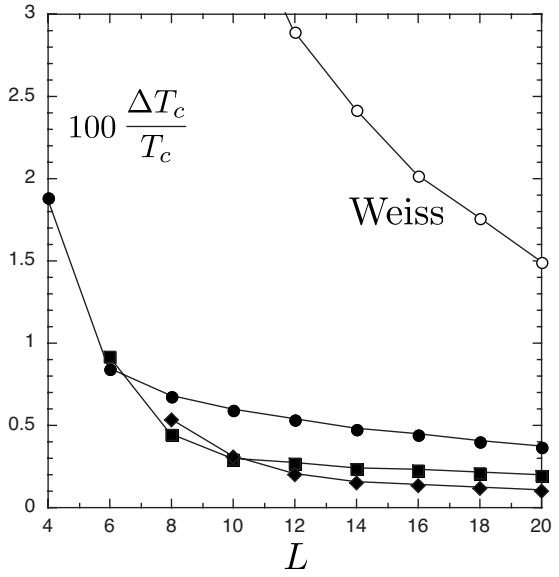

FIG. 4. Percentage of the overestimation in the transition temperatures with respect to the very accurate value $k_B T^*/J \approx 4.5115$ [15] for several three-dimensional cubic systems and approximations: Weiss (open circles) and the present method for depth 0 (closed circles), depth 1 (squares), and depth 2 (diamonds).

By choosing the test spins closer to the center of the system (increasing the depth) the estimation of the transition temperatures is better, but it must be mentioned that this improvement entails a decrease in the precision in the calculation of the derivatives and a larger number of Monte Carlo steps must be performed to have a good convergence toward the solution of the self-consistent equations.

Figure 5 points up the advantages of the inclusion of the self-consistency in the correlations to estimate the evolution of the magnetization with temperature close to the critical point. The absolute value of the order parameter obtained by

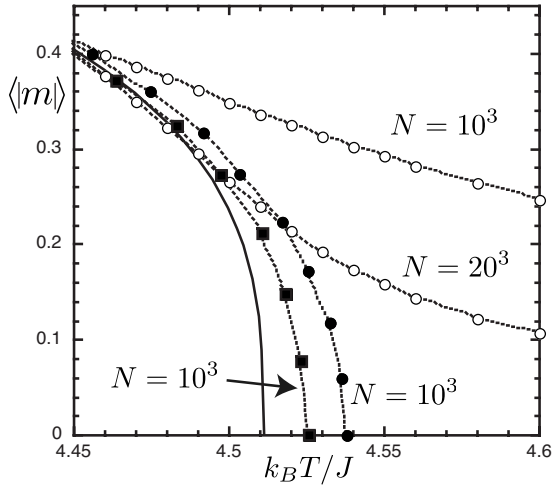

FIG. 5. Evolution of the absolute value of the magnetization with the temperature for different three-dimensional system sizes calculated by standard Monte Carlo simulations with periodic boundary conditions (open circles), the present method with depth 0 (closed circles), and depth 1 (squares) and the very accurate results (solid line) of Ref. [15].

TABLE II. Estimation of the critical temperatures and critical exponents of the susceptibility calculated by applying CAM theory to a sequence of different system sizes for the two- and three-dimensional Ising models.

	2D		3D	
	T_c	γ	T_c	γ
Depth 0	2.266(1)	1.820(3)	4.5226(7)	1.166(1)
Depth 1	2.267(2)	1.804(4)	4.517(1)	1.142(2)

standard Monte Carlo simulations with periodic boundary conditions is also shown for comparison. The behavior of the simulations with constrained mean values and correlations is much closer to the exact behavior of the Ising model even for smaller system sizes, the rounding effect due to the finite size of the system is not present and the transition temperature can be located easily, showing that close to a phase transition the present method gives a better estimation of nonuniversal magnitudes than the periodic boundary conditions.

As the method involves a mean-field approximation, the critical exponents are not correct, but, in principle, CAM theory [6] can be used to obtain accurate estimations of them. Close to the critical temperature $T_c^{(L)}$ the susceptibility for a system of size L has the form

$$\chi_L \sim \bar{\chi}_L \frac{T_c^{(L)}}{T - T_c^{(L)}},$$

where $\bar{\chi}_L$ is the critical coefficient. If the series are well behaved, for a sequence of different sizes, the critical coefficient has a singularity:

$$\bar{\chi}_L \sim \frac{1}{(T_c^{(L)} - T_c^*)^{\varphi}}, \tag{11}$$

where T_c^* is the exact critical temperature. The critical exponent of the susceptibility can be obtained by $\gamma = 1 + \varphi$.

Following Ref. [7], we have obtained the critical coefficients of the susceptibility ($\bar{\chi}$) for the system sizes represented in Figs. 3 and 4 and fitted the values according to Eq. (11) to extract an estimation of the critical temperature and critical exponent of the susceptibility for the two- and three-dimensional Ising systems. As can be seen in Table II, the transition temperatures are quite accurate but the estimation of the γ exponent obtained from convergence of the series constructed with the present method are not satisfactory. Additional simulations with larger systems combined with an FSS analysis of the data should give a more reliable evaluation of the potentiality of the method to estimate more accurately transition temperatures and critical exponents.

VI. CONCLUSIONS

The application of self-consistent constraints to correlations between nearest neighbors improves the estimation of

nonuniversal magnitudes (transition temperatures and behavior of the order parameter) in small systems in comparison with standard periodic boundary conditions. The procedure involves a Monte Carlo simulation to perform two tasks simultaneously: the self-consistent equations are solved to obtain the parameters of the mean-field Hamiltonian (an effective field and an effective coupling) and statistics are acquired such as in a standard Monte Carlo run. The method opens the possibility of obtaining reliable estimations of transition temperatures and other non universal quantities by performing inexpensive simulations with systems of small size. However the estimation of critical exponents seems to be out of the scope of the method in comparison with more powerful techniques such as series expansions, Monte Carlo renormalization group, or finite-size scaling.

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