Cluster-algorithm renormalization-group study of universal fluctuations in the two-dimensional Ising model

G. Palma* and D. Zambrano
Departamento de Física, Universidad de Santiago de Chile, Casilla 307, Santiago 2, Chile
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In this paper we propose a method to study critical systems numerically, which combines collective-mode algorithms and renormalization group on the lattice. This method is an improved version of the Monte Carlo renormalization group in the sense that it has all the advantages of cluster algorithms. As an application we considered the 2D Ising model and studied whether scale invariance or universality are possible underlying mechanisms responsible for the approximate "universal fluctuations" close to a so-called bulk temperature $T^*(L)$. "Universal fluctuations" were first proposed in the work of Bramwell, Holdsworth, and Pinton [Nature (London) **396**, 552 (1998)] and stated that the probability density function of a global quantity for very dissimilar systems, such as a confined turbulent flow and a two-dimensional (2D) magnetic system, properly normalized to the first two moments, becomes similar to the "universal distribution," originally obtained for magnetization in the 2D *XY* model in the low-temperature region. The results for the critical exponents and the renormalization-group flow of the probability density function are very accurate and show no evidence to support that the approximate common shape of the PDF should be related to both scale invariance or universal behavior.

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I. INTRODUCTION

Critical phenomena are present in a large number of quite different physical systems: superfluid He-3, low-temperature superconductors, ferromagnetic-paramagnetic systems, turbulent fluids, plasmas, polymers, among many others. Nevertheless, an important common feature of these systems is the scale independent fluctuations at the critical temperature: although the underlying intermolecular forces, responsible for the existence of phase transitions, have a well-defined length scale, the structures they give rise to do not. This leads, very close to the critical temperature (scaling region), to a power-law behavior of the physical quantities, which is a fundamental feature of universality [1].

The main challenge of the theory of critical phenomena is to explain how dissimilar systems exhibit the same critical behavior. Renormalization-group (RG) theory developed by Wilson and Kogut [2] provides a consistent framework to understand the existence of equivalence classes of critical systems. On the lattice, a very cunning method of applying a RG analysis to Monte Carlo simulations of general systems was first proposed in Ref. [3].

Nevertheless, the numerical simulation of critical systems has a serious limitation due to the critical slowing down effect. Indeed, as a critical system approaches the critical temperature, the decorrelation time diverges with the power of the correlation length of the system ξ to the dynamical critical exponent z: $\tau \sim \xi^z$, where z is approximately 2 for local-flip algorithms such as the Metropolis algorithm. In order to beat or at least reduce this effect, a cluster algorithm was first developed in Ref. [4].

In this paper, we develop a self-consistent method along the line proposed by Swendsen in Ref. [3], which will be explained in Sec. II, to perform a lattice renormalization-group (RG) analysis of the probability density function (PDF) as a function of the magnetization, in the 2D Ising model. His proposal amounts to compute by a direct Monte Carlo simulation of the fundamental Hamiltonian, a sequence of approximations to the linearized RG matrix $T_{\alpha\beta^*}$. From its eigenvalues the critical exponents can be obtained in a direct way. In order to reduce critical slowing down, we used instead of a local (Metropolis-type) algorithm the collective-mode algorithm developed in Ref. [5] to simulate the fundamental Hamiltonian. We call this method the cluster algorithm renormalization group (CARG) [6].

Our physical motivation is to study, in the context of the 2D Ising model, whether scale invariance and universality are the underlying mechanism which could give rise to the approximate "universal curve." This phenomenon links a large class of dissimilar systems defined on different dimensions and including nonequilibrium systems, in which the PDF of a global quantity—such as the power consumption in a confined turbulent system or the magnetization in a finite ferromagnetic system—properly normalized to the first two moments, is described by a single curve [7]. This claim is not free of controversy and in the last years it has been the central task of several publications [8–15]. This "universal curve" was shown to correspond to the PDF of the 2D-*XY* model in the zero temperature limit [11].

The paper is organized as follows. In Sec. II the CARG method is explained for a general critical system. In the third section we explain the concept of approximate "universal fluctuations" of the PDF of the magnetization for the 2D Ising model. In Sec. IV the critical exponents ν and η are computed using fundamental lattices of lattice sizes $L=45$, 64, and 108, performing two and three RG steps, to check the accuracy of the method. It is shown that relative errors of the critical exponents increase monotonically with the departure from the critical temperature. Finally, the RG flow of the

*guillermo.palma@usach.cl

PDF itself is computed and it is shown that when conveniently normalized, it is invariant. The underlying reason for this invariance is discussed in connection with the so-called "generalized universality" conjecture. The results are discussed and conclusions are formulated in the last section.

II. THE CARG METHOD

To describe the method, we first introduce the notation. We consider a model defined in a square lattice of lattice spacing a, and linear size L, with periodic boundary conditions (PBCs). The spin variables σ_i are defined on each site i of the lattice and the Hamiltonian has the form

$$H = \sum_{\alpha} K_{\alpha} S_{\alpha}, \tag{1}$$

where each S_α is some kind of combination of the spin variables, with the only requirement of translation invariance subject to PBCs. For our study we will consider the 2D Ising model, including up to three even interactions (nearest neighbor, second neighbor, and four spin) and one odd interaction (a weak magnetic field).

The aim of RG theory is to study the critical properties of a model. The critical exponents, for example, can be obtained from the linearized RG transformation matrix $T_{\alpha\beta^*}$, defined in Eq. (8), by computing its eigenvalues. $T_{\alpha\beta^*}$ can be obtained numerically from the coupled equations

$$\frac{\partial \langle S_\gamma^{(n)} \rangle}{\partial K_\beta^{(n-1)}} = \sum_{\alpha} \frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(n-1)}} \frac{\partial \langle S_\gamma^{(n)} \rangle}{\partial K_\alpha^{(n)}}. \tag{2}$$

Here, the superindices $(n-1)$ and (n) denote the original and the renormalized quantity, respectively, after one RG transformation, and the thermal average $\langle F(\phi) \rangle$ is defined by the usual formula

$$\langle F(\sigma) \rangle = \frac{1}{Z} \sum_{\{\sigma\}} F(\sigma) \exp[-H(\sigma)]. \tag{3}$$

The left and right quantities appearing in Eq. (2) can be obtained through the identities

$$\frac{\partial \langle S_\gamma^{(n)} \rangle}{\partial K_\beta^{(n-1)}} = -\langle S_\gamma^{(n)} S_\beta^{(n-1)} \rangle + \langle S_\gamma^{(n)} \rangle \langle S_\beta^{(n-1)} \rangle, \tag{4}$$

$$\frac{\partial \langle S_\gamma^{(n)} \rangle}{\partial K_\alpha^{(n)}} = -\langle S_\gamma^{(n)} S_\alpha^{(n)} \rangle + \langle S_\gamma^{(n)} \rangle \langle S_\alpha^{(n)} \rangle. \tag{5}$$

Due to the definition of the renormalized Hamiltonian, the thermal expectation of any function F of the variables $\sigma^{(n)}$ yield the same value, whether one evaluates it using $H^{(n)}$ or $H^{(n-1)}$, i.e.,

$$\frac{1}{Z^{(n)}} \sum_{\{\sigma^{(n)}\}} F(\sigma^{(n)}) e^{-H^{(n)}(\sigma^{(n)})} = \frac{1}{Z^{(n-1)}} \sum_{\{\sigma^{(n-1)}\}} F(\sigma^{(n-1)}) e^{-H^{(n-1)}(\sigma^{(n-1)})}. \tag{6}$$

Therefore, the quantities appearing in Eqs. (4) and (5) can be computed directly by a numerical simulation of the original Hamiltonian on the fundamental lattice. Because the simulations must be performed close to the critical point of the system, the configurations produced by a local-update algorithm are not statistically independent, which leads to inaccurate thermal averages. This phenomenon is called in the literature critical slowing down [1]. In order to avoid this effect we use the collective-mode algorithm developed by Wolff [5] for the Ising model.

The expectation values appearing in Eqs. (4) and (5) should be computed by using a simulation with a cluster algorithm on the fundamental lattice. These numerical values inserted into Eq. (2) lead to coupled algebraic equations, which allow one to obtain a sequence of approximations to the linearized RG transformation $T_{\alpha\beta^*}$, as the renormalization transformation is iterated to the fixed point Hamiltonian H^*, defined in the vicinity of the fixed point by

$$K_\alpha^{(n+1)} - K_{\alpha^*} = \sum_{\beta} T_{\alpha\beta^*} (K_\beta^{(n)} - K_{\beta^*}), \tag{7}$$

where the linearized RG transformation is defined by

$$T_{\alpha\beta^*} = \left[\frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(n-1)}} \right]_{H^*}. \tag{8}$$

To evaluate $T_{\alpha\beta^*}$ one in principle needs a "linear region" close to the critical temperature, where its derivatives are essentially constant. This region can be found by using FSS analysis of the lattice shifted critical temperature [6], and in the case of the 2D Ising model, by using the binder cumulant (see Sec. IV).

Finally, the critical exponents are obtained from the eigenvalues of $T_{\alpha\beta^*}$ from Eq. (8) in the standard way. For the 2D Ising model they are given by the fundamental relations $\nu = \ln s / \ln \lambda_1^e$ and $\eta = d + 2 - 2 \ln \lambda_1^o / \ln b$, where $\lambda_1^{e(o)}$ is the largest even (odd) eigenvalue.

III. UNIVERSAL FLUCTUATIONS IN THE 2D ISING MODEL

The two-dimensional Ising model is well known and it is defined by the Hamiltonian

$$H(\sigma) = \frac{J}{k_B T} \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{9}$$

where σ_i is the spin variable defined on the lattice site i, $J > 0$ is the ferromagnetic constant, k_B is the Boltzmann's constant, and $\Sigma_{\langle i,j \rangle}$ stands for sum over nearest neighbors $\langle i,j \rangle$. We use a system of units where Boltzmann's constant is set equal to unity throughout the paper and identify T with the reduced temperature T/J. It is well known that for an infinite square lattice $(L \to \infty)$, this model has a second order phase transition at the critical temperature T_c defined by $\sinh(1/T_c) = 1$ or, equivalently, $T_c = 2/\ln[1 + \sqrt{(2)}]$, which was first computed by Onsager [16].

Universality of rare fluctuations in turbulence and critical phenomena, as it was first proposed in Ref. [17], linked two quite different physical systems: a confined turbulent flow and the finite volume 2D XY model in the low temperature

regime. The (generalized) universality of both systems was based on the collapse of the probability distribution functions of the corresponding global quantities, the power consumption in the turbulent experiment and the magnetization in the critical system. The PDFs were conveniently normalized to their first two moments, and fell onto a common curve, which was called "universal fluctuations."

A further generalization of the phenomenon described above was performed in Ref. [7], including nonequilibrium models such as the autoigniting forest fire model and the Bak-Tang-Wiesenfeld sandpile model, and the equilibrium 2D Ising model at temperature $T^*(L)$, which they called "bulk temperature."

Nevertheless, using the 2D and 3D Ising model Zheng *et al.* [8] showed a dependence of the "universal fluctuations" on the equivalence class of the model. In a high precision MC simulation of the finite volume 2D *XY* model, a slight but systematic dependence of the "universal fluctuations" on the system temperature was first suggested [9]. This claim was proved analytically in Ref. [11]. Moreover, by computing the skewness and the kurtosis in the harmonic 2D *XY* model (the second and third moments of the PDF) the temperature dependence of the PDF was confirmed numerically and analytically in Refs. [12,13], respectively.

The precise physical definition of $T^*(L)$ is still in progress. In more recent papers, $T^*(L)$ has been linked to intermittency of the magnetization [14].

To address this issue we used the CARG method described in the above section and we have simulated the 2D Ising model in square lattices of sizes $L=45$, 64, and 108, with periodic boundary conditions, in a range of temperatures within the bulk $T^*(L)$ and the lattice shifted critical temperature $T_c(L)$ which can be defined, for example, as the temperature at which the magnetic susceptibility has a peak.

IV. NUMERICAL RESULTS

As it was mentioned in Sec. II, an estimation for the critical temperature for the 2D Ising model can be obtained by using the binder cumulant [18]

$$u(L,T) = 1 - \frac{1}{3}\frac{\langle M^4\rangle}{\langle M^2\rangle^2}. \tag{10}$$

where $\langle M\rangle$ is the averaged magnetization. It follows that $u(L,T)$ depends on the system size and temperature through the ratio of the averaged fourth power to the averaged square

TABLE I. The critical exponents obtained by the CARG method (PZ) and by Swendsen's method (S) for $L=45$ are displayed.

RG step	λ_1^e	λ_1^o	ν	η
1_S	2.887	7.712	1.036	0.2812
1_{PZ}	2.8900	7.7408	1.0352	0.2744
2_S	3.006	7.835	0.998	0.2524
2_{PZ}	3.0083	7.8508	0.9975	0.2487
Exact	3	7.8452	1	0.250

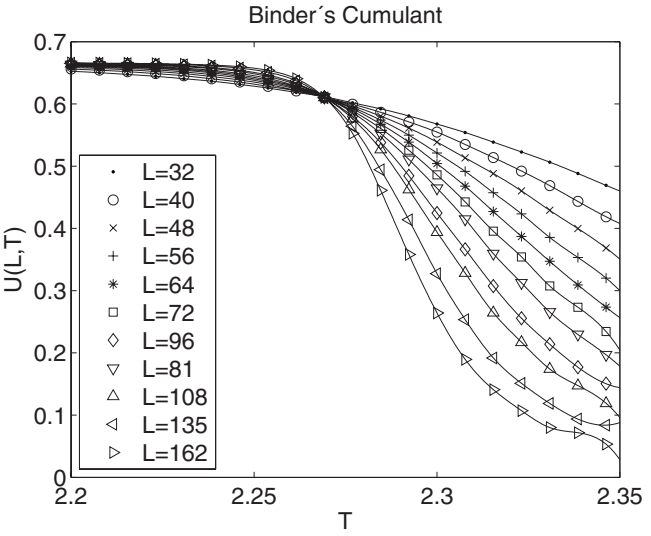

FIG. 1. The binder cumulant is shown for different lattice sizes. From their interception the critical temperature for infinite volume $T_c(\infty)=2.26903\pm0.00059$ is obtained. It differs in 0.7 per one thousand from Onsager's exact result.

of the magnetization. Nevertheless, from finite size scaling analysis, close to the critical temperature it is independent of the lattice size and, therefore, the curves representing the binder cumulant corresponding to different lattice sizes must collapse onto one point. This behavior is displayed in Fig. 1. The value obtained agrees with Onsager's critical temperature within an error of 0.7 per one thousand.

Now we use the CARG method to compute the critical exponents ν and η, associated to the Ising model. In order to compare with the results obtained in Ref. [3], we use a square lattice of size $L=45$ to compute the quantities appearing in the RG equations (4) and (5) close to the critical temperature, obtained as explained above, and perform two RG steps. Using the Wolff algorithm [5], 10^5 sweeps were used to thermalize the system and 10^6 configurations were used to compute thermal averages.

For the RG analysis up to three even interactions (nearest neighbor, second neighbor, and four spin or plaquette) and one odd interaction (magnetic field) were considered. In order to compare our results with the corresponding ones obtained by Ref. [3], we display in Table I the results of a lattice of size $L=45$, where the scale factor $b=3$ was used. After two RG steps, the values compare quite well. Compared to their exact values of the infinite volume limit, they agree up to 0.25% for ν and 0.52% for η.

In Table II we display the results for the critical exponents ν and η, for a lattice of lattice size $L=64$. The scale factor $b=2$ was used. The results are even better than with the

TABLE II. Critical exponents for $L=64$ and $T=2.259$.

RG step	λ_1^e	λ_1^o	ν	η
1	1.9586	3.6856	1.0311	0.2362
2	1.9986	3.6676	1.0010	0.2503
Exact	2	3.6680	1	0.250

TABLE III. The critical exponents obtained by the CARG method (PZ) and those obtained by Swendsen [19] for $L=108$.

RG step	λ_1^e	λ_1^o	ν	η
1_S	2.852	7.705	1.048	0.2828
1_{PZ}	2.8635	7.7062	1.0443	0.2825
2_S	3.021	7.828	0.994	0.2540
2_{PZ}	3.0027	7.8269	0.9992	0.2542
3_S	3.007	7.831	0.998	0.2534
3_{PZ}	3.0013	7.8361	0.9996	0.2521
Exact	3	7.8452	1	0.250

smaller lattice, with errors of order less than 0.13%. The reason for this behavior is physically intuitive: An important feature of the RG method is that the smallest system considered should be still large compared to the range of the fixed-point Hamiltonian, so that any significant truncation should be avoided. The validity of this requirement is improved with the larger lattice sizes.

In spite of the good accuracy obtained for the critical exponents performing only two RG steps, we iterated the RG transformations to three RG steps in order to compare our results with the ones obtained in Ref. [19]. The comparison is displayed in Table III. Both methods achieve a remarkable accuracy, compared to the exact results. The main difference is related to the computational time needed to obtained these values.

In order to compare both methods, we have measured the computational time needed to obtain the critical exponents η and ν first by using the Metropolis algorithm with a decorrelation of five sweeps, and second by using the Wolff's algorithm without decorrelation. We used different lattice sizes including $L=64$ and 162. In both cases 10^3 sweeps were used to thermalize the system and 10^4 configurations were used to compute thermal averages. When the ratio of the computational time using the Metropolis algorithm to the corresponding one by using the Wolff's algorithm is measured, it turned out that the CARG method is faster than Swendsen's method by a factor which increases monotonically with the lattice size, from six for $L=64$ until ten for $L=162$.

We want now to address the question of whether the model displays or not a critical behavior at the bulk temperature $T^*(L)$, which would lead to scale invariance of the system. By definition, at $T^*(L)$ the PDF of the magnetization has a similar form to the distribution originally obtained for the magnetization in the 2D XY model in the zero-temperature limit [11]. The scale invariance is usually expressed as a power law behavior of the physical quantities involved and therefore we use the CARG method to look for critical exponents in the whole inertial range $[T^*(L), T_c(L)]$ [8].

In Ref. [14], $T^*(L)$ was defined as the temperature for which the skewness (the third normalized moment of the PDF of the magnetization) is equal to that for the 2D XY model in the low-temperature region. According to this definition, and for a lattice of lattice size $L=64$ the numerical value $T^*(L)=2.11$ was found. In this article it was argued that at $T^*(L)$ there are (strong) correlations on all scales up to a length of the order of the system size L, which is an important feature of critical behavior. Furthermore, the fluctuations of the magnetization were linked to intermittency. To address this issue we have simulated a lattice with $L=64$ as well.

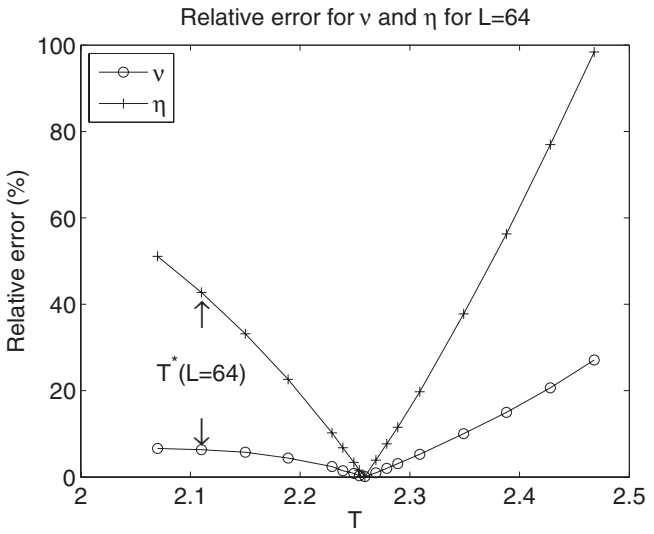

FIG. 2. Relative errors for the critical exponents η and ν obtained in the second renormalization step with lattice size $L=64$ and $NAV=10^6$. The minimum error occurs at $T_c(64)=2.259$ and the critical exponents for this temperature are shown in Table II.

In Fig. 2, the relative errors between the exact values of the infinite volume critical exponents ν and η and the corresponding numerical result are displayed as a function of the system temperature. They are expressed in percents and from this figure we conclude that the relative errors increase monotonically as the temperature moves away from $T_c(L)$, which includes the particular value $T^*(L)$, at which the relative errors are large. It is therefore rather unjustified to expect scale invariance of the physical quantities close to $T^*(L)$.

Now we study a possible scaling behavior of the order parameter—the magnetization—in the vicinity of both the bulk and the shifted critical temperatures $[T^*(L)$ and $T_c(L)]$, respectively. It is well known that the magnetization near the critical temperature behaves as a power law of the kind

$$\langle M \rangle \sim \tau^{\beta}, \tag{11}$$

where the reduced temperature τ is given by

$$\tau = \frac{|T - T_c(L)|}{T_c(L)} \tag{12}$$

and β is the critical exponent. A direct numerical computation of this exponent is rather subtle because of the reflection symmetry of the Hamiltonian (9), which leads in numerical simulations close to the phase transition to the use of the absolute value of the magnetization instead of the magnetization itself. One can instead compute β by using the scaling relation $\beta=\nu(d+\eta-2)/2$.

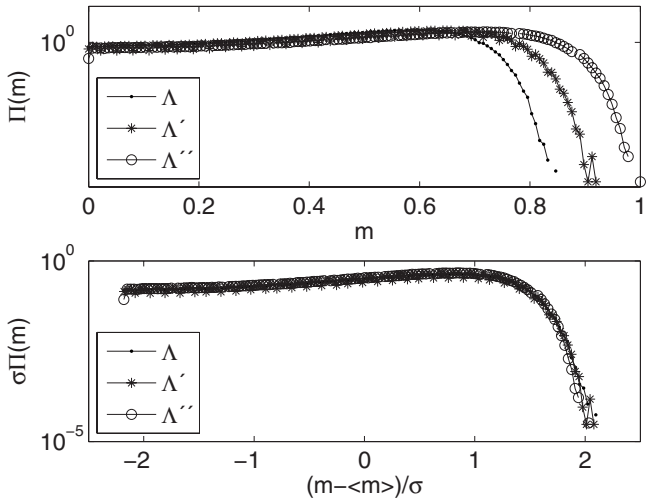

FIG. 3. PDFs (raw and normalized data) for the fundamental lattice ($L=64$) at temperature $T_c(L)=2.3008$ and for the two coarse grained lattices ($L=32$ and $L=16$).

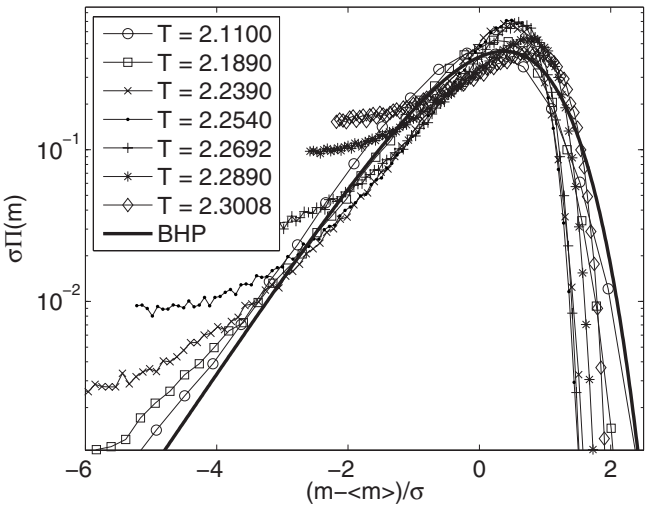

FIG. 4. The PDF is displayed for temperatures in the "inertial range" and for the lattice size $L=64$.

In Ref. [14] the stochastic evolution of the magnetization was computed and it was argued that the system displays "larger fluctuations" at $T^*(L)$ than at $T_c(L)$. This apparent phenomenon has been called "intermittency." Nevertheless, according to the discussion associated with Fig. 2, no underlying scale invariance is responsible for this phenomenon. This apparent behavior is rather related to the fact that, in order to avoid metastable states in numerical simulations, the observable used in MC simulations is the absolute value of the magnetization instead of the magnetization itself. This quantity is bounded from below and therefore at $T_c(L)$ its fluctuations appear suppressed by a factor of order 2 compared to the corresponding at $T^*(L)$, where this lower bound plays no role as the magnetization does not vanishes in its neighborhood.

RG flow of the probability density function. We proceed to study of the PDF by using the CARG method. In particular we have computed the RG flow of the PDF starting on a square lattice of size $L=64$, which we called fundamental lattice, and which we denote by Λ. We have performed two RG transformations. Two further lattices were defined with lattice sizes $L=32$ and 16, which are denoted by Λ' and Λ'', respectively. In Fig. 3 the PDF is displayed for the three lattices. It follows that, properly normalized to the first two moments, the PDF remains invariant along a renormalized trajectory, the see second graphic in Fig. 3. For the present computation we used Swendsen-Wang's cluster algorithm [4] to update the fundamental lattice. We used the block spin parameter $b=2$ and $T_c(L=64)=2.3008$ for the lattice shifted critical temperature.

The invariance of the PDF under RG transformations can be understood by observing that it can be written as a Fourier transform of a partition function of an auxiliary theory, which differs from the original theory by a dimension zero perturbation, with a very small imaginary coefficient. This was first pointed out in Ref. [11]. From the RG theory we know that partition functions are invariant under RG transformations.

Finally we plot in Fig. 4 the PDF in the whole "inertial range" of temperatures. The curves depend slightly on the temperature close to $T^*(L)$, but this particular value, as we have argued, is not related to scale invariance or power law behavior of the system. Moreover, different curves normalized to the first two moments are difficult to distinguish from one another, close to the maximum. This has been pointed out in Ref. [15], where the PDF at the particular value $T^*(L)$ was fitted by a Gumbel distribution, which plays an important role in statistics of extremes.

V. CONCLUSIONS

In this paper we have introduced a very accurate method, which we call the CARG method, to study critical systems close to a critical point. Compared to the original method proposed by Swendsen, our method is faster by a factor which grows linearly with the lattice size from 6 for $L=64$ until 10 for $L=162$, due to the use of cluster algorithms to simulate the fundamental Hamiltonian. This advantage allows us to simulate larger lattices in reasonable computational times, and to improve the accuracy of the results, as shown in Table III.

We illustrated the method by using the 2D Ising model defined in a square lattice of lattice size L, and we have shown how to obtain very accurate values for the critical exponents without the previous knowledge of the critical temperature. We used further the 2D Ising model to study scale invariance and universality as the underlying mechanism which could give rise to the approximate generalized universal behavior of fluctuations. We computed the probability density function (PDF) of the magnetization and its RG trajectory close to the lattice shifted critical temperature.

Critical behavior is associated with scale invariance, which is commonly represented as a power law behavior: the physical quantities are described close enough to a critical point, by critical exponents, which characterize the equivalence class the system belongs to. In the special case of the

2D Ising model, from Fig. 2 we conclude that, at the bulk temperature $T^*(L)$, neither scale invariance nor universal behavior is really present. Therefore the approximate collapse of the PDF onto the "universal distribution" seems not to be related to critical behavior but rather to a numerical phenomenon associated to approximated scaling relations and extreme statistics, as proposed in Ref. [15], and to the constraint character of the global quantity used to compute the PDF.

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