Improving the efficiency of Monte Carlo simulations of systems that undergo temperature-driven phase transitions

L. Velazquez\(^1\) and J.C. Castro-Palacio\(^2\)

\(^1\)Departamento de Física, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile.
\(^2\)Department of Chemistry, University of Basel, Klingelbergstr. 80, 4056 Basel, Switzerland

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Abstract

Recently, Velazquez and Curilef have proposed a methodology to extend Monte Carlo algorithms based on canonical ensemble, which is aimed to overcome slow sampling problems associated with temperature-driven discontinuous phase transitions. We show in this work that Monte Carlo algorithms extended with this methodology also exhibit a remarkable efficiency near a critical point. Our study is performed for the particular case of 2D four-state Potts model on the square lattice with periodic boundary conditions. This analysis reveals that the extended version of Metropolis importance sample is more efficient than the usual Swendsen-Wang and Wolff cluster algorithms. These results demonstrate the effectiveness of this methodology to improve the efficiency of Monte Carlo simulations of systems that undergo any type of temperature-driven phase transition.

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I. INTRODUCTION

Many different algorithms have been proposed to overcome slow sampling problems in large-scale Monte Carlo (MC) simulations. Most of them are based on two types of strategies: (1) the substitution of local MC moves by the so-called cluster MC methods \([1-10]\), and (2) the use of histograms to extract information from MC simulations combined with re-weighting techniques to improve the statistics, such as the multicanonical method and its variants \([11-12]\). Cluster MC methods are useful to overcome slow sampling problems associated with a continuous Phase Transition (PT). However, the application of nonlocal moves, by itself, does not help so much in the presence of a discontinuous PT. For such cases, the consideration of a re-weighting technique as the multicanonical method is more appropriate, which reduces the size dependence of the decorrelation time from exponential to a power-law behavior.

Not one of the above strategies seem to be sufficiently general to overcome any type sampling problems of MC simulations. The success of clusters MC algorithms is not universal because of the proper cluster moves seem to be highly dependent on the system. In fact, efficient cluster MC methods have only been found for a reduced number of models \([1-10]\). Multicanonical method and its variants have a general applicability. However, the efficiency of these algorithms is not so significant to justify their application to overcome slow sampling problems associated with continuous PTs \([14]\).

Recently, Velazquez and Curilef have introduced a different methodology to overcome slow sampling problems associated with a temperature-driven discontinuous PT \([16, 17]\). Their proposal is based on the general equilibrium situation associated with fluctuation relation \([18, 19]\),

\[
C = \beta^2 \langle \delta U^2 \rangle + C \langle \delta \beta \omega \delta U \rangle ,
\]

which generalizes canonical relation \([20, 21]\):

\[
C = \beta^2 \langle \delta U^2 \rangle
\]

between the heat capacity \(C\) and the energy fluctuations \(\delta U\). This relation describes the existence of a feedback perturbation of the environment during its thermodynamic interaction with the system. This mechanism is characterized by the correlation function \(\langle \delta \beta \omega \delta U \rangle\) between the system internal energy \(U\) and the environmental inverse temperature \(\beta_\omega = 1/T^\omega\). A relevant feature of fluctuation relation \([11]\) is its compatibility with the existence of negative heat capacities \(C < 0\) \([22-24]\).

The consideration of the above arguments in MC simulations enables a considerable reduction of the dependence of the decorrelation times on system size \(N\), from exponential \(\tau(N) \propto \exp(\gamma N)\) to a very weak power-law behavior \(\tau(N) \propto N^\alpha\) \([30]\). For example, dynamic critical exponent \(\alpha\) ranges from 0.14 to 0.2 in the case of 2D seven and ten-state Potts model regardless one employees local or nonlocal MC moves \([16, 17]\). Such an improvement is significantly better than the one achieved applying the multicanonical method and its variants to the same model systems, whose typical exponent \(\alpha\) ranges from 2 to 2.5 \([11, 12]\). We shall show in this work that canonical MC algorithms extended with this methodology also exhibit a good performance near a critical point. This claim is illustrated for the particular case of 2D four-state Potts model \([14]\). Our results evidence the effectiveness of the present methodology to overcome slow sampling problems associated with temperature-driven PT regardless its continuous or discontinuous character.

II. OVERVIEW OF METHODOLOGY

A. Theoretical backgrounds

Methodology reviewed in this section is based on the consideration of generalized ensembles. Many generalized
ensembles that are employed in MC simulations have no physical meaning, e.g.: multicanonical ensemble \[ \text{[11,13–15]} \]. However, this is non necessarily the case of equilibrium situation considered in Ref.\[13\] to derive fluctuation relation \[ \text{(1)} \]: a closed system composed of two systems A and B with finite heat capacities \( C_A \) and \( C_B \), which are in put in thermal contact among them and isolated of any external influence. This situation can be implemented in a physical laboratory with an acceptable accuracy. Moreover, this is the arrangement considered in statistical mechanics to discuss thermal equilibrium conditions \[ \text{[20,21]} \]. Curiously, standard textbooks of statistical mechanics never refer to implications of equilibrium conditions concerning to states with negative heat capacities \[ \text{[22–24]} \]. For its own importance in this work, let us start this section clarifying this question. We recommend readers to see Ref.\[18\] for further details.

As usual, the total energy \( U_T \) and entropy \( S_T \) of the closed system are assumed as additive quantities, \( U_T = U_A + U_B \) and \( S = S_A + S_B \). Maximization of entropy \( S_T \) at constant energy \( U_T \) demands the stationary condition:

\[
\frac{\partial S_T}{\partial U_A} = \frac{\partial S_A}{\partial U_A} - \frac{\partial S_B}{\partial U_B} = 0 \Rightarrow \frac{1}{T_A} = \frac{1}{T_B} (= \beta),
\]

as well as the stability condition:

\[
\frac{\partial^2 S_T}{\partial U_A^2} = \frac{\partial^2 S_A}{\partial U_A^2} + \frac{\partial^2 S_B}{\partial U_B^2} < 0 \Rightarrow \frac{C_A C_B}{C_A + C_B} > 0.
\]

We have considered here the microcanonical expressions:

\[
\frac{1}{T_A} = \frac{\partial S_A}{\partial U_A} \quad \text{and} \quad \frac{\partial^2 S_A}{\partial U_A^2} = -\frac{1}{T_A^2}.
\]

with \( \alpha = (A,B) \). Accordingly, systems A and B can be found in thermal equilibrium if they exhibit the same temperature and their heat capacities satisfy one of the following stability conditions: (i) both systems exhibit positive heat capacities, or (ii) a system exhibits a negative heat capacity, e.g.: \( C_A < 0 \), and the other a positive heat capacity \( C_B > 0 \) that satisfies the following inequality:

\[
C_B < |C_A|.
\]

Condition \[ \text{(6)} \] was obtained by Thirring almost forty years ago \[ \text{[25]} \]. Accordingly, a system with negative heat capacity cannot be found in thermal equilibrium with an environment that exhibits an infinite heat capacity, e.g.: under thermodynamic influence of the natural environment. In other words, canonical ensemble is unable to study systems with negative heat capacities. However, these systems can be analyzed considering the thermal contact with an environment that exhibits a finite heat capacity. This conclusion is specially relevant for MC simulations. An unexpected consequence of the above analysis concerns to so-called zeroth law of thermodynamics \[ \text{[24]} \], which states: if two systems are both in thermal equilibrium with a third system then they are in thermal equilibrium with each other. Although this law helps to define the notion of temperature, its validity is restricted to systems exhibiting positive heat capacities. Two identical systems, that are initially prepared in the same macroscopic state, cannot be in thermal equilibrium if such macroscopic state exhibits a negative heat capacity. Noteworthy that each system can remain in thermal equilibrium with a third system exhibiting a positive heat capacity, whenever its obeys Thirring inequality \[ \text{[4]} \]. This violation of zeroth law of thermodynamics was recently discussed in the literature \[ \text{[27]} \].

Let us now regard system B as an environment in order to study thermodynamic properties of system A. Since heat capacity of this environment is finite, its temperature \( T_B \) will be affected by the energy interchange with the system A. Considering \( \delta T_B = -\delta U_A/C_B \Rightarrow \delta \beta_B = \beta^2 \delta U_A/C_A \), one obtains from \[ \text{(1)} \] the following result:

\[
\frac{C_A C_B}{C_A + C_B} = \beta^2 \langle \delta U_A^2 \rangle.
\]

Stability condition \[ \text{(1)} \] is derived from positivity of r.h.s. of Eq.\[7\], but this time from a fluctuational viewpoint. Relation \[ \text{(7)} \] drops to canonical fluctuation relation \[ \text{(2)} \] in the limit \( C_B \to +\infty \), as well as the microcanonical result \( \langle \delta U_A^2 \rangle \to 0 \) when \( C_B \to 0^+ \). Accordingly, this type of equilibrium situation can be associated with a family of generalized ensembles that contains microcanonical and canonical ensembles as particular cases. As expected, the exact mathematical form of each ensemble depends on the system B acting as environment.

Phenomenon of negative heat capacity has been regarded as an anomalous behavior. Precisely, their existence is incompatible with results of classical fluctuation theory \[ \text{[20,21]} \], e.g.: fluctuation relation \[ \text{(2)} \]. However, this incompatibility arises because of the restricted applicability of some conventional assumptions. Specifically, the macroscopic state of the environment can be affected by influence of the system under study. Such an environmental feedback perturbation is systematically omitted when one employs traditional ensembles such as Boltzmann-Gibbs distributions \[ \text{[20,21]} \]:

\[
\omega_{BG} (U, X|T, Y) = \frac{1}{Z} \exp \left[-\beta (U + XY)\right],
\]

where the environmental inverse temperature \( \beta = 1/T \) and the external generalized forces \( Y \) (e.g.: pressure \( p \), magnetic and electric fields \( H \) and \( E \), etc.) are assumed as constant control parameters for the energy \( U \) and the generalized displacements \( X \) (e.g.: volume \( V \), magnetization \( M \) and electric polarization \( P \), etc.). As expected, more general equilibrium situations involve non-vanishing correlations such as \( \langle \delta \beta U \rangle \) or \( \langle \delta Y \delta X \rangle \). Fluctuation theorems associated with these equilibrium situations provide a suitable treatment for states with negative heat capacities as well as other anomalies in response functions \[ \text{[28]} \].
B. Application to MC simulations

The inclusion of a feedback effect \( \langle \delta \beta_\omega \delta U \rangle \) to extend any canonical MC algorithm is achieved replacing the constant inverse temperature \( \beta \) of the canonical ensemble by an effective inverse temperature \( \beta_\omega(U) \):

\[
\beta_\omega(U) = -\frac{\partial}{\partial U} \log \omega(U),
\]

which depends on the energy \( U \) of system under study. This effective inverse temperature corresponds to an environmental influence whose probability weight \( \omega(U) \) differs from the one associated with canonical ensemble:

\[
\omega(U) \neq \omega_c(U|\beta) = \frac{1}{Z(\beta)} \exp(-\beta U). \tag{10}
\]

This type of arguments were employed by Gerling and Hülle to propose dynamic ensemble MC method \[29\]. These authors considered as environment an ideal gas with \( N \) degrees of freedom. Analysis of detailed balance led them to introduce an effective inverse temperature \( \beta_\omega = \langle N - 2 \rangle/2Nk_b \). Here, \( k_b = (U_T - U)/N \) is the mean kinetic energy per particle for the ideal gas, while \( U_T \) is the total energy. Effective inverse temperature \( \beta_\omega \) is adjusted dynamically during the course of MC simulation. Data are then obtained by computing the mean value of the energy \( \langle U \rangle \) and the mean value of the temperature from \( 2(k_b) \). This method allows to detect the presence of states with negative heat capacities whenever Thirring inequality \[10\] is fulfilled.

Methodology proposed by Velazquez and Curilef includes three important modifications for dynamic ensemble MC method of Gerling and Hülle \[16, 17\]: (i) the consideration of a more suitable generalized ensemble, (ii) the employment of a point statistical estimation to obtain the relevant microcanonical dependencies and reduce incidence of finite size effects, and finally, (iii) the optimization of efficiency considering a more active control on the system fluctuating behavior. For the rest of this section, let us detailedly explain these modifications.

C. Gaussian ensemble and its implementation

Let us consider the power-expansion of environmental inverse temperature \( \beta_\omega(U) \) around the mean value of the energy \( U_e(U) = \langle U \rangle \):

\[
\beta_\omega(U) = \beta + \sum_{n=1}^{\infty} a_n(U - U_e)^n. \tag{11}
\]

Assuming that energy fluctuations \( \delta U = U - U_e \) are sufficiently small, power-expansion \[12\] can be restricted to first-order approximation, \( \beta_\omega = \beta + \lambda \delta U/N \). Coupling constant \( \lambda = Na_1 \) plays a role of control parameter in conjunction with the expectation value of inverse temperature \( \beta = \langle \beta_\omega \rangle \). Substituting this ansatz into Eq.\[1\], one obtains the fluctuation relations:

\[
\langle \delta U^2 \rangle = \frac{N}{\beta^2 N/C + \lambda} \quad \text{and} \quad \langle \delta \beta_\omega^2 \rangle = \frac{1}{N} \frac{\lambda^2}{\beta^2 N/C + \lambda} \tag{12}
\]
as well as the stability condition:

\[
\beta^2 N/C + \lambda > 0. \tag{13}
\]

Noteworthy that the size dependencies of the energy \( \Delta U \) and inverse temperature \( \Delta \beta_\omega \) dispersions \( (\Delta x \equiv \sqrt{\langle (\delta x)^2 \rangle}) \) behave as \( \Delta U \propto \sqrt{N} \) and \( \Delta \beta_\omega \propto 1/\sqrt{N} \) for a short-range interacting system. As expected, linear approximation \( \beta_\omega = \beta + \lambda \delta U/N \) is good as long as the system size \( N \) is sufficiently large. If coupling constant \( \lambda \) obeys the stability condition \[14\], statistical ensemble associated with the present equilibrium situation becomes equivalent to the microcanonical ensemble in the thermodynamic limit:

\[
\lim_{N \to \infty} \frac{\Delta U}{U} = \lim_{N \to \infty} \Delta \beta_\omega = 0 \tag{14}
\]

regardless the positive or negative character of heat capacity \( C \) of the system under study. The origin of the exponential dependence with \( N \) of the decorrelation time in MC simulations \( \tau(N) \propto \exp(\gamma N) \) is due to the multimodal character of the energy distribution function within the canonical ensemble \[14\]. Such a bimodal character of energy distributions is associated with the existence of macrostates with negative heat capacities. Since the ensemble equivalence ensures the existence of only one peak, MC simulations based on the present equilibrium situation cannot undergo this type of slow sampling problem.

Equilibrium situation previously described is implemented assuming a linear dependence of the environmental inverse temperature on the system energy, \( \beta_\omega(U) = \beta_s + \lambda_s(U - U_s)/N \), with \( (U_s, \beta_s, \lambda_s) \) being three seed parameters, where \( U_s \) and \( \beta_s \) are roughly estimates of the expectation values \( \langle U \rangle \) and \( \langle \beta \rangle \). According to Eq.\[9\], this choice corresponds to the gaussian ensemble \[30, 31\]:

\[
\omega_G(U) = \frac{1}{Z(\beta_s)} \exp \left[ -\beta_s U - \frac{1}{2N} \lambda_s(U - U_s)^2 \right] \tag{15}
\]

with parameter \( \lambda_s \geq 0 \). Gaussian ensemble describes intermediate equilibrium situations between the usual thermal contact (canonical ensemble) when \( \lambda_s \to 0 \) and energy isolation (microcanonical ensemble) when \( \lambda_s \to +\infty \). The bath associated with this ensemble corresponds to a hypothetical substance whose heat capacity decreases with temperature as \( C_B \propto 1/T^2 \) \[25\]. Gaussian ensemble \[15\] provides several advantages to improve canonical MC simulations. In particular, its mathematical form makes more easy the analysis of detailed balance and the point statistical estimation.

Let \( W^c(U_i \to U_j; \beta) \) be the transition probability of a given canonical MC algorithm, which satisfies detailed
balance condition:

\[ \frac{W^c (U_i \rightarrow U_j; \beta)}{W^c (U_j \rightarrow U_i; \beta)} = \exp \left( - \beta \delta U_{ij} \right), \]

where \( \delta U_{ij} = U_j - U_i \) is energy change after transition. The detailed balance condition corresponding to gaussian ensemble \( \text{[13]} \) can be satisfied considering the following transition probability \( W (U_i \rightarrow U_j) \):

\[ W (U_i \rightarrow U_j) = W^c (U_i \rightarrow U_j; \beta^\nu), \]

where \( \beta^\nu = (\beta^\omega + \beta^\nu) / 2 \) is the transition inverse temperature \( \text{[17]} \), with \( \beta^\nu \) and \( \beta^\omega \) being the environmental inverse temperatures at the initial and the final configurations respectively, \( \beta^\mu = \beta (U_i) \) and \( \beta^\nu = \beta (U_j) \). This result follows from the identity:

\[ \frac{W (U_i \rightarrow U_j)}{W (U_j \rightarrow U_i)} = \frac{\omega_G (U_j)}{\omega_G (U_i)} = \exp \left( - \beta^\mu \delta U_{ij} \right), \]

which is obtained from the mathematical form of gaussian ensemble. Accordingly, one should replace the constant inverse temperature \( \beta \) of any canonical MC algorithm by the transition inverse temperature \( \beta^\nu \). Unfortunately, the application of this result demands to know, \textit{a priori}, the final configuration \( X_f \) of the system with energy \( U_j \). Therefore, this method can only be applied to extend local MC algorithms such as Metropolis importance sample \( \text{[32, 33]} \) or Glauber dynamics \( \text{[34]} \). The extending of cluster canonical MC algorithms is also possible, but their implementation is carried out dividing each MC moves into two steps \( \text{[13]} \).

1. To obtain a virtual configuration \( X_j \) with energy \( U_j \) through a canonical cluster MC method using the inverse temperature \( \beta^\omega \) of the initial configuration \( X_i \) with energy \( U_i \);

2. To accept the virtual configuration \( X_j \) using the acceptance probability \( w_{i\rightarrow j} \):

\[ w_{i\rightarrow j} = \min \left\{ 1, \frac{W^c_{i\rightarrow j}}{W^c_{j\rightarrow i}} \exp \left( - \beta^\mu \delta U_{ij} \right) \right\}. \]

The terms \( W^c_{i\rightarrow j} = W^c [U_i \rightarrow U_j; \beta^\omega] \) and \( W^c_{j\rightarrow i} = W^c [U_j \rightarrow U_i; \beta^\nu] \) represent the transition probabilities of the direct and the reverse process, respectively. Thus, the transition probability of the global process can be expressed as:

\[ W (U_i \rightarrow U_j) = W^c (U_i \rightarrow U_j; \beta^\nu) w_{i\rightarrow j}. \]

In general, values of the acceptance probability \( w_{i\rightarrow j} \) are close to the unity because of the change of the inverse temperature \( \delta \beta^\nu = \beta^\nu - \beta^\omega \) and the energy change \( \delta U_{ij} \) are very small if the system size \( N \) is sufficiently large.

D. Point statistical estimation

By definition, statistical expectation values of macroscopic observables are \textit{ensemble-dependent}, that is, they depend on the concrete equilibrium situation associated with a given statistical ensemble. To avoid this arbitrariness, one should perform the calculation of microcanonical quantities derived from the system entropy \( S(U) \), such as the microcanonical caloric curve \( \beta (U) = \partial S(U) / \partial U \) and the curvature curve \( \kappa (U) = -N \partial^2 S(U) / \partial U^2 \). Notice that this second quantity is directly related to the microcanonical heat capacity \( C \) as \( \kappa = \beta^2 N / C \).

In multicanonical algorithms and other re-weighting techniques, the microcanonical dependencies \( \beta (U) \) and \( \kappa (U) \) can be obtained by direct numerical differentiation of the entropy \( S(U) \), which was previously estimated using energy histograms. However, this procedure increases the statistical errors associated with any MC calculations, whose incidence is more significant with a larger order of differentiation \( \text{[15]} \). A more precise calculation is performed using the \textit{point statistical estimation} at the equilibrium energy \( U_e \), which is related to the thermal equilibrium condition \( \beta_e (U_e) = \beta (U_e) = \beta_e \). The estimation of microcanonical quantities \( (U_e, \beta_e, \kappa_e) \) is based on the asymptotic property of the energy distribution to adopt a \textit{gaussian form} in the thermodynamic limit \( N \rightarrow +\infty \). In analogous way to dynamic ensemble MC method \( \text{[29]} \), estimation of microcanonical dependencies is only exact in the thermodynamic limit. However, the incidence of finite size effects is considerably reduced using the following expressions \( \text{[17]} \):

\[ U_e = \langle U \rangle - \frac{1 - \psi_1}{2 (\delta U^2)} \langle \delta U^3 \rangle + O \left( \frac{1}{N^4} \right), \]

\[ \beta_e = \langle \beta \rangle - \frac{1 - \psi_1}{2 N (\delta U^2)} \langle \delta U^3 \rangle + O \left( \frac{1}{N^4} \right), \]

\[ \kappa_e = \frac{1 - \psi_1 - \lambda \langle \delta U^2 \rangle / N}{\langle \delta U^2 \rangle / N} + O \left( \frac{1}{N^2} \right), \]

where \( \psi_1 = \frac{8}{3} \epsilon_2 + \frac{11}{60} \epsilon_1 \) is a second-order correction term defined from the cumulants \( \epsilon_1 \) and \( \epsilon_2 \):

\[ \epsilon_1 = \frac{\langle \delta U^3 \rangle^2}{\langle \delta U^2 \rangle^3}, \quad \epsilon_2 = 1 - \frac{\langle \delta U^4 \rangle}{3 \langle \delta U^2 \rangle^2}. \]
and the four-order derivatives of the entropy:

\[ \zeta_2 = N^2 \frac{\partial^2 S(U_c)}{\partial U^2} = N^2 \left( \frac{\delta U^3}{\delta U^2} \right)^2 (1 - 3\psi_1) + O \left( \frac{1}{N^2} \right), \]
\[ \zeta_4 = N^3 \frac{\partial^4 S(U_c)}{\partial U^4} = -\psi_2 N^3 \frac{\delta U^3}{\delta U^2} + O \left( \frac{1}{N} \right), \]

(23)

where \( \psi_2 = \frac{1}{N^2} + \frac{1}{N}. \) Derivation of the above formulæ was discussed in appendix section of Ref.[17]. The same ones were obtained for the particular case of gaussian ensemble [15], and their applicability is associated to licitness of gaussian approximation for describing system fluctuating behavior. This means that the seed parameters \((U_s, \beta_s, \lambda_s)\) of gaussian ensemble [15] should be carefully chosen to guarantee applicability of gaussian approximation. The way to achieve this goal will be explained at the end of the next subsection.

E. Efficiency factor and its optimization

The efficiency of MC methods is commonly characterized by the decorrelation time \( \tau \), that is, the minimum number of MC steps needed to generate effectively independent, identically distributed samples in the Markov chain [14]. This quantity will be calculated as follows:

\[ \tau = \lim_{k \to \infty} \tau_k = \lim_{k \to \infty} \frac{k \cdot \text{var}(u_k)}{\text{var}(u_1)}, \]

(24)

where \( \text{var}(u_k) = \langle u_k^2 \rangle - \langle u_k \rangle^2 \) is the variance of \( u_k \), which is defined as the arithmetic mean of the energy per particle \( u = U/N \) over \( k \) samples (consecutive MC steps):

\[ u_k = \frac{1}{k} \sum_{i=1}^{k} u_i. \]

(25)

However, the decorrelation time \( \tau \) provides a partial characterization about the efficiency in the case of the extended canonical MC methods. To clarify this idea, let us consider the number of MC steps \( S \) needed to obtain a point of the caloric curve \( \beta(u) \) with a precision \( \delta u + \delta \beta^2 < a^2 \). This quantity can be estimated in terms of the total dispersion \( \Delta_T^2 \) and the decorrelation time \( \tau \) as follows:

\[ S = \tau \Delta_T^2 / Na^2. \]

(26)

The total dispersion \( \Delta_T^2 \) is kept fixed for canonical ensemble, and hence, a canonical MC algorithm is more efficient as smaller is its decorrelation time \( \tau \). However, the total dispersion \( \Delta_T^2 \) is ensemble-dependent, e.g.: this quantity depends on the control parameters \((U_s, \beta_s, \lambda_s)\) of gaussian ensemble [15]. According to expression [20], an extended canonical MC algorithm is more efficient as smaller is its efficiency factor:

\[ \eta = \tau \Delta_T^2. \]

(27)

The efficiency factor (27) depends on both decorrelation time \( \tau \) and the system fluctuating behavior. Moreover, decorrelation time \( \tau \) depends on both the statistical ensemble and the concrete canonical MC algorithm. The explicit mathematical form of the decorrelation time \( \tau \) in terms of control parameters of a given MC calculation is difficult to precise. The simplest criterion to reduce the efficiency factor \( \eta \) is minimizing the total dispersion \( \Delta_T^2 \), that is, by introducing a more active control on the system fluctuating behavior [16,17]. Using the expressions of equation (12), the lower-bound of the total dispersion \( \Delta_T^2 \) and the optimal value of the control parameter \( \lambda_s \) are the following:

\[ \lambda_s = \lambda_\Delta(\kappa_e) = \sqrt{1 + \kappa_e^2} \quad \text{and} \quad \min(\Delta_T^2) = 2\lambda_\Delta, \]

(28)

where \( \kappa_e \) is the curvature at the energy point \( U_e \). Accordingly, the optimal value for the parameter \( \lambda_s \) demands to consider a roughly estimation of the curvature \( \kappa_e \).

Seeds parameters \((U_s, \beta_s, \lambda_s)\) for a given MC run can be specified using the microcanonical estimates \((U_e, \beta_e, \kappa_e)\) obtained from a previous simulation run. We have employed in this work the following iterative scheme:

\[ U_{j+1} = U_j + \varepsilon; \beta_{j+1} = \beta_j - \kappa_e \varepsilon \quad \text{and} \quad \lambda_{j+1} = \lambda_\Delta(\kappa_e), \]

(29)

with \( \varepsilon \) being a small energy step. Noteworthy that scheme for \( \beta_{j+1} \) is simply first-order power-expansion of microcanonical inverse temperature, \( \beta_{j+1} = \beta(U_j + \varepsilon) = \beta(U_e^j + \varepsilon) + O(\varepsilon^2) \). Moreover, we have assumed a zero-order approximation for curvature \( \kappa_{j+1}^\varepsilon = \kappa(U_e^j + \varepsilon) = \kappa_e + O(\varepsilon) \). The initial values of the seed parameters \((U_s, \beta_s, \lambda_s)\) could be estimated from any canonical MC algorithm far from the region of temperature-driven PT. Sometimes, it is recommendable to consider a variable energy step \( \varepsilon \), overall, in those energy regions where the absolute values of microcanonical curvature curve \( \kappa(U) \) are sufficiently large. We have employed in this work the following rule \( \varepsilon = \varepsilon_0\sqrt{1 + \kappa_e^2} \), with \( \varepsilon_0 \) being the energy step near critical point where \( \kappa_e \approx 0 \). Notice that this rule guarantees, approximately, a constant arc-length between neighboring points of microcanonical caloric curve \( \beta \) versus \( U \). This feature can be checked in FIG.

III. EFFICIENCY NEAR A CRITICAL POINT

A. Temperature-driven continuous PT

Ensemble equivalence is always ensured in the case of a temperature driven-continuous PT. Slow sampling problems in systems that undergo this type of PT are consequence of the large increasing of the energy fluctuations and the heat capacity \( C \) when the inverse temperature \( \beta \) of canonical ensemble approaches the critical point \( \beta_c \). As discussed elsewhere [20], the fluctuating behavior observed here can be associated with the existence of large correlation length \( \xi \) among the system constituents.
The incidence of slow sampling problems could be significantly reduced if such strong correlations could be avoided by some external influence. If possible, the relaxation times of averages of physical observables could be good enough even using local MC moves. Such a reduction of correlation length $\xi$ can also be achieved considering the feedback perturbation of the system boundary. According to Eqs. (12) and (13), the coupling constant $\lambda$ acts as a control parameter of the system thermodynamic stability and fluctuating behavior. Canonical fluctuation acts as a control parameter of the system thermodynamic limit $L \rightarrow \infty$ when $C \rightarrow \infty$. However, the quantity $\Delta U$ remains finite whenever the stability condition (13) applied, that is, if the coupling constant $\lambda > 0$ when $C \rightarrow \infty$. Since the energy fluctuations are kept finite at the critical point, the underlying correlation length $\xi$ among the system constituents should be reduced.

B. Potts model and its MC algorithms

For the sake of convenience, let us consider the $q$-state Potts model [14]:

$$H = -\sum_{i,j} \delta_{\sigma_i,\sigma_j}$$ (30)

defined over a square lattice $L \times L$ with periodic boundary conditions, where $\sigma_i = (1, 2, \ldots, q)$ is the spin variable of the $i$-th site and the sum in (30) involves all nearest-neighbors. This family of toy models undergoes both continuous and discontinuous PT at $\beta_c = \ln (1 + \sqrt{q})$ in the thermodynamic limit $L \rightarrow \infty$. Their MC study can be performed using different canonical MC algorithms. Specifically, we will consider Metropolis importance sample [22] as a local MC method, as well as Swendsen-Wang and Wolff cluster algorithms [11,12] as examples of nonlocal MC methods. These cluster MC methods are easily extended with the application of the present methodology. Firstly, we need to obtain the transition probabilities $W_{i\rightarrow j}$ and $W_{j\rightarrow i}$, that appear in the acceptance probability (19). Denoting by $p_i = 1 - e^{-\beta \sigma}$ and $p_j = 1 - e^{-\beta \sigma}$ the acceptance probabilities of bonds for the direct and reverse processes, the transition probabilities $W_{i\rightarrow j}$ and $W_{j\rightarrow i}$ are expressed as follows:

$$W_{i\rightarrow j} = p_i^{b_i} (1 - p_i)^{b_p + b_d}, W_{j\rightarrow i} = p_j^{b_i} (1 - p_j)^{b_p + b_d}.$$ (31)

Here, $b_o$ and $b_p + b_d$ are the numbers of inspected bonds which have been accepted and rejected in the direct process, respectively. Moreover, $b_d$ is the number of rejected bonds which have been destroyed in the final configuration $X_j$, while $b_c$ is number of created bonds. Notice that the energy change $\delta U_{i\rightarrow j} = b_d - b_c$. The integer numbers $(b_o, b_d, b_c, b_p)$ should be obtained for each cluster move.

C. Numerical simulations

We have shown in FIG[1] several microcanonical dependencies of $q$-state Potts model with $L = 32$ and $q = 2 - 6$, which were estimated using the extended version of Wolff cluster algorithm and the point statistical estimation (21). Each point of these curves was obtained considering $M = 4 \times 10^3 \tau$ iterations for each MC run, with $\tau$ being its associated decorrelation time. The convergence of four-order derivative $\zeta^4(u)$ is less significant than the other microcanonical dependencies. However, this is a reasonable result taking into consideration that $\zeta^4(u)$ is associated with high-order fluctuating behavior beyond gaussian approximation.

According to the minimal total dispersion, $\min(\Delta f^2) = 2\lambda_{\Delta}(\kappa)$, the system exhibits its largest energy fluctuations when the curvature $\kappa$ reaches its minimum value $\kappa_{\min}$. The character of the PT depends on the signature of the curvature $\kappa_{\min}$. It is continuous for $\kappa_{\min} \geq 0$ ($q = 2 - 4$), while discontinuous for $\kappa_{\min} < 0$ ($q > 4$). The extended version of Wolff algorithm is able to describe both continuous and discontinuous temperature-driven PTs. Since 2D four-state Potts model exhibits the largest fluctuating behavior near critical point, this particular case will be considered to analyze the impact of the present methodology on the efficiency of MC simulations.

For comparison purposes, the microcanonical quantities will be estimated using the entropy $S(U)$ derived from Wang-Landau method [13]. To avoid statistical errors associated with numerical differentiation of the entropy $S(U)$, we shall consider the formulae (21) of the point statistical estimation. Statistical expectation values can be evaluated as follows:

$$\langle a(U) \rangle = \frac{\sum_i a(U_i) \exp[-\phi(U_i) + S(U_i)]}{\sum_i \exp[-\phi(U_i) + S(U_i)]},$$ (32)

where $\phi(U) = \beta_s (U - U_s) + \lambda_s (U - U_s)^2 / 2N$. The estimates of the entropy per site $s = S/N$ and the inverse temperature $\beta$ versus energy per site $u = U/N$ are shown in FIG[2] for the case of 2D four-state Potts model with $L = 32$. As clearly illustrated here, results obtained from a direct numerical differentiation of entropy $S(U)$ are strongly affected by the statistical errors associated with MC calculations of energy histograms. Fortunately, the point statistical estimation overcomes this difficulty providing a smoothly dependence for the microcanonical caloric curve $\beta$ versus $u$. Results from Wang-Landau method are considered as a reference in FIG[3] which illustrates microcanonical estimates derived from three canonical MC algorithms and their extended versions. We have considered a variable number of steps $M = 4 \times 10^3 \tau$ for each simulation run, with $\tau$ being its decorrelation time. Dependencies associated with Wang-Landau method were obtained from two simulation runs with $M = 2 \times 10^7$ and $M = 1.1 \times 10^8$ steps.

Results derived from the extended versions of canonical MC algorithms and Wang-Landau method exhibit a...
great agreement among them. Discrepancy among these MC methods is only observed for estimation of curvature curve \( \kappa(u) \) near critical region (see in FIG.3.b). This discrepancy was also observed in FIG.2 of Ref. [17]. In principle, extended canonical MC algorithms and Wang-Landau method should provide same microcanonical estimates when the number of steps \( M \) is sufficiently large. However, the entropy per site \( s(u) \) obtained from Wang-Landau method is not sufficiently equilibrated to perform a more precise estimation of curvature curve \( \kappa(u) = -\partial^2 s(u)/\partial u^2 \) near critical point. The convergence of results obtained from estimation formulae (21) is not uniform everywhere. Even using the optimal values for the seed parameters \( U_s, \beta_s, \lambda_s \) of gaussian ensemble (15), the largest fluctuating behavior is always observed near critical point. This fact evidences a particular advantage of extended canonical MC algorithms. These methods enable the study of a small energy region in a given simulation run. Thus, the number of steps \( M \) of each run can be locally extended as large as needed to guarantee the convergence of microcanonical estimates. On the contrary, Wang-Landau method sweeps the whole energy range in a single run. Although this feature is regarded as an advantage in many applications, this is not the case of calculations of partial derivatives \( \partial^n s(u)/\partial u^n \). Statistical errors of entropy per site \( s(u) \) are only reduced increasing the number of steps of Wang-Landau method for whole energy range. According to results shown in FIG.3.b, there exist a certain converge of results of Wang-Landau method towards results of extended canonical MC methods when number of steps \( M \) is increased from \( 2 \times 10^7 \) to \( 1.1 \times 10^8 \) [38]. However, the fully convergence requires much more calculations. This exigence contrasts with the high-performance of extended Wolff cluster algorithm. Using this last MC method, we have only employed a total of \( M = 7.3 \times 10^6 \) steps, with an average of \( M = 2.2 \times 10^5 \) steps for each calculated point.

Microcanonical estimates derived from usual canoni-
tical MC algorithms undergo large systematic deviations. This behavior is not associated with a poorly equilibration of MC averages, but the large energy fluctuations experienced by the model system near critical point within canonical ensemble. Canonical ensemble is a particular case of gaussian ensemble with $\lambda_s = 0$, so that, formulae (21) of the point statistical estimation are applicable to this ensemble whenever the associated energy distribution satisfies gaussian approximation. This requirement cannot be satisfied near critical point, which is illustrated in FIG. 4. We show here energy distributions near critical point obtained from MC simulations using both Wolff cluster algorithm and its extended version for $\beta \simeq 1.098$. Distribution obtained from usual Wolff cluster algorithm (canonical ensemble) cannot be described by a gaussian approximation. On the contrary, gaussian approximation is fully licit for distribution obtained from extended Wolff cluster algorithm, which considers a gaussian ensemble with optimal values of the seed parameters $(U_s, \beta_s, \lambda_s)$. A way to reduce the incidence of finite size effects of microcanonical estimates derived from canonical ensemble is by considering higher-order correction terms in formulae (21). This exigency presupposes calculation of energy moments $\langle \delta U^n \rangle$ with $n > 4$, which demands larger simulation runs to achieve their convergence.

The size dependencies of the decorrelation time $\tau$ and the efficiency factor $\eta$ at the critical point are shown in FIG. 5 for canonical and extended versions of three different MC algorithms for lattice sizes $L$ ranging from 8 to 128. For all extended versions, size dependency of decorrelation time $\tau$ and the efficiency factor $\eta$ exhibit power-law behaviors $\tau(N) = C_\tau N^{\alpha_\tau}$ and $\eta(N) = C_\eta N^{\alpha_\eta}$ weaker than their canonical counterparts. For a better quantitative characterization, estimates of dynamic critical exponents $\alpha_\tau$ and $\alpha_\eta$ are shown in Table I. The size dependency associated with Metropolis importance sample is reduced, but the improvement of its decorrelation time $\tau$ is less significant than the one achieved by cluster algorithms. Greater impact of the present methodology is manifested when the efficiency is described in terms of the efficiency factor $\eta$. Precisely, the efficiency factor $\eta$ determines the number of iterations needed to achieve the convergence of the microcanonical caloric curve $\beta(u)$. All extended MC algorithms exhibit a better efficiency factor $\eta$ than their original canonical counterparts. Extended version of Metropolis importance sample, in particular,
is slightly more efficient than canonical Swendsen-Wang and Wolff cluster algorithms. The exponents for extended cluster algorithms near critical point $\alpha_\eta \approx 0.1$, which are very similar to the typical values of systems that undergo temperature-driven discontinuous PT. Dynamic critical exponents $\alpha_\eta$ and $\alpha_\eta$ are practically the same for extended canonical MC algorithms. On the contrary, dynamic critical exponents of canonical MC algorithms exhibit a constant difference $\delta = \alpha_\eta - \alpha_\eta \approx 0.36$ that is directly associated with the incidence of size effects in the total dispersion $\Delta^2_T$.

IV. FINAL REMARKS

Methodology proposed by Velazquez and Curilef [16, 17] leads to a significant improvement of the efficiency of MC simulations in presence of any type of temperature-driven phase transitions. Although extended canonical cluster algorithms exhibit the highest efficiencies, a local MC method as extended Metropolis importance sample has a universal applicability and a very good efficiency. For the particular case of 2D four-state Potts model, this extended local MC methods exhibits an efficiency comparable to canonical cluster algorithms of Swendsen-Wang and Wolff. Consequently, this extended local MC algorithm can be specially useful in MC simulations of systems whose canonical cluster algorithms are still unavailable in the literature.

Before to end this section, let us refer to some open problems. Firstly, the present methodology should be extended to those MC algorithms based on Boltzmann-Gibbs distributions [20]. An important antecedent of this problem was considered by Velazquez and Curilef in Ref. [28], where general equilibrium fluctuation theorem [11] was generalized for the case of many thermodynamic variables. However, some relevant developments still missing, as example, the extending of formulae [21] for the point statistical estimation. On the other hand, the present methodology can be combined with re-weighting techniques such as multi-histogram method to improve statistics [14], which can provide a better estimation for the higher-order derivatives of the entropy $S(U)$.

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\begin{table}[!h]
\centering
\begin{tabular}{|c|c|c|}
\hline
MC method & $\alpha_\eta$ & $\alpha_\eta$ \\
\hline
Metropolis & 1.06 $\pm$ 0.01 & 1.42 $\pm$ 0.01 \\
extended Metropolis & 0.777 $\pm$ 0.006 & 0.790 $\pm$ 0.008 \\
Swendsen-Wang & 0.432 $\pm$ 0.007 & 0.792 $\pm$ 0.008 \\
extended Swendsen-Wang & 0.098 $\pm$ 0.004 & 0.117 $\pm$ 0.004 \\
Wolff & 0.474 $\pm$ 0.005 & 0.833 $\pm$ 0.007 \\
extended Wolff & 0.094 $\pm$ 0.006 & 0.103 $\pm$ 0.006 \\
\hline
\end{tabular}
\caption{Dynamic critical exponents $\alpha_\eta$ and $\alpha_\eta$ associated with the size dependencies of decorrelation time $\tau$ and efficiency factor $\eta$ shown in FIG.5}
\end{table}

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