Extending canonical Monte Carlo methods: II

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Abstract. We have previously presented a methodology for extending canonical Monte Carlo methods inspired by a suitable extension of the canonical fluctuation relation $C = \beta^2 \langle \delta E^2 \rangle$ compatible with negative heat capacities, $C < 0$. Now, we improve this methodology by including the finite size effects that reduce the precision of a direct determination of the microcanonical caloric curve $\beta(E) = \partial S(E)/\partial E$, as well as by carrying out a better implementation of the MC schemes. We show that, despite the modifications considered, the extended canonical MC methods lead to an impressive overcoming of the so-called supercritical slowing down observed close to the region of the temperature driven first-order phase transition. In this case, the size dependence of the decorrelation time $\tau(N)$ is reduced from an exponential growth to a weak power-law behavior, $\tau(N) \propto N^{\alpha}$, as is shown in the particular case of the 2D seven-state Potts model where the exponent $\alpha = 0.14–0.18$.

Keywords: rigorous results in statistical mechanics, classical Monte Carlo simulations
1. Introduction

In a previous paper [1], we have proposed a methodology that enables Monte Carlo (MC) methods based on the Gibbs canonical ensemble:

\[ \frac{d}{dE} \frac{c(E|\beta_B)}{Z(\beta_B)} = \frac{1}{Z(\beta_B)} \exp(-\beta_B E) \Omega(E) dE \]  \hspace{1cm} (1)

to account for the existence of an anomalous region with negative heat capacities \( C < 0 \) [2]–[7] and to overcome the so-called supercritical slowing down observed near the first-order phase transition [8]. Here, \( \Omega(E) \) is the system density of states, \( Z(\beta_B) \) is the partition function, and \( \beta_B = 1/T \) is the constant inverse temperature of the environment associated with the canonical ensemble. Our development is inspired by the consideration of the following fluctuation relation [9]–[11]:

\[ C = \beta^2 \langle \delta E^2 \rangle + C \langle \delta \beta_{\omega} \delta E \rangle, \]  \hspace{1cm} (2)

which appears as a suitable extension of the known canonical identity \( C = \beta^2 \langle \delta E^2 \rangle \) involving the heat capacity \( C \) and the expectation value of the energy fluctuations \( \langle \delta E^2 \rangle \). This last expression accounts for the realistic perturbation of the internal state of a certain environment as a consequence of the thermodynamic interaction with the system. The same effect is characterized here in terms of the function \( \langle \delta \beta_{\omega} \delta E \rangle \) describing the correlation between the system internal energy \( E \) and the environment inverse temperature \( \beta_{\omega} \). Use of the canonical ensemble (1) entails dismissing the existence of this feedback effect due to the constant character of the inverse temperature \( \beta_B \) associated with this ensemble, which is only compatible with positive heat capacity. Conversely, the general case allows access

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to anomalous macrostates with negative heat capacities $C < 0$ whenever the condition $\langle \delta \beta_\omega \delta E \rangle > 1$ is obeyed.

The incidence of non-vanishing correlated fluctuations $\langle \delta \beta_\omega \delta E \rangle$ can be easily implemented in MC simulations. Roughly speaking, the extension of canonical MC methods is achieved by replacing the canonical inverse temperature $\beta_B$ by a variable inverse temperature $\beta_\omega(E)$. The resulting framework constitutes a suitable extension of the Gerling and H"uller methodology on the basis of the so-called dynamic ensemble [12], where the microcanonical curve $\beta(E) = \partial S(E)/\partial E$ and the heat capacity $C(E)$ can be estimated in terms of the energy and temperature expectation values $\langle E \rangle$ and $\langle \beta_\omega \rangle$ as well as their fluctuating behavior described by equation (2). This method successfully reduces the exponential divergence of the decorrelation time $\tau \propto \exp(\lambda N)$ with the increase of the system size $N$ of canonical MC methods to a weak power-law divergence $\tau \propto N^\alpha$, with a typical exponent $\alpha \simeq 0.2$ for the case of the 2D ten-state Potts model [1]. By combining this type of argument with clusters algorithms, one obtains very efficient MC schemes that constitute attractive alternatives to the known multicanonical method and its variants [8]. In this work, we shall improve the present methodology to consider the existence of the finite size effects that reduce the precision of a direct determination of the microcanonical caloric curve $\beta(E)$, as well as by carrying out a better implementation of the MC schemes.

2. Methodology

2.1. Overview

The simplest way to implement the incidence of non-vanishing correlations $\langle \delta \beta_\omega \delta E \rangle$ corresponds to a linear coupling of the environment inverse temperature $\beta_\omega$ with the thermal fluctuations of the system energy:

$$\beta_\omega(E) = \beta_e + \lambda \delta E/N,$$

where $\lambda$ is a coupling constant that appears as an additional control parameter. While the case with $\lambda = 0$ corresponds to the canonical ensemble (1), where $\beta_\omega = \text{const}$, in general, a constant character of the inverse temperature $\beta_\omega$ can only be ensured for the expectation value $\beta_e = \langle \beta_\omega \rangle$. Equation (3) can be substituted into equation (2) to obtain the following results:

$$\langle \Delta E \rangle^2 = \frac{N}{\beta^2 N/C + \lambda}, \quad \langle \Delta \beta_\omega \rangle^2 = \frac{1}{N} \frac{\lambda^2}{\beta^2 N/C + \lambda},$$

where $\Delta x \equiv \sqrt{\langle \delta x^2 \rangle}$ denotes the thermal dispersion of a given quantity $x$. Since $\Delta \beta_\omega$ and $\Delta E$ should be nonnegative, one arrives at the following stability condition:

$$\beta^2 N/C + \lambda > 0.$$

For $\lambda = 0$, one obtains the constraint $C > 0$ that emphasizes the unstable character of macrostates with negative heat capacities within the canonical description. However, these anomalous macrostates can be observed in a stable way in a general situation with $\lambda \neq 0$ when this control parameter satisfies equation (5). Assuming an extensive character of the heat capacity $C \sim N$ in short-range interacting systems, the energy dispersion $\Delta E$ grows with the increase of the system size $N$ as $\Delta E \sim \sqrt{N}$, so the dispersion of the energy
per particle $\varepsilon = E/N$ behaves as $\Delta \varepsilon \sim 1/\sqrt{N}$. Since $\delta \beta_\omega \equiv \lambda \delta E/N$ in the case of the ansatz (3), the dispersion of the inverse temperature also behaves as $\Delta \beta_\omega \sim 1/\sqrt{N}$. Thus, the present equilibrium situation constitutes a physical scenario that ensures the stability of macrostates with negative heat capacities $C < 0$ with the incidence of small thermal fluctuations.

This type of equilibrium situation is schematically represented in figure 1. Here, we show the typical microcanonical caloric curve $\beta(E) = \partial S(E)/\partial E$ corresponding to a finite short-range interacting system that undergoes a first-order phase transition, as well as the energy distribution function $\rho(E)$ associated with the thermal coupling of this system within an environment with inverse temperature $\beta_\omega(E)$. Notice that the ansatz (3) can be regarded as the first-order approximation in the power expansion of an arbitrary dependence $\beta_\omega(E)$:

$$\beta_\omega(E) = \beta_e + \sum_{n=1}^{\infty} a_n (E - E_e)^n,$$

where $a_1 = \partial \beta_\omega(E_e)/\partial E \equiv \lambda/N$. The intersection points $E_e$, derived from the condition of thermal equilibrium:

$$\beta(E_e) = \beta_\omega(E_e),$$

determine the position of maxima and minima of the distribution function $\rho(E)$. While in the canonical ensemble there could exist three intersections points ($e$, $c_1$ and $c_2$) because of the constant character of the inverse temperature, it is possible to ensure the existence of only one intersection point $E_e$ by appropriately choosing the inverse temperature dependence $\beta_\omega(E)$. If the system size $N$ is sufficiently large, the energy distribution function $\rho(E)$ adopts a bell shape, which is approximately described by using the Gaussian distribution:

$$\rho(E) \simeq A \exp \left[ -\frac{1}{2\sigma_E^2} (E - E_e)^2 \right],$$

Figure 1. Schematic representation of the typical microcanonical caloric curve $\beta(E) = \partial S(E)/\partial E$ associated with a finite short-range interacting system undergoing a first-order phase transition, as well as the energy distribution function $\rho(E)$ resulting from the thermal coupling of this system with a certain environment with inverse temperature $\beta_\omega(E)$.
where $\sigma_E = \Delta E$. The expectation values $\langle E \rangle$ and $\langle \beta_\omega \rangle$ provide a good estimation of the energy $E_e$ and inverse temperature $\beta_e = \beta(E_e)$ at the intersection point illustrated in figure 1:

$$E_e = \langle E \rangle, \quad \beta_e = \langle \beta_\omega \rangle.$$  

(9)

The previous procedure is equivalent to one employed by Gerling and H{"u}ller in the framework of the dynamical ensemble [12], whose probabilistic weight:

$$\omega_D(E) = A(E_T - E)^B$$  

(10)
accounts for the thermal coupling of the system with a bath exhibiting a constant heat capacity $C_B = B^2$, e.g., an ideal gas, whose inverse temperature obeys the following dependence on the system energy $E$:

$$\beta_\omega(E) = \frac{B}{(E_T - E)}.$$  

(11)

Our proposal improves the Gerling and H{"u}ller methodology. In fact, the energy dependence (11) is less convenient for calculations than the linear ansatz (3), which is a feature particularly useful for performing the analysis of finite size effects (see section 2.2 below). Moreover, one can also obtain the value of the heat capacity $C(E)$, or more exactly, the so-called curvature curve $\kappa(E)$:

$$\kappa(E) = \beta^2 N/C \equiv -N \frac{\partial^2 S(E)}{\partial E^2}$$  

(12)

at the intersection point $E_e$, $\kappa_e = \kappa(E_e)$, through the energy dispersion $\Delta E$ in an analogous way to the MC calculation by using the canonical ensemble (1):

$$\kappa_e = \frac{1 - \lambda \langle \delta E^2 \rangle / N}{\langle \delta E^2 \rangle / N}.$$  

(13)

This last equation was obtained from equation (12) by rewriting the first relation of equation (4) and considering $\Delta E \equiv \sqrt{\langle \delta E^2 \rangle}$.

Since the energy and the inverse temperature dispersions in equation (4) are controlled by the coupling constant $\lambda$, it is desirable to reduce them as much as possible. One can verify that the energy dispersion $\Delta E$ decreases with the increasing of the coupling constant $\lambda$. However, the value of this parameter should not be excessively large. Its increase leads to the increase of the inverse temperature dispersion $\Delta \beta_\omega$, which affects the precision of the inverse temperature $\beta_e$ of the system indirectly derived from the expectation value $\langle \beta_\omega \rangle$. A thermodynamic criterion that provides an optimal value for the coupling constant $\lambda$ can be obtained by minimizing the total dispersion $\Delta^2_T$:

$$\Delta^2_T = \frac{(\Delta E)^2}{N} + N (\Delta \beta_\omega)^2 = \frac{1 + \lambda^2}{\lambda + \kappa_e},$$  

(14)

which provides the precision of the intersection point determination, $(E_e, \beta_e)$. This analysis leads to the following result:

$$\lambda_\Delta = \lambda_\Delta(\kappa_e) = \sqrt{1 + \kappa_e^2} - \kappa_e, \quad \min \Delta^2_T = 2\lambda_\Delta.$$  

(15)

2 Here, $E_T = E + E_B$ is the total energy of the composite system (system + bath), with $E_B$ being the internal energy of the bath.
2.2. Finite size effects

The energy distribution function that corresponds to the thermal coupling of the system with an environment can be expressed by the following equation:

\[ \rho(E) \, dE = \omega(E) \Omega(E) \, dE. \]  

(16)

Here, \( \omega(E) \) is a probabilistic weight that characterizes such a thermodynamic influence, which is related to the environment inverse temperature \( \beta_\omega(E) \) as follows:

\[ \beta_\omega(E) = -\frac{\partial \log \omega(E)}{\partial E}. \]  

(17)

Through a direct integration it is verified that the probabilistic weight associated with the linear ansatz (3) is simply the Gaussian ensemble [13]:

\[ \omega_G(E) = \frac{1}{Z(\beta_e)} \exp \left[ -\beta_e E - \frac{1}{2N} \lambda (E - E_e)^2 \right], \]  

(18)

which is introduced by Hetherington [14], and approaches the microcanonical ensemble in the limit \( \lambda \to +\infty \):

\[ \omega_M = \frac{1}{\Omega} \delta(E - E_e). \]  

(19)

As already explained, the estimation of the microcanonical caloric curve \( \beta(E) \) as well as the fluctuation relation (2) is based on the consideration of a Gaussian shape for the energy distribution function \( \rho(E) \). Such an approximation naturally arises as the asymptotic distribution as long as the system size \( N \) is large enough. If the system size \( N \) is not very large, small deviations from the Gaussian profile (8) are naturally expected. Fortunately, the particular mathematical form of the Gaussian ensemble (18) allows us to consider some simple correction formulae for dealing with the existence of these finite size effects and for improving the precision of the present methodology. For details, see the appendix.

The first-order correction of equation (9) is given by the following formulae:

\[ E_e = \langle E \rangle - \frac{1}{2} \frac{\psi_1}{\langle \delta E^2 \rangle} \langle \delta E^3 \rangle, \]  

(20)

\[ \beta_e = \langle \beta_\omega \rangle - \lambda \frac{1}{2N \langle \delta E^2 \rangle} \langle \delta E^3 \rangle, \]  

(21)

which require the calculation of the cubic dispersion of the energy fluctuation \( \langle \delta E^3 \rangle \). This approximation level does not introduce any change in equation (13) for the estimation of the curvature \( \kappa_e \) at the intersection point \( E_e \).

The second-order approximation leads to the following formulae:

\[ E_e = \langle E \rangle - \frac{1 - \psi_1}{2} \frac{\psi_1}{\langle \delta E^2 \rangle} \langle \delta E^3 \rangle, \]  

(22)

\[ \beta_e = \langle \beta_\omega \rangle - \lambda \frac{1 - \psi_1}{2N \langle \delta E^2 \rangle} \langle \delta E^3 \rangle, \]  

(23)

\[ \kappa_e = \frac{1 - \psi_1 - \lambda \langle \delta E^2 \rangle / N}{\langle \delta E^2 \rangle / N}. \]  

(24)
Here, $\psi_1$ is a second-order term:

$$\psi_1 = \frac{6}{5}\epsilon_2 + \frac{11}{30}\epsilon_1$$

(25)

that is defined by the cumulants $\epsilon_1$ and $\epsilon_2$:

$$\epsilon_1 = \frac{\langle \delta E^3 \rangle^2}{\langle \delta E^2 \rangle^3}, \quad \epsilon_2 = 1 - \frac{\langle \delta E^4 \rangle}{3\langle \delta E^2 \rangle^2},$$

(26)

which need to assess the cubic and the fourth-order dispersion of the energy fluctuation, $\langle \delta E^3 \rangle$ and $\langle \delta E^4 \rangle$. It is easy to verify that while the surviving finite size effects of the above correction for the caloric curve $\beta(\varepsilon)$ in terms of the energy per particle $\varepsilon$ are of order $O(1/N^3)$, the other effects corresponding to the curvature curve $\kappa$ versus $\varepsilon$ are of order $O(1/N^2)$. As a by-product of the previous analysis, one can obtain the third and fourth derivatives of the entropy per particle $s(\varepsilon)$ as follows:

$$\zeta_3^e = \frac{\partial^3 s(e)}{\partial \varepsilon^3} = 2N^2 \frac{\langle \delta E^3 \rangle}{\langle \delta E^2 \rangle^3} (1 - 3\psi_1),$$

(27)

$$\zeta_4^e = \frac{\partial^4 s(e)}{\partial \varepsilon^4} = -\psi_2 \frac{N^3}{\langle \delta E^2 \rangle^2},$$

(28)

where $\psi_2$ is another second-order term given by

$$\psi_2 = \frac{12}{5}\epsilon_2 + \frac{41}{15}\epsilon_1.$$  

(29)

While the underlying finite size effects of the dependence $\zeta_3$ versus $\varepsilon$ estimated by using equation (27) are of order $O(1/N^2)$, the ones corresponding to the dependence $\zeta_4$ versus $\varepsilon$ estimated by equation (28) are of order $O(1/N)$.

At first glance, one may expect the expressions (22)–(24) to reduce to the results $\beta_\omega = \langle \beta_\omega \rangle$ and $E_\omega = \langle E \rangle$ for the particular case of the canonical ensemble where $\lambda = 0$. The first equality does indeed emerge from equation (23), but as equation (22) does not depend on $\lambda$, one does not recover the second one. Actually, there is nothing wrong with such an expression. The expectation value $\langle E \rangle$ only provides a direct estimation of the interception energy $E_\omega$ when the distribution function $\rho(E)\,dE$ exactly adopts the Gaussian form (8), where $\langle \delta E^3 \rangle = 0$ and $\langle \delta E^4 \rangle = 3\langle \delta E^2 \rangle \Rightarrow \psi_1 = \psi_2 = 0$.

2.3. Implementation

As already commented in section 1, a general way to extend a particular canonical MC algorithm with transition probability $W(X_i \rightarrow X_f; \beta_B)$ using the present methodology is to replace the constant inverse temperature $\beta_B$ of the canonical ensemble (1) with a variable inverse temperature, $\beta_B \rightarrow \beta_\omega(E)$. The fulfilment of the detailed balance condition:

$$p_\omega(X_i)W(X_i \rightarrow X_f; \beta_\omega) = p_\omega(X_f)W(X_f \rightarrow X_i; \beta_\omega)$$

(30)

requires the use of a certain value $\beta_\omega^\dagger$ of the environment inverse temperature for both the direct and reverse processes defined from the condition

$$\frac{p_\omega(X_i)}{p_\omega(X_f)} = \exp(\beta_\omega^\dagger \delta E_{df}),$$

(31)

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which is hereafter referred to as the **transition inverse temperature**. Here, $p_{\omega}(X) \equiv \omega[E(X)]$ represents the distribution function associated with the environmental inverse temperature $\beta_{\omega}(E)$, and $\delta E_{df} = E_f - E_i$, the energy variation of the system during the transition, where $E_i = E(X_i)$ and $E_f = E(X_f)$. The linear ansatz (3) is a special case where the transition inverse temperature $\beta^t_\omega$ is simply given by

$$\beta^t_\omega = \frac{1}{2}(\beta^i_\omega + \beta^f_\omega),$$

where $\beta^i_\omega$ and $\beta^f_\omega$ are the bath inverse temperatures for the initial and the final configurations, respectively, $\beta^i_\omega = \beta_\omega(E_i)$ and $\beta^f_\omega = \beta_\omega(E_f)$.

The direct applicability of the above result is restricted due to the final configuration $X_f$ having to be previously known in order to obtain the transition inverse temperature $\beta^t_\omega$. While such a requirement can be always satisfied in a local MC study as a Metropolis importance sample [15, 16], the final configuration $X_f$ is a priori unknown in non-local MC methods such as cluster algorithms [17]–[25]. For these cases, one is forced to employ an approximate value of the transition inverse temperature $\beta^t_\omega$, e.g., the inverse temperature $\beta^i_\omega$ for the initial configuration. Although the resulting MC algorithm does not obey detailed balance, we have shown that the deviation of the asymptotic distribution function $\tilde{p}_{\omega}(X)$ from the exact distribution function $p_{\omega}(X)$ can be disregarded when the system size $N$ is large [1]. This is why this method is particularly useful for overcoming slow sampling problems in large scale MC simulations.

The use of an approximate value for the transition inverse temperature $\beta^t_\omega$ is no longer appropriate when the interest extends to the study of systems with relatively small size $N$. Such an approximation introduces uncontrollable finite size effects that cannot be dealt with by using the working equations (22)–(24). In this case, it is necessary to fulfil the detailed balance condition (30) to obtain the Gaussian profile (18) as an asymptotic distribution function. The most general way to achieve this aim is to introduce a posteriori the acceptance probability $w_i \rightarrow f$:

$$w_i \rightarrow f = \min \left\{ 1, \frac{W_{f \rightarrow i}}{W_{i \rightarrow f}} \exp(-\beta^t_\omega \delta E_{df}) \right\}$$

for accepting or rejecting the final configuration $X_f$. Here, the terms

$$W_{i \rightarrow f} = W[X_i \rightarrow X_f; \beta^t_\omega] \quad \text{and} \quad W_{f \rightarrow i} = W[X_f \rightarrow X_i; \beta^t_\omega]$$

represent the transition probabilities of the direct and the reverse processes, respectively, which should be calculated for the given canonical cluster MC algorithm.

### 2.4. Iterative schemes

Given a certain dependence of the environment inverse temperature $\beta^{(i)}_\omega(E)$, one may obtain from a MC run a point estimation of the system inverse temperature $\beta_i$, the curvature $\kappa_i$, as well as the third and fourth derivatives of the entropy per particle $\zeta^3_i$ and $\zeta^4_i$ at the $i$th intersection point $\varepsilon_i$. One can use these values to provide the next dependence $\beta^{(i+1)}_\omega(E)$. The linear ansatz (3) can be rewritten in terms of the energy per particle as follows:

$$\beta_\omega = \beta^*_i + \lambda_i(\varepsilon - \varepsilon^*_i),$$

where $\beta^*_i$ and $\lambda_i$ are determined from the values of $\beta^t_\omega$ and $\beta^i_\omega$.

$$\beta^t_\omega = \frac{1}{2}(\beta^i_\omega + \beta^f_\omega).$$

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where $\varepsilon_i^*$ and $\beta_i^*$ are rough estimates of the correct values $\varepsilon_i$ and $\beta_i$, which are employed here as seed parameters. The coupling constant $\lambda_i$ is provided through its optimal dependence (15):

$$\lambda_i = \lambda_{\Delta}(\kappa_i^*)$$

by using an estimation $\kappa_i^*$ of the curvature at the intersection point $\varepsilon_i$. The seed values $(\varepsilon_i^*, \beta_i^*, \kappa_i^*)$ are obtained from the previous estimated values $(\varepsilon_i, \beta_i, \kappa_i)$ using the power expansions:

$$\varepsilon_{i+1}^* = \varepsilon_i + \Delta \varepsilon$$

$$\beta_{i+1}^* = \beta_i - \kappa_i \Delta \varepsilon + \frac{1}{2} \zeta_3^i \Delta \varepsilon^2,$$

$$\kappa_{i+1}^* = \kappa_i - \zeta_3^i \Delta \varepsilon,$$

where $\Delta \varepsilon$ is the energy step. Here, it is recommended that one consider the power expansion up to the third derivative of the entropy per particle $\zeta_3^i$, because the calculation of the fourth derivative $\zeta_4^i$ can only be achieved with sufficient precision after performing a very large MC run.

### 2.5. Efficiency

The efficiency of MC methods is commonly characterized in terms of the so-called *decorrelation time* $\tau$, that is, the minimum number of MC steps needed to generate effectively independent, identically distributed samples in the Markov chain [8]. Its calculation in this approach can be performed by using the expression

$$\tau = \lim_{M \to \infty} \frac{M \cdot \text{var}(\varepsilon_M)}{\text{var}(\varepsilon_1)},$$

where $\text{var}(\varepsilon_M) = \langle \varepsilon_M^2 \rangle - \langle \varepsilon_M \rangle^2$ is the variance of $\varepsilon_M$, which is defined as the arithmetic mean of the energy per particle $\varepsilon$ over $M$ samples (consecutive MC steps):

$$\varepsilon_M = \frac{1}{M} \sum_{i=1}^{M} \varepsilon_i.$$  

However, the decorrelation time $\tau$ only provides a partial view of the efficiency in the case of the extended canonical MC methods discussed in this work. In general, the efficiency is more appropriately characterized by the number of MC steps $S$ needed to achieve the convergence of a given run. The question is whether the number of MC steps $S$ needed to achieve a convergence of the expectation value $\langle x \rangle$ of a given observable $x$ also depends on its thermal dispersion $\Delta x$. For example, to obtain an estimation of the expectation value $\langle x \rangle$ with a statistical error $\epsilon_x < a$, the number of MC steps $S$ should obey the following inequality:

$$S > \frac{\tau(\Delta x)^2}{a^2}.$$  

While the fluctuating behavior of a given observable $x$ is an intrinsic system feature in canonical MC methods, this is no longer valid in the present framework. In this case, the fluctuating behavior crucially depends on the nature of the external influence acting on

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the system; e.g., the thermal dispersion of the system energy $\Delta E$ depends on the coupling constant $\lambda$ in equation (4). In particular, the number of MC steps $S$ needed to obtain a point of the caloric curve $(\varepsilon, \beta)$ with a precision $\sqrt{\varepsilon^2 + \beta^2} < a$ should be evaluated in terms of the total dispersion $\Delta T^2$ introduced in equation (14) as follows:

$$S = \frac{\tau \Delta T^2}{Na^2}.$$  \hspace{1cm} (43)

We refer to the quantity $\eta = \tau \Delta T^2$ as the efficiency factor. Clearly, an extended canonical MC method is as efficient as its efficiency factor $\eta$ is small.

3. Applications

3.1. The Potts model and its extended canonical MC algorithms

For convenience, let us again consider the model system studied in our previous paper [1], namely the $q$-state Potts model [8]:

$$H_q = \sum_{\{ij\}} (1 - \delta_{\sigma_i \sigma_j}), \hspace{1cm} (44)$$

which is defined on the square lattice $L \times L$ with periodic boundary conditions. The sum $\{ij\}$ is over nearest neighbor sites, with $\sigma_i = 1, 2, \ldots, q$ being the spin variable on the $i$th site. According to this model, the system undergoes a continuous phase transition when $q = 2$–4, which turns discontinuous for $q > 4$.

The direct way to implement an extended canonical MC simulation of this model is by the use of a Metropolis importance sample [15, 16], whose transition probability is given by

$$W_i \to f; \beta = \min\{1, \exp(-\beta \delta E_{it})\}.$$  \hspace{1cm} (45)

Besides this last local algorithm, the MC study of the model (44) can be also carried out by using non-local MC methods such as the well known Swendsen–Wang [17, 18] and Wolff [19] clusters algorithms. As discussed elsewhere [8], such clusters algorithms are based on the consideration of the Fortuin–Kasteleyn theorem [26, 27]:

$$Z = \sum_{\text{spins}} e^{-\beta H_q} = \sum_{\text{bonds}} p^b (1 - p)^{N_b} q^{N_c}, \hspace{1cm} (46)$$

which allows a mapping of this model system to a random clusters model of percolation. Here, $p = 1 - e^{-\beta}$ is the acceptance probability of bonds, $N_c$ is the number of clusters, $b$ is the number of bonds, $N_b$ is the total number of possible bonds, and $q$ is the number of different states of any spin variable $\sigma$ ($q = 2$ for the Ising model).

To implement the extended clusters algorithms, let us denote by $p_i = 1 - e^{-\beta_i}$ the acceptance probability for bonds for the direct process. The transition probability $W_{i \to f}$ in this case can be expressed as follows:

$$W_{i \to f} = p_i^b (1 - p_i)^{b_a + b_d}, \hspace{1cm} (47)$$

where $b_o$ ($b_p + b_d$) is the number of inspected bonds which have been accepted (rejected). At this point, it is also important to identify the number of rejected bonds $b_d$ which have
been destroyed in the final configuration $X_f$, as well as the number $b_c$ of created bonds. Notice that these bonds are responsible of the energy variation $\delta E_{if}$ after the transition, $\delta E_{if} = b_d - b_c$. In the reverse process, the accepted bonds $b_a$ of the direct process are also accepted with probability $p_f = 1 - e^{-\beta^f}$, while the created bonds $b_c$ as well as the rejected bonds $b_p$ that have not been destroyed in the final configuration $X_f$ are now rejected with probability $1 - p_f$. Thus, the transition probability of the reverse process $W_{f \rightarrow i}$ can be expressed as follows:

$$W_{f \rightarrow i} = p_f^{b_a} (1 - p_f)^{b_p + b_c}. \quad (48)$$

For within the canonical ensemble, where $p_i = p_f = 1 - e^{-\beta^i}$, it is easy to see that the transition probability obeys the detailed balance condition:

$$\frac{W_{f \rightarrow i}}{W_{i \rightarrow f}} = \exp(\beta^i E_{ij}), \quad (49)$$

In the general case with $\lambda > 0$, one introduces the a posteriori acceptance probability (33) to fulfil the detailed balance, which can be expressed as follows:

$$w_{i \rightarrow f} = \min\left[1, \frac{p_f^{b_a} (1 - p_f)^{b_p + b_c}}{p_i^{b_a} (1 - p_i)^{b_p + b_d}} \exp(-\beta^i \omega \delta E_{if})\right] = [1, \exp(\theta_{if})], \quad (50)$$

where the argument $\theta_{if}$ depends on the integer numbers $(b_a, b_p, b_c, b_d)$:

$$\theta_{if} = b_a \log \left(\frac{p_f}{p_i}\right) - \frac{1}{2N} \lambda (b_d - b_c)(2b_p + b_c + b_d). \quad (51)$$

This last result can be easily obtained by considering the definitions

$$p_i = 1 - e^{-\beta^i}, \quad p_f = 1 - e^{-\beta^f}, \quad (52)$$

and noticing the relations

$$\beta^i_{\omega} = \beta^f_{\omega} - \lambda \delta E_{if} / 2N, \quad \beta^f_{\omega} = \beta^i_{\omega} + \lambda \delta E_{if} / 2N, \quad (53)$$

with $\delta E_{if} = b_d - b_c$.

### 3.2. Results and discussion

Results derived from the extended versions of the Metropolis importance sample, as well as the Swendsen–Wang and Wolff clusters algorithms, are shown in figure 2 for the particular case of the 2D seven-state Potts model with $L = 25$. Each point of these dependences has been obtained from MC runs with $10^6$ steps. For comparison purposes, we have also carried out the calculation of the caloric $\beta(\varepsilon)$ and the curvature $\kappa(\varepsilon)$ curves, performing a direct numerical differentiation of the entropy per particle $s(\varepsilon) = \log \Omega(E)/N$ obtained from the Wang–Landau sampling method [29], which is shown in the inset panel ($N = L^2$). Although there is a good agreement among all these MC results, the ones obtained from the Wang–Landau method seem to be less significant; overall, the results correspond to the curvature curve $\kappa(\varepsilon)$.

Previous results constitute a clear illustration of the finite size corrections introduced in section 2.2 providing a significant improvement in the precision of these kinds of MC calculations. In this particular example with $L = 25$, the first-order corrections of the
finite size effects in the caloric curve $\beta(\epsilon)$ have a typical order of $\delta_1 \sim 10^{-3}$, while those corresponding to the second-order correction are of order $\delta_2 \sim 10^{-5}$. Nevertheless, the most significant correction of the finite size effects in non-local canonical MC methods comes from the fulfillment of the detailed balance condition (30) obtained after introducing an a posteriori acceptance probability (33) whose correction has a typical order of $\delta_{db} \sim 10^{-2}$. This fact can be observed in figure 3 for the case of the Swendsen–Wang clusters algorithm.

Although the acceptance probability $w_{1 \rightarrow f}$ for clusters flipping is lower than unity, its expectation value $p = \langle w_{1 \rightarrow f} \rangle$ is significantly high for every energy value (see also figure 3). Since the consideration of such an a posteriori acceptance probability $w_{1 \rightarrow f}$ amends a finite size error $\delta_\beta = |\beta^i - \beta^t|$ associated with the estimation of the transition inverse temperature $\beta^t$, one should expect a growth of the expectation value $\langle w_{1 \rightarrow f} \rangle$ as $N$ increases. Such a behavior is indeed observed in figure 4 for the extended clusters algorithms. While all these dependences have a similar qualitative behavior, the expectation value of the acceptance probability $\langle w_{1 \rightarrow f} \rangle$ of the extended Wolff clusters algorithm in the paramagnetic region is larger than the one corresponding to the extended Swendsen–Wang method. This is a quite expected qualitative result. The acceptance probability $w_{1 \rightarrow f}$ rectifies a finite size error $\delta_\beta = |\beta^i - \beta^t|$ related to the flipping of only one cluster in the case of the extended Wolff method, while the finite size error $\delta_\beta$ associated with the extended Swendsen–Wang method is larger due to this MC algorithm involving the flipping of all system clusters.

At low energies or in the ferromagnetic region, these methods have practically the same performance, since the number of spins belonging to the cluster is comparable to the system size $N$. (For a more detailed comparison, see the inset panel in figure 4.)

The qualitative behavior of the dependence $\langle w_{1 \rightarrow f} \rangle$ versus $\epsilon$ finds a simple explanation in terms of the explicit dependence of the acceptance probability $w_{1 \rightarrow f}$ on the coupling

$$s = \log \Omega / N$$

obtained by using the Wang–Landau sampling method.

Figure 2. Microcanonical caloric and curvature curves associated with the 2D seven-state Potts model obtained from the application of the extended canonical MC algorithms (MIS: Metropolis importance sample, SW: Swendsen–Wang, and WF: Wolff clusters algorithm). Such results can be compared with the ones obtained from a direct numerical differentiation of the entropy per particle $s = \log \Omega / N$ obtained by using the Wang–Landau sampling method.
Figure 3. Microcanonical caloric curves $\beta(\epsilon)$ showing the different corrections of finite size effects corresponding to the Swendsen–Wang clusters algorithm. We also show here the expectation value of the acceptance probability $p = \langle w_{i\rightarrow f} \rangle$ versus energy per particle $\epsilon$ corresponding to the extended Swendsen–Wang algorithm obeying detailed balance.

Figure 4. Size dependence of the expectation value of the a posteriori acceptance probability $p = \langle w_{i\rightarrow f} \rangle$ for extended clusters algorithms.

constant $\lambda$. While the acceptance probability $w_{i\rightarrow f} \equiv 1$ within the canonical ensemble where $\lambda = 0$, this quantity undergoes a reduction with increase of the coupling constant $\lambda$. Moreover, the optimal value of the coupling constant $\lambda_{\Delta} = \sqrt{1 + \kappa^2} - \kappa$ employed in the present MC simulations increases with reduction of the system curvature $\kappa$. Indeed, the lowest values of $\langle w_{i\rightarrow f} \rangle$ are observed in the energy region where the system curvature also exhibits its lower values, that is, the anomalous region with negative heat capacities $C < 0$. 

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Figure 5. Main panel: size dependence of the decorrelation time $\tau$ and the efficiency factor $\eta = \tau \Delta^2 T$ for the extended canonical MC simulations with the environment inverse temperature $\beta_\omega(\varepsilon) = \beta_e + \lambda (\varepsilon - \varepsilon_e)$. Here, $\beta_e = \beta_{pt}$, $\varepsilon_e = \varepsilon_2$, $\lambda = \lambda_\Delta(\kappa_2)$ and $\kappa_2 = \kappa(\varepsilon_2)$, where $\beta_{pt}$ is the estimated inverse temperature that corresponds to the discontinuous PT, while $\varepsilon_2$ is the stationary solution derived from the thermal equilibrium condition $\beta(\varepsilon_2) = \beta_{pt}$ located within the region with negative heat capacities $C < 0$. Inset panel: size dependence of the entropy per particle $s(\varepsilon)$, or more exactly, the quantity $s^*(\varepsilon) = s(\varepsilon) - \beta_{pt}\varepsilon + \text{const}$, which allows us to show the convex intruder associated with the region with negative heat capacities. The energies corresponding to the two maxima $(\varepsilon_1, \varepsilon_3)$ and the minimum $\varepsilon_2$ are the three stationary solutions derived from the thermal equilibrium condition $\beta(\varepsilon_{1,2,3}) = \beta_{pt}$.

The size dependences of the decorrelation time $\tau$ and the efficiency factor $\eta = \tau \Delta^2 T$ within the anomalous region with $C < 0$ are shown in the main panel of figure 5; these were obtained from MC simulations with lattice sizes $L = (8, 16, 32, 64, 128)$. Since the absolute values of the curvature $\kappa$ are close to zero, $|\kappa| \simeq 0$, the total dispersion is approximately given by the constant value $\Delta^2 T \simeq 2$, in accordance with equation (15). This is why the dependences $\tau(N)$ and $\eta(N)$ are almost displaced by a constant value along the vertical direction of the log–log graph shown in figure 5.

As expected, the extended version of the Metropolis importance sample exhibits the largest values of the decorrelation time $\tau$ for the lattice sizes $L$ studied in this work. Curiously, the size dependence of its decorrelation time $\tau(N)$ shows an abrupt transition from a power-law regime with exponent $\alpha_1 \simeq 0.72$ to another one with exponent $\alpha_2 \simeq 0.14$ close to $N \simeq 10^3$ ($L = 32$). Despite the extended Metropolis importance sampling being a local MC method, the effective exponent $\alpha_2$ for the larger system sizes is comparable to the ones associated with the extended clusters MC methods, $\alpha_{SW} \simeq 0.18$ (Swendsen–Wang) and $\alpha_{WF} \simeq 0.15$ (Wolff). Notice also that the efficiency of these extended clusters methods is still significant despite the consideration of the a posteriori acceptance probability (50) employed here to ensure the detailed balance condition (30).

The above examples confirm that the efficiency achieved with the application of the present methodology is remarkable. In fact, it is more significant than the one achieved
with the application of reweighting techniques such as the multicanonical method and its variant, whose typical values of the exponent $\alpha$ range from 2 to 2.5 in the case of Potts models [28]. As already evidenced in figure 2, while the Wang–Landau sampling method provides a good estimation of the entropy per particle $s(\varepsilon)$, its underlying statistical errors are still notorious for the curvature curve $\kappa(\varepsilon) = -\partial^2 s(\varepsilon)/\partial \varepsilon^2$ regardless of whether or not the simulation is extended until the modifying factor fulfills the condition $f_i < \exp(10^{-10})$. Such an observation evidences that the results obtained from this last method are not sufficiently relaxed to provide a precise estimation of the curvature curve $\kappa(\varepsilon)$. By considering the CPU time/cost needed to achieve the convergence, it is more convenient to perform a point estimation of the caloric $\beta(\varepsilon)$ and curvature $\kappa(\varepsilon)$ curves using the present methodology instead of carrying out a direct numerical differentiation of the microcanonical entropy $s(\varepsilon)$ obtained from a reweighting technique.

4. Conclusions

In this work, the methodology for extending canonical MC methods inspired by the consideration of the fluctuation relation (2) has been improved to achieve fulfillment of the detailed balance condition (30) and to account for the existence of finite size effects. Remarkably, despite the consideration of the a posteriori acceptance probability (33), it has been shown that the relaxation times needed to ensure the convergence with this method are more significant than the ones achieved with reweighting techniques. For the particular case of the seven-state Potts model, the consideration of any extended canonical MC algorithm enables a suppression of the supercritical slowing down from an exponential growth to a very weak power-law dependence with exponent $\alpha = 0.14–0.18$.

There are still some open questions as regards the potential applications of the present methodology. For example, although this method has been specially conceived to overcome the slow relaxations of canonical MC simulations near to a region with a first-order phase transition, in principle, there is no limitation and the same approach can also be employed to improve canonical MC simulations near to a critical point of a continuous phase transition. Moreover, a similar extension can be carried out for the MC methods based on the consideration of the Boltzmann–Gibbs distributions:

$$dp_{BG}(E, X) = \frac{1}{Z(\beta, Y)} \exp[-\beta(E + YX)] \, dE \, dX \quad (54)$$

To account for the existence of anomalous values in other response functions, besides the heat capacity. The analysis of these questions deserves special attention in future works.

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Appendix. Derivation of correction formulae

The energy distribution function $\rho(E) = \omega_G(E)\Omega(E)$ in terms of the energy per particle $\varepsilon = E/N$ can be expressed as follows:

$$\rho(\varepsilon) = \frac{1}{Z_\lambda} \exp[-N\phi(\varepsilon)], \quad (A.1)$$

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where the function \( \phi(\epsilon) \equiv \beta e + \frac{1}{2} \lambda (\epsilon - \epsilon_e)^2 - s(\epsilon) \), with \( s(\epsilon) \) being the entropy per particle, and \( \beta_e \), given by

\[
\beta_e = \frac{\partial s(\epsilon_e)}{\partial \epsilon_e},
\]

is the system inverse temperature at the stationary point \( \epsilon_e \). Let us now develop a power expansion:

\[
\phi(\epsilon + x) = \phi(\epsilon) + \frac{1}{2} (\lambda + \kappa_e) x^2 + \sum_{n=3}^{\infty} a_n x^n,
\]

with \( \kappa_e = -\frac{\partial^2 s(\epsilon_e)}{\partial \epsilon^2} \) being the curvature. The Gaussian approximation is developed by ignoring those terms with \( n > 2 \). Here, the energy deviation \( x \) obeys a Gaussian distribution:

\[
\rho^{(0)}(x) \, dx \simeq \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \, dx
\]

with standard deviation \( \sigma \):

\[
\sigma^2 = \frac{1}{N(\lambda + \kappa_e)}.
\]

and the partition function \( Z_\lambda \) can be approximated as

\[
Z_\lambda = e^{-N\phi(\epsilon_e)} \sqrt{2\pi\sigma}.
\]

Notice that equation (A.5) is fully equivalent to equation (13) since the standard deviation \( \sigma \equiv \Delta E/N \). Equation (A.6) can be rewritten as follows:

\[
P_\lambda \simeq \beta_e E_e - S(E_e) + \frac{1}{2} \log(2\pi\sigma^2),
\]

where \( P_\lambda = -\log Z_\lambda \) can be referred to as the Planck thermodynamic potential corresponding to the Gaussian ensemble (18). By taking the thermodynamic limit \( N \to \infty \), this thermodynamic function can be related to the known Legendre transformation with the microcanonical entropy

\[
p_\lambda = \lim_{N \to \infty} \frac{P_\lambda}{N} = \beta_e \epsilon_e - s(\epsilon_e).
\]

Clearly, the Gaussian ensemble (18) provides a suitable extension of the Gibbs canonical ensemble (1) that is able to deal with the existence of macrostates with negative heat capacities \( C < 0 \). In fact, it is a particular example of the so-called generalized canonical ensembles that preserve some of its more relevant features \([11,30,31]\).

The first correction of the Gaussian approximation (A.4) is obtained by ignoring terms with \( n > 3 \) in the power expansion (A.3):

\[
N\phi(x) = N\phi_0 + \frac{1}{2\sigma^2} x^2 + \xi x^3 + O(x^4),
\]

where

\[
\xi = -\frac{1}{6} N \frac{\partial^3 s(\epsilon_e)}{\partial \epsilon^3}.
\]
For convenience, let us introduce the dimensionless variable \( \theta = x/\sigma \). By considering the size dependences \( \xi \sim N \) and \( \sigma \sim 1/\sqrt{N} \), it is possible to verify that the cubic term \( \xi x^3 \equiv \xi \sigma^3 \theta^3 \) decreases as \( 1/\sqrt{N} \) with increase of the system size \( N \). Thus, one arrives at the distribution function

\[
\rho^{(1)}(\theta) \, d\theta \sim \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(\theta^2)} \left(1 - \xi \sigma^3 \theta^3\right) \, d\theta. \tag{A.11}
\]

This last result leads to the following expectation values:

\[
\langle \theta \rangle = -3\xi \sigma^3, \quad \langle \theta^2 \rangle = 1, \quad \langle \theta^3 \rangle = -15\xi \sigma^3, \tag{A.12}
\]

which allow us to express the expectation value of the energy deviation \( \langle x \rangle \) as well as its second- and third-order dispersions, \( \langle \delta x^2 \rangle \) and \( \langle \delta x^3 \rangle \), as follows:

\[
\langle x \rangle = -3\xi \sigma^4 + O\left(\frac{1}{N^2}\right), \quad \langle \delta x^2 \rangle = \sigma^2 + O\left(\frac{1}{N^2}\right), \tag{A.13}
\]

\[
\langle \delta x^3 \rangle = -6\xi \sigma^6 + O\left(\frac{1}{N^3}\right). \tag{A.14}
\]

The previous results can be combined with the linear ansatz (3) to obtain the following first-order correction of equation (9):

\[
E_e = \langle E \rangle - \frac{1}{2} \langle \delta E^2 \rangle \langle \delta E^3 \rangle, \tag{A.15}
\]

\[
\beta_e = \langle \beta \rangle - \lambda \frac{1}{2N} \langle \delta E^2 \rangle \langle \delta E^3 \rangle. \tag{A.16}
\]

The second-order correction of the Gaussian contributions is carried out by ignoring terms with \( n > 4 \) in power expansion (A.3):

\[
N \phi(x) = \frac{1}{2\sigma^2} x^2 + \xi x^3 + \xi_2 x^4 + O(x^5), \tag{A.17}
\]

where

\[
\xi_2 = -\frac{1}{24} N \frac{\partial^4 s(\varepsilon)}{\partial \varepsilon^4}. \tag{A.18}
\]

These terms lead to the following correction of the distribution function:

\[
\rho^{(2)}(\theta) \, d\theta \sim \frac{e^{-\frac{1}{2}(\theta^2)}}{A\sqrt{2\pi}} \left(1 - \xi \sigma^3 \theta^3 - \xi_2 \sigma^4 \theta^4 + \frac{1}{2} \xi_2 \sigma^6 \theta^6\right) \, d\theta, \tag{A.19}
\]

whose third and fourth terms account for finite size effects of order \( O(1/N) \). On denoting the auxiliary constants \( C_1 \) and \( C_2 \) as follows:

\[
C_1 = \xi \sigma^3, \quad C_2 = \xi_2 \sigma^4, \tag{A.20}
\]

direct calculations allow us to obtain the normalization constant \( A \):

\[
A = 1 - 3C_2 + \frac{15}{2} C_1^2. \tag{A.21}
\]
as well as the following expectation values:

\[ \langle \theta \rangle = -3C_1, \quad \langle \theta^2 \rangle = 1 - 12C_2 + 45C_1^2, \quad (A.22) \]

\[ \langle \theta^3 \rangle = -15C_1, \quad \langle \theta^4 \rangle = 3 - 102C_2 + 465C_1^2. \quad (A.23) \]

While the expressions (A.13) and (A.14) for the expectation values \( \langle x \rangle \) and \( \langle \delta x^3 \rangle \) remain invariable under the second-order approximation, the second- and fourth-order dispersions \( \langle \delta x^2 \rangle \) and \( \langle \delta x^4 \rangle \) exhibit the following corrections:

\[ \langle \delta x^2 \rangle = \sigma^2 \left( 1 - \frac{12}{N}C_2 + \frac{36}{N^3} \right), \quad (A.24) \]

\[ \langle \delta x^4 \rangle = \left( 3 - \frac{102}{N}C_2 + \frac{339}{N^4} \right) \sigma^4 + O \left( \frac{1}{N^4} \right). \quad (A.25) \]

On introducing the cumulants \( \epsilon_1 \) and \( \epsilon_2 \):

\[ \epsilon_1 = \frac{\langle \delta E^3 \rangle^2}{\langle \delta E^2 \rangle^3}, \quad \epsilon_2 = 1 - \frac{\langle \delta E^4 \rangle}{3 \langle \delta E^2 \rangle^2}, \quad (A.26) \]

the auxiliary constants \( C_1^2 \) and \( C_2 \) can be expressed as follows:

\[ C_1^2 = \frac{1}{36} \epsilon_1, \quad C_2 = \frac{1}{10} \epsilon_2 + \frac{41}{360} \epsilon_1. \quad (A.27) \]

Thus, the main working equations (9) and (13) can be expressed in this second-order approximation as follows:

\[ E_e = \langle E \rangle - \frac{1 - \psi_1}{2 \langle \delta E^2 \rangle} \langle \delta E^3 \rangle, \quad (A.28) \]

\[ \beta_e = \langle \beta_\omega \rangle - \lambda \frac{1 - \psi_1}{2N \langle \delta E^2 \rangle} \langle \delta E^3 \rangle, \quad (A.29) \]

\[ \kappa_e = \frac{1 - \psi_1 - \lambda \langle \Delta E \rangle^2 / N}{\langle \Delta E \rangle^2 / N}, \quad (A.30) \]

where \( \psi_1 \) is a second-order term defined by the cumulants \( \epsilon_1 \) and \( \epsilon_2 \) as

\[ \psi_1 \equiv \frac{6}{5} \epsilon_2 + \frac{11}{30} \epsilon_1. \quad (A.31) \]

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