Enhancing Monte Carlo methods by using a generalized fluctuation theory

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Abstract
According to the recently obtained thermodynamic uncertainty relation \( \langle \delta \beta \delta E \rangle = 1 + \frac{\partial^2 S}{\partial E^2} \langle \delta E^2 \rangle \), the microcanonical regions with a negative heat capacity can be accessed within a canonical-like description by using a thermostat with a fluctuating inverse temperature. This far-reaching conclusion is used in this Letter for enhancing the potentialities of the well-known Swendsen-Wang cluster algorithm in order to access to the anomalous microcanonical states of the \( q = 10 \) state Potts model on a square lattice \( L \times L \), which exhibits a first-order phase transition in its thermodynamical description.

The present approach for enhancing the Monte Carlo methods based on the equilibrium distributions of the Statistical Mechanics [1] is straightforwardly followed as a direct application of a non Riemannian framework of the Equilibrium Thermodynamics recently proposed in the refs. [2, 3]. A fundamental result derived from this theory is the following thermodynamic identity:

\[
\langle \delta \beta \delta E \rangle = 1 + \frac{\partial^2 S}{\partial E^2} \langle \delta E^2 \rangle,
\]

where \( \beta \) characterized the effective inverse temperature of certain generalized thermostat and \( E \) the total energy of the interest system. This expression generalizes the well-known relation \( C = \beta^2 \langle \delta E^2 \rangle \) between the heat capacity \( C = dE/dT \) and the energy fluctuations within the Gibbs canonical description towards all those microcanonical regions hidden by the ensemble inequivalence, that is, all those energetic regions characterized by the presence of negative heat capacities [1]:

\[
C = - \left( \frac{\partial S}{\partial E} \right)^2 \left( \frac{\partial^2 S}{\partial E^2} \right)^{-1},
\]

associated to the convex character of the Boltzmann entropy \( S = \ln W \).

The thermodynamic identity [1] naturally appears within the generalized framework under the hypothesis of the ensemble equivalence. Thus, the ordinary condition \( \delta \beta = 0 \) associated to the Gibbs canonical description is only admissible wherever the entropy be a concave function \( \partial^2 S/\partial E^2 < 0 \) (convex-down). The identity [1] leads to the following inequality:

\[
\langle \delta \beta \delta E \rangle \geq 1
\]

wherever the entropy be locally convex \( \partial^2 S/\partial E^2 \geq 0 \) (convex-up). This means that the anomalous regions with a negative heat capacity could be only accessed by using a generalized thermostat exhibiting correlated fluctuations of its effective inverse temperature \( \beta \) with the fluctuations of the total energy \( E \) of the interest system. This far-reaching conclusion could be a fundamental ingredient for allowing the improvement of many Monte Carlo algorithms based on the Gibbs canonical ensemble for deal with the presence of first-order phase transitions without the necessity of appealing to multicanonical methods [1]. The aim of the present Letter is to show a numerical evidence which seems to support the above ideas.

The reader can also notice that the inequality [1] looks-like an uncertainty relation, which allows us to claim that the inverse temperature of the thermostat \( \beta \) and the total energy of the interest system \( E \) can be considered as complementary thermodynamical quantities within the regions of ensemble inequivalence. The energy fluctuations \( \delta E \) can not be reduced there without an increasing the fluctuations of the inverse temperature \( \delta \beta \) of the generalized thermostat, and vice versa. Thus, the identity [1] can be referred as a thermodynamic uncertainty relation since it imposes certain restrictions to the determination of the microcanonical caloric curve.

The understanding of the methodology introduced in this Letter demands to carry out a summary of the geometric foundations leading to the thermodynamic uncertainty relation [1]. I shall only exposed here the fundamental points, so that, the interested reader should see the refs. [2, 3] for more details.

Let be an isolated Hamiltonian system \( \hat{H}_N \) whose macroscopic description can be performed starting from microcanonical basis by considering only the total energy \( E = \hat{H}_N \). Let \( \Theta = \Theta (E) \) be any diffeomorphism (a bijective and piece-wise differentiable function) of the total energy \( E \). It is said that the functional \( \hat{\Theta}_N = \Theta (\hat{H}_N) \) constitutes a reparametrization of the Hamiltonian \( \hat{H}_N \). It is easy to show that the Physics within the microcanonical description is reparametrization invariant:

\[
\hat{\omega}_M (E) = \frac{1}{\Omega (E, N)} \delta \left[ E - \hat{H}_N \right],
\]

\[
\equiv \frac{1}{\Omega (\Theta, N)} \delta \left[ \Theta - \hat{\Theta}_N \right] = \hat{\omega}_M (\Theta). \tag{4}
\]

The demonstration is straightforwardly followed from the properties of the Dirac function. Such feature implies that the microcanonical average \( \langle A \rangle = SP \left( \hat{\omega}_N \hat{A} \right) \) of any microscopic observable \( \hat{A} \) is also reparametriz-
tion invariant, \( \langle A \rangle (E) = \langle A \rangle (\Theta) \), that is, these averages can be taken as scalar functions under the energy reparametrization changes. The microcanonical partition function \( \Omega(\Theta, N) = Sp \left \{ \exp \left[ -\frac{1}{\eta} \Theta N \right] \right \} \) allows us to introduce the invariant measure of the phase space volume:

\[
d\mu = \Omega(\Theta, N) d\Theta = \Omega(E, N) dE,
\]

which leads to an reparametrization invariant definition of the microcanonical entropy \( S = \ln W_\alpha \), where \( W_\alpha = \int_{\Sigma_\alpha} d\mu \), being \( \Sigma_\alpha \) a subset of certain coarsed grained partition of the phase space. Such a coarsed grained nature of the entropy can be disregarded in the thermodynamic limit \( N \to \infty \) and this thermodynamic potential can be considered as a continuous scalar function. The estimation \( W_\alpha \simeq \Omega(\Theta, N) \delta \Theta_0 \) can be used whenever the subset \( \Sigma_\alpha \) be small, a condition which is always justified when \( N \) is large enough without any lost of generality \cite{2}.

The concavity of a scalar function as the microcanonical entropy \( S \) depends crucially on the reparametrization used for describing the thermodynamical properties, which is explained by the presence of the term \( \partial S/\partial \Theta \) in the transformation rule of the entropy Hessian during the reparametrization \( E \leftrightarrow \Theta \):

\[
\frac{\partial^2 S}{\partial E^2} = \left( \frac{\partial \Theta}{\partial E} \right)^2 \frac{\partial^2 S}{\partial \Theta^2} + \frac{\partial^2 \Theta}{\partial E^2} \frac{\partial S}{\partial \Theta}.
\]

A trivial example is the concave function \( s(x) = \sqrt{x} \) with \( x > 0 \), which becomes a convex function \( s(y) = y^2 \) after consider the reparametrization \( y = \sqrt{x} \).

The concavity of the microcanonical entropy is an important condition for the ensemble equivalence. The modifying of the entropy convex properties during the energy reparametrization changes is a very simple alternative for ensure the ensemble equivalence within a canonical-like description. This kind of framework demands the introduction of the called generalized Gibbs canonical ensemble:

\[
\omega_{GC}(\eta) = \frac{1}{Z(\eta, N)} \exp \left[ -\frac{1}{\eta} \Theta N \right],
\]

which describes the equilibrium conditions of the interest system under the external influence of a generalized thermostat with generalized canonical parameter \( \eta \). It is easy to show that this distribution function is derived within the Jaynes reinterpretation of the Thermodynamics in terms of the Information theory \cite{3} by imposing the constrain:

\[
\langle \Theta \rangle = \sum_k \Theta(E_k) p_k,
\]

instead of the usual energy constrain with \( \Theta(E) = E \), a viewpoint recently developed by Toral in the ref.\cite{3}. This last observation clarifies us that the role of the generalized thermostat is precisely to impose the constrain \cite{3}.

The generalized partition function \( Z(\eta, N) = Sp \left \{ \exp \left[ -\frac{1}{\eta} \Theta N \right] \right \} \) can be rewritten in terms of the microcanonical partition function \( \Omega(E, N) \) as follows:

\[
Z(\eta, N) = \int \exp \left[ -\frac{1}{\eta} \Theta \right] \Omega(E, N) dE
\]

\[
\equiv \int \exp \left[ -\frac{1}{\eta} \Theta \right] \Omega(\Theta, N) d\Theta,
\]

where the invariant character of the measure possibilities us to rephrase the generalized partition function as an usual Laplace transformation. The imposition of the thermodynamic limit \( N \to \infty \) leads to the validity of the Legendre transformation between the Thermodynamic potentials \( P \) and \( S \):

\[
P(\eta) = \inf_{\Theta} \left \{ \eta \Theta - S(\Theta, N) \right \},
\]

being \( P(\eta, N) = -\ln Z(\eta, N) \) the Planck potential associated to the generalized canonical ensemble \cite{7}, whenever there is only one point \( \Theta^* \) satisfying the stationary conditions:

\[
\eta = \frac{\partial S(\Theta^*, N)}{\partial \Theta} \quad \text{and} \quad \kappa_\Theta = \frac{\partial^2 S(\Theta^*, N)}{\partial \Theta^2} < 0.
\]

within the energy reparametrization \( \Theta = \Theta(E) \).

While the microcanonical ensemble is reparametrization invariant \cite{2}, the generalized Gibbs canonical description \cite{7} depends crucially on the energy reparametrization. Nevertheless, these equilibrium statistical descriptions becomes asymptotic equivalent with the imposition of the thermodynamic limit \( N \to \infty \) with the exception of all those microcanonical regions where the convex-down character of the entropy \( S \) in the energy reparametrization \( \Theta \) can not be ensured.

The reader can notice that the using of energy reparametrizations \( \Theta = \Theta(E) \) allows us to extend many results and methodologies of the standard Thermodynamics and Boltzmann-Gibbs Statistical Mechanics with a simple change of reparametrization \( (\beta, E) \to (\eta, \Theta) \). This viewpoint was considered in the ref.\cite{3} for introduce a variant of the Metropolis importance sample algorithm \cite{4} based on the generalized canonical weight \( \exp \left[ -\frac{1}{\eta} \Delta \Theta \right] \) instead on the usual \( \exp \left( -\beta \Delta E \right) \), being \( \Delta \Theta = \Theta(E + \Delta E) - \Theta(E) \). Since \( |\Delta E| \ll |E| \) during a Metropolis move when \( N \) is large enough, the approximation \( \Delta \Theta \simeq \partial \Theta(E)/\partial E \Delta E \) allows us to rephrase the corresponding acceptance probability \( p \):

\[
p \simeq \min \left \{ 1, \exp \left[ -\beta \Delta E \right] \right \},
\]

as an ordinary Metropolis move with a variable inverse temperature:

\[
\beta = \beta(E; \eta) = \frac{\partial \Theta(E)}{\partial E}.
\]
This results allows us to understand that the generalized thermostat associated to the ensemble (13) can be taken without any lost of generality when \( N \) is large enough as an ordinary Gibbs thermostat with a variable inverse temperature (19) which fluctuates around the equilibrium value \( \beta^* = \beta (E^*; \eta) \), being \( E^* \) the equilibrium energy corresponding to the stationary point \( \Theta^* = \Theta (E^*) \). The inverse temperature fluctuations of such generalized thermostat \( \delta \beta = \beta (E; \eta) - \beta (E^*; \eta) \simeq (\eta \partial \Theta (E^*) / \partial E^2) * \delta E \) are correlated to the energy fluctuations of the interest system \( \delta E = E - E^* \) as follows:

\[
\langle \delta \beta \delta E \rangle \simeq \eta \partial \Theta (E^*) / \partial E^2 \langle \delta E^2 \rangle . \tag{14}
\]

Taking into account the approximation \( \delta \Theta = \Theta (E) - \Theta (E^*) \simeq [\partial \Theta (E^*) / \partial E] * \delta E \) and the well-known relation between the fluctuations \( \langle \delta \Theta ^2 \rangle \) with the entropy Hessian \( \partial^2 S / \partial \Theta^2 \) within the Gaussian approximation \( \langle \delta \Theta ^2 \rangle \simeq - (\partial^2 S / \partial \Theta^2)^{-1} \) (now in terms of the energy reparametrization \( \Theta \)), the inverse of the average square dispersion of the energy \( \langle \delta E^2 \rangle \) can be expressed as follows:

\[
\langle \delta E^2 \rangle ^{-1} = - (\partial \Theta (E^*) / \partial E)^2 \partial^2 S (\Theta^*) / \partial \Theta^2 . \tag{15}
\]

Finally, by combining the stationary condition (11) and the transformation rule (9):

\[
\eta \partial \Theta / \partial E^2 = \partial S \partial \Theta / \partial E^2 = \partial^2 S / \partial E^2 - (\partial \Theta / \partial E)^2 \partial^2 S / \partial \Theta^2 , \tag{16}
\]

as well as the equation (15), the thermodynamic uncertainty relation (1) is obtained.

Let us now consider that the interest system becomes extensive with the imposition of the thermodynamic limit and the same one exhibits an ensemble inequivalence inside the energy interval \( (\varepsilon_1, \varepsilon_2) \), where \( \partial^2 s (\varepsilon_i) / \partial \varepsilon^2 < 0 \), being \( \varepsilon = E/N \) and \( s = S/N \) the energy and the entropy per particle respectively. Everything that should be taking into consideration for the convergence of the Metropolis algorithm described above is the use of an appropriate energy reparametrization \( \Theta = \Theta (E) \). Obviously, there exist an undeterminable number of possibilities in order to perform such selection.

A convenient choice of the energy reparametrization under the above background conditions is given by \( \Theta (E) = N \varphi (E/N) \), where the first derivative of the bijective function \( \varphi (\varepsilon) \) is taken as follows:

\[
\xi (\varepsilon) = \partial \varphi (\varepsilon) / \partial \varepsilon = \exp (-\lambda (\varepsilon_2 - \varepsilon)) \tag{17}
\]

being \( \lambda \) a large enough positive constant. Thus, the effective inverse temperature of the thermostat in terms of the instantaneous value of the energy per particle \( \varepsilon \) of the interest system is given by \( \beta (\varepsilon; \eta) = \eta \xi (\varepsilon) \). It can be verified that an unnecessary large value of \( \lambda \) leads to an increasing of the inverse temperature fluctuations. An appropriate prescription for the value of \( \lambda \) is given by \( \lambda \gtrsim \beta_c^{-1} \), being \( \beta_c \) an estimation of the critical inverse temperature of the first-order phase transition. Each point of the caloric curve \( \beta \) versus \( \varepsilon \) is determined from the averages \( \langle \varepsilon \rangle \) and \( \langle \beta (\varepsilon; \eta) \rangle \) taken from a Metropolis dynamics by keeping fixed the canonical parameter \( \eta \) of the generalized thermostat. The second derivative of the entropy per particle is obtained from the thermodynamic uncertainty relation (11). The whole simulation can start from \( \eta = \beta_2 \), being \( \beta_2 \) the corresponding inverse temperature at the point \( \varepsilon_2 \), where \( \eta \) is increased until the caloric curve be obtained for all the energetic interval \( (\varepsilon_1, \varepsilon_2) \).

The variant of the Metropolis algorithm described above seems to be a very general alternative to avoid the anomalies related with the presence of a first-order phase transitions in the short-range interacting systems. An example of application was presented in the ref.[3] in order to obtain the microcanonical calorific curve of the \( q = 10 \) states Potts model:

\[
\hat{H}_N = \sum_{\{\sigma\}} (1 - \delta_{\sigma_i, \sigma_j}) , \tag{18}
\]

on a square lattice with \( N = L \times L \) with periodic boundary conditions, whose microcanonical description shows the existence of a first-order phase transition. The sum is over pairs of nearest neighbor lattice points only and \( \sigma_i \) is the spin state at the \( i \)-th lattice point.

Generally speaking, any Metropolis algorithm is more inefficient than other nonlocal Monte Carlo methods involving clusters algorithms. However, the use of such clusters algorithms can be limited by the phenomenon of the ensemble inequivalence. For example, the clusters algorithms for the Potts model (9) are based on a mapping of this model system to a random clusters model of percolation throughout the equation:

\[
Z = \sum_{\{\sigma\}} \exp \left[ -\beta \hat{H}_N \right] = \sum_{\{\pi\}} q^{N_c} p^b (1 - p)^{N_d - b} , \tag{19}
\]

where \( p = 1 - \exp (1) \), \( b \) is the number of bonds, \( N_c \) the number of clusters and \( d \) the dimension of the lattice. Whilst such Monte Carlo methods allow in general an efficient calculation of the thermodynamic properties of the Potts models, they can undergo a supercritical slowing down whenever an ensemble inequivalence exists within the canonical description.

The ensemble inequivalence can be avoided by using the generalized canonical description (17) instead of the usual canonical description. A very important question is how to develop suitable clusters algorithms within the framework of the generalized canonical ensemble (4). A serious obstacle is the nonlinear character of the energy reparametrization \( \Theta = \Theta (E) \), i.e.: the linear character of the energy reparametrization \( \Theta (E) = E \) is crucial for the
mapping of the Potts model described by the equation [10]. However, there could be a very simple way to avoid such difficulties. The reader can notice that the thermodynamic uncertainty relation [11] does not make an explicit reference to the particular energy reparametrization $\Theta (E)$ used during its derivation. This remarkable feature suggests us that actually there is not needing to perform an exact Monte Carlo implementation of the generalized canonical ensemble [7] when the system size $N$ is large enough, that is, all that it needs to demand in order to avoid the ensemble inequivalence is the use of a generalized thermostat with a fluctuating inverse temperature.

Such a working hypothesis leads to propose the following scheme for enhancing the potentialities of any Monte Carlo algorithm based on the Gibbs canonical ensemble in order to deal with the ensemble inequivalence: (1) To generate a new configuration $X_i$ from the previous configuration $X_{i-1}$ by using a Monte Carlo method with constant inverse temperature $\beta$; (2) Redefine the inverse temperature of the thermostat $\beta = \beta (E; \eta)$ of the next configuration by using the energy $E = H_N (X_i)$ of the present configuration $X_i$. The function $\beta (E; \eta)$ can be taken as the effective inverse temperature [13] associated to the Metropolis algorithm based on the generalized canonical ensemble [7]. The microcanonical calorific curve $\beta (\varepsilon) = \partial s (\varepsilon) / \partial \varepsilon$ can be obtained from the average values of the energy $\langle \varepsilon \rangle$ and the inverse temperature $\langle \beta \rangle \simeq \eta \langle \xi (\varepsilon) \rangle$, while the curvature or the second derivative of the entropy per particle $\kappa (\varepsilon) = \partial^2 s (\varepsilon) / \partial \varepsilon^2$ by means of the relation $\kappa (\varepsilon) = (\sigma_\beta^2 - 1) / \sigma_\varepsilon^2$, being $\sigma_\varepsilon^2 = N \langle \delta \varepsilon^2 \rangle$, $\sigma_\beta^2 = N \langle \delta \beta^2 \rangle$ and $\xi (\varepsilon)$ the function [17].

A complete analysis about the applicability and the convergence of the procedure proposed above to any Monte Carlo algorithm based on the Gibbs canonical ensemble seems to be at first glance a very difficult mathematical task. Nevertheless, the thermodynamic relation [11] constitutes by itself a general result supporting in principle the applicability of such methodology.

Numerical evidences seems to be in agreement with the present viewpoint. The FIG. 1 shows a study where the above procedure was employed in order to combine the potentialities of the well-known Swendsen-Wang cluster algorithm (SW) [9] and the use of a generalized thermostat with a fluctuating inverse temperature in order to access to the microstates with a negative heat capacity presented in the thermodynamical description of the $q = 10$ states Potts model [18]. A previous simulation (by using the usual Metropolis or SW algorithms) allows to set the interest energetic window between $\varepsilon_1 = 0.2$ and $\varepsilon_2 = 1.2$ which encloses the region of ensemble inequivalence of this model for $L = 25$. The inverse critical temperature was estimated as $\beta_c \simeq 1.4$, allowing us to set $\lambda = 0.8$. The reader can notice that while the SW algorithm with a constant temperature is unable to reproduce the backbending behavior of the microcanonical calorific curve, the use of a thermostat with a fluctuating inverse temperature avoids such limitation both for this cluster algorithm as well as the Metropolis one. The agreement between these last Monte Carlo methods is remarkable.

Thus, the analysis of the thermodynamic uncertainty relation [11] consequences opens a whole world of theoretical developments and numerical studies about the enhancing of the available Monte Carlo methods based on the canonical ensemble in order to deal with the ensemble inequivalence phenomenon without appealing to the multicanonical methods [1].

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