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Hybrid Monte Carlo method for conserved-order-parameter systems

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We introduce a method based on the hybrid Monte Carlo (HMC) algorithm [S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, Phys. Lett. B **195**, 216 (1987)] to sample the canonical distribution in systems with a conserved order parameter. We show that the standard HMC method and the one introduced here are special cases of a general class of HMC methods. As an application we compute the scaling function of the interface excess energy for the ϕ^4 model.

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The hybrid Monte Carlo (HMC) algorithm [1] was introduced as an alternative to other computer simulation methods [2] (such as Metropolis sampling, Langevin integration, or molecular dynamics) in order to sample the equilibrium probability distribution given by the Gibbs measure, $\exp(-\mathcal{H})$, for continuous models. The HMC algorithm combines the standard acceptance or rejection decision of the Metropolis algorithm with a molecular dynamics evolution for proposing new configurations. The HMC algorithm was originally proposed for lattice gauge theories because the global updating scheme minimizes the number of computations of the Gibbs factor necessary for the acceptance procedure (one of the main problems in these theories). One of the main advantages of the HMC methods is that their general formulation is applicable to a great variety of systems, however complicated the Hamiltonian $\mathcal{H}$ may be. Recently, they have been used to study critical universality for the ϕ^4 model [3] and the equilibrium properties of a system of Lennard-Jones particles [4] (these two papers discuss the advantages of using HMC methods with respect to normal Monte Carlo methods in the context of statistical physics). Furthermore, HMC methods are unbiased, in the sense that they do not show any systematic discretization errors; the only errors are of statistical origin and can consequently be diminished by increasing the number of samplings.

In this Rapid Communication we introduce a hybrid Monte Carlo scheme suitable for studying systems with a conserved order parameter. Our method shows all the advantages of the standard hybrid Monte Carlo algorithm, offering a very convenient way to study these conserved-order-parameter systems. We also show that the standard HMC method and the one introduced here are particular cases of a general class of HMC methods.

The only previous Monte Carlo method known to us [5] for studying continuous systems with a conserved order parameter is a generalization of the Kawasaki exchange dynamics for Ising systems [6]. However, the authors in Ref. [5] did not use the method to study equilibrium properties, but rather as an alternative to the numerical integration of the Cahn-Hilliard-Cook [7] equation in order to study spinodal decomposition in binary systems described by a continuous concentration field.

Conserved-order-parameter systems are defined by a set of variables $(\phi_1, \phi_2, \ldots, \phi_N) \equiv [\phi]$ such that the order parameter $\Phi \equiv \sum_{i=1}^{N} \phi_i$ takes a fixed value. Index $i \equiv (i_1, i_2, \ldots, i_d)$ runs over the $N = L^d$ sites of a d-dimensional hypercubic lattice, with periodic boundary conditions. The statistical properties of the system are defined by its Hamiltonian $\mathcal{H}[\phi]$.

Let us briefly review the standard hybrid Monte Carlo algorithm for nonconserved-order-parameter systems. In these schemes one introduces a set of auxiliary variables $(p_1, p_2, \ldots, p_N) \equiv [p]$. Furthermore, one defines a canonical mapping G, $[\phi, p] \to [\phi', p'] = G([\phi, p])$ of phase space. The new configuration $[\phi']$ is accepted or rejected according to the usual Metropolis criterion. In order to sample the equilibrium probability distribution defined by the Hamiltonian of the model, the method is constructed such that detailed balance is fulfilled.

The variables $[\phi]$ are considered to be generalized coordinates and the auxiliary variables $[p]$ are the conjugate momenta associated with a kinetic energy $\mathcal{H}_K = \sum_{i=1}^{N} p_i^2/2$. The transformation G is conventionally defined in terms of a suitable approximation to the Hamiltonian dynamics associated with the total Hamiltonian $\hat{\mathcal{H}} = \mathcal{H}_K + \mathcal{H}$:

$$\begin{aligned} \frac{d\phi_i}{dt} &= \frac{\partial \hat{\mathcal{H}}}{\partial p_i} = p_i, \\ \frac{dp_i}{dt} &= -\frac{\partial \hat{\mathcal{H}}}{\partial \phi_i} = F_i, \end{aligned} \tag{1}$$

where $F_i([\phi]) = -\partial \mathcal{H}/\partial \phi_i$ is the force acting on the variable ϕ_i. The conservation of energy follows from this Hamiltonian dynamics: $d\hat{\mathcal{H}}/dt = 0$. In [1] a leap-frog discretization is used to approximate the solution of the previous set of equations, thus introducing a discrete mapping $G^{\delta t}$ dependent on the time step δt:

$$\begin{aligned} \phi_i' &= \phi_i + \delta t \left(p_i + \frac{\delta t}{2} F_i([\phi]) \right), \\ p_i' &= p_i + \frac{\delta t}{2} \{ F_i([\phi]) + F_i([\phi']) \}. \end{aligned} \tag{2}$$

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The mapping G is then defined as $G = (G^{\delta t})^M$, M being the number of leap-frog steps. The time discretization causes a discretization error in the energy, $\delta E = \hat{\mathcal{H}}([\phi', p']) - \hat{\mathcal{H}}([\phi, p])$, which can be controlled by varying δt and M. The resulting configuration $[\phi']$ is then accepted with a probability $\min\{1, \exp(-\delta E)\}$ according to the usual Metropolis algorithm. The key point is that, since the Hamilton equations exactly conserve energy, the discretization error δE can be made small so that the average acceptance probability can be adjusted to a reasonable value. In order to fulfill detailed balance [1] the following (sufficient) conditions are required.

(i) The mapping $G^{\delta t}$ must be time reversible, i.e., if $[\phi', p'] = G^{\delta t}([\phi, p])$ then $G^{\delta t}([\phi', -p']) = [\phi, -p]$.

(ii) The mapping $G^{\delta t}$ must be area preserving, i.e., the Jacobian associated with the transformation must have unit determinant, $|J([\phi', p']/[\phi, p])| = 1$.

(iii) The momenta variables $[p]$ must be refreshed after each acceptance/rejection (i.e., after M leap-frog steps) according to the distribution $\exp(-\mathcal{H}_K)$ (a Gaussian distribution for independent random variables).

It turns out that the mapping defined by the leap-frog approximation [1] to the solution of the Hamiltonian dynamics satisfies properties (i) and (ii) above. However, the order parameter Φ is not conserved. We propose a modification of the previous algorithm, which, still fulfilling the previous requirements needed to satisfy detailed balance, leaves the order parameter Φ conserved. The modification goes as follows: to every field variable ϕ_i, we assign a vector variable $\mathbf{p}_i \equiv (p_i^1, p_i^2, \ldots, p_i^d)$ of dimension d (the space dimension). The associated kinetic energy is then $\mathcal{H}_K = \sum_{i=1}^N \mid \mathbf{p}_i \mid^2 /2$ and the total Hamiltonian is again $\hat{\mathcal{H}} = \mathcal{H} + \mathcal{H}_K$. The next step is to substitute the previous Hamiltonian based mapping by one based on the following set of equations:

$$\frac{d\phi_i}{dt} = \boldsymbol{\nabla}_R \cdot \left\{ \frac{\partial \hat{\mathcal{H}}}{\partial \mathbf{p}_i} \right\} = \boldsymbol{\nabla}_R \cdot \mathbf{p}_i$$

$$\frac{d\mathbf{p}_i}{dt} = \boldsymbol{\nabla}_L \left\{ \frac{\partial \hat{\mathcal{H}}}{\partial \phi_i} \right\} = -\boldsymbol{\nabla}_L F_i, \qquad i = 1, \ldots, N \tag{3}$$

or, in more compact notation,

$$\frac{d\phi}{dt} = \boldsymbol{\nabla}_R \cdot \mathbf{p},$$

$$\frac{d\mathbf{p}}{dt} = -\boldsymbol{\nabla}_L F. \tag{4}$$

Here, $\boldsymbol{\nabla}_R$ and $\boldsymbol{\nabla}_L$ are the lattice gradient operators defined as $\boldsymbol{\nabla}_R f_i \equiv (f_{i_{+1}} - f_i, f_{i_{+2}} - f_i, \ldots, f_{i_{+d}} - f_i)$ and $\boldsymbol{\nabla}_L f_i \equiv (f_i - f_{i_{-1}}, f_i - f_{i_{-2}}, \ldots, f_i - f_{i_{-d}})$, where i_{+k} and i_{-k} are the two nearest neighbors of the site i, in the direction k, i.e., $i_{\pm k} \equiv (i_1, \ldots, i_k \pm 1, \ldots, i_d)$ (remember that periodic boundary conditions are assumed). The kth component ($k = 1, \ldots, d$) of vector operator $\boldsymbol{\nabla}_R$, ∇_R^k, is an $N \times N$ matrix, $\mathcal{A}^k$. One has $\mathcal{A}^k = \mathcal{T}^k - 1$, $\mathcal{T}^k$ being the matrix associated with the translation operator in direction k. The $\mathcal{A}^k$ components are explicitly given by $(\mathcal{A}^k)_{ij} = \delta(i_{+k}, j) - \delta(i, j)$, $\delta(i, j)$ being the Kronecker delta function. Analogously, if $\mathcal{B}^k$ is the matrix associated with ∇_L^k, then $\mathcal{B}^k = 1 - (\mathcal{T}^k)^{-1}$. Since $\mathcal{T}^k$ is orthogonal, one has $\mathcal{B}^k = -(\mathcal{A}^k)^T$.

An interesting and essential property of Eqs. (3) is that although they are non-Hamiltonian, they still exactly conserve the energy $\hat{\mathcal{H}}$, i.e., $d\hat{\mathcal{H}}/dt = 0$. Moreover, the order parameter is also conserved during the evolution, $d\Phi/dt = 0$.

We introduce a mapping $G_C^{\delta t}$, defined in terms of the leap-frog approximation to the solution of Eqs. (3):

$$\phi_i' = \phi_i + \delta t \, \boldsymbol{\nabla}_R \cdot \left(\mathbf{p}_i - \frac{\delta t}{2} \boldsymbol{\nabla}_L F_i([\phi]) \right),$$

$$\mathbf{p}_i{}' = \mathbf{p}_i - \frac{\delta t}{2} \boldsymbol{\nabla}_L \{ F_i([\phi]) + F_i([\phi']) \}. \tag{5}$$

It is trivially proven that this mapping still exactly conserves the order parameter. Furthermore, the discretization (5) satisfies the properties mentioned above: (i) it is time reversible; (ii) it is area preserving, i.e., the $[(d+1)N \times (d+1)N]$ dimensional Jacobian $|J([\phi', \mathbf{p}']/[\phi, \mathbf{p}])|$ is equal to 1; (iii) the detailed balance condition is then fulfilled if after M leap-frog iteration steps the change in energy $\delta E = \hat{\mathcal{H}}([\phi', p']) - \hat{\mathcal{H}}([\phi, p])$ is computed and the configuration $[\phi']$ is accepted with probability $\min\{1, \exp(-\delta E)\}$ and if the momenta variables $[\mathbf{p}]$ are then refreshed according to the Gaussian distribution $\exp(-\mathcal{H}_K)$.

As before, the mapping G_C is defined as an iteration of the basic mapping $G_C^{\delta t}$ after M leap-frog steps, $G_C = (G_C^{\delta t})^M$. We have hence constructed a mapping G_C given by M iterations of the transformation (5), which is an approximation to a set of differential equations that exactly conserves the energy, fulfills all the conditions required for satisfying detailed balance and conserves the order parameter. This is the main result of this Rapid Communication.

We will now rewrite the algorithm in a more general form. We notice that, since the matrix associated with operator $-\nabla_L^k$ is $(\mathcal{A}^k)^T$, Eqs. (4) can be written as

$$\frac{d\phi}{dt} = \sum_{k=1}^{D} \mathcal{A}^k p^k,$$

$$\frac{dp^k}{dt} = (\mathcal{A}^k)^T F, \qquad k = 1, \ldots, D \tag{6}$$

with $D = d$. We can now consider these equations as the basic ingredient for constructing a variety of hybrid Monte Carlo methods by considering that the matrices $\mathcal{A}^k$, for $k = 1, \ldots, D$, are arbitrary matrices and that the number D of auxiliary variables $(p^1, \ldots, p^D)$ need not be equal to the space dimension d. First of all, let us note that these equations still exactly conserve the energy for any set of matrices $\mathcal{A}^k$, $d\hat{\mathcal{H}}/dt = 0$. The leap-frog approximation to the solution of these differential equations is

$$\phi' = \phi + \delta t \sum_{k=1}^{D} \mathcal{A}^k p^k + \frac{(\delta t)^2}{2} \sum_{k=1}^{D} \mathcal{A}^k (\mathcal{A}^k)^T F([\phi]),$$

$$p'^k = p^k + \frac{\delta t}{2} (A^k)^T (F([\phi]) + F([\phi'])). \tag{7}$$

It is easily proven that the mapping $G_{\mathcal{A}}^{\delta t}$ associated with this transformation is also time reversible. By refreshing the variables $(p^1, \ldots, p^D)$ after M leap-frog steps according to the Gaussian distribution $\exp(-\mathcal{H}_K)$ and using the usual Metropolis acceptance rules, we also satisfy property (iii) above. By using different matrices $\mathcal{A}^k$ with different symmetries, different ensembles could be simulated. The case $D = 1$, $\mathcal{A} = 1$ corresponds to the usual hybrid Monte Carlo method. If $\mathcal{A}^k = \mathcal{T}^k - 1$ and $D = d$ we reproduce the conserved-order-parameter method introduced in this work. It is possible to include long-range correlations in matrices $\mathcal{A}^k$ in such a way that the updating has an important nonlocal component. It might then be conceivable that an appropriate choice of the set of matrices $\mathcal{A}^k$ would result in algorithms in which the autocorrelation time can be reduced [8]. In fact, the approach given here extends and makes "exact" (in the sense of being independent of the discretization step) previous algorithms based on approximations to generalized Langevin equations with a matrix time step [9].

Let us now come back to the conserved-order-parameter algorithm introduced above, i.e., take $\mathcal{A}^k = \mathcal{T}^k - 1$ and $D = d$. With this choice of matrices, the requirement $D = d$ is necessary in order not to introduce any spurious conservation laws. If we had used $D = 1$ independent of dimension d, then we would have had conservation for the magnetization along every row of the system. With the choice of matrices given here and by using $D = d$ we ensure that the only linear conservation law is that of the total magnetization.

Further insight into the method is given by noticing that, if the number M of leap-frog steps equals 1, an interesting relation is obtained with the Cahn-Hilliard-Cook (CHC) dynamics [7]. In this case, the variables $[\mathbf{p}]$ are refreshed every time step and their evolution can be effectively neglected (after they have been used in the Metropolis acceptance step) and they can be considered simply as independent random variables following the Gaussian distribution. In this case of $M = 1$, the evolution equation for the field variables is

$$\phi_i' = \phi_i - \frac{(\delta t)^2}{2} \Delta F_i([\phi]) + \delta t \xi_i, \tag{8}$$

where the new random variable $\xi_i \equiv \nabla_R \cdot \mathbf{p}_i$ has mean zero and $\langle \xi_i \xi_j \rangle = -\Delta \delta(i,j)$, where $\Delta \equiv \nabla_R \cdot \nabla_L$ is the lattice Laplacian operator. This is to be compared with the Euler discretization of the CHC equation for a time (τ)-dependent field $\phi_i(\tau)$

$$\frac{\partial \phi_i(\tau)}{\partial \tau} = -\Delta F_i(\tau) + \sqrt{2} \xi_i(\tau), \tag{9}$$

where the noise term satisfies the correlations $\langle \xi_i(\tau) \xi_j(\tau') \rangle = -\Delta \delta(i,j) \delta(\tau - \tau')$. The Euler discretization reads [10]

$$\phi_i(\tau + \delta\tau) = \phi_i(\tau) - \delta\tau \Delta F_i(\tau) + \sqrt{2\delta\tau} \xi_i(\tau). \tag{10}$$

This equation is similar to Eq. (8), provided the time step $\delta\tau$ used in the Euler method is taken to be $(\delta t)^2/2$. We could say that the acceptance step in the HMC method makes the Euler approximation to the CHC equation "exact" in the sense that the equilibrium statistical properties are unbiased and independent of the time step used in the numerical integration. A similar relation holds between the nonconserved HMC algorithm and the model-A Langevin equation [11].

As an application we have considered the ϕ^4 model in two dimensions, which is given by the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \left[-\frac{\theta}{2} \phi_i^2 + \frac{\chi}{4} \phi_i^4 + \frac{1}{2} \mid \nabla_L \phi_i \mid^2 \right]. \tag{11}$$

Here, χ is considered to be constant and θ is some function of temperature such that high values for θ correspond to a low-temperature point in the phase diagram. To every value of χ corresponds a critical point defined by a value $\theta = \theta_c(\chi)$. We have used both the Hybrid Monte Carlo conserved-order-parameter and nonconserved-order-parameter algorithms to sample the equilibrium probability distribution of the model near the critical point for $\chi = 1$, $\theta_c = 1.265(5)$ [12]. We have used in all our simulations extrapolation techniques[13] applicable to the canonical distribution that allow one to draw continuous curves from a set of simulation data. For the conserved case, simulations are made with the zero-order parameter, i.e., zero magnetization. The conserved system develops at equilibrium two interfaces, separating regions of opposite magnetization sign. These interfaces become sharper as the temperature is lowered. We have computed the excess energy, given by

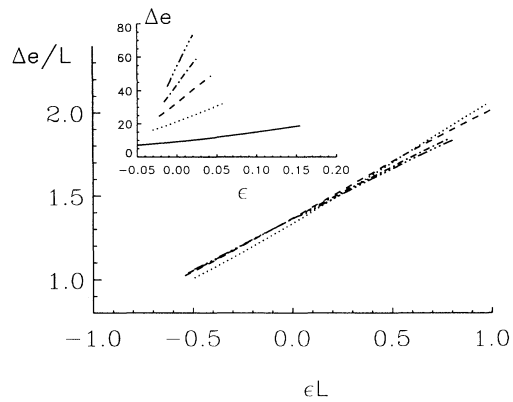

FIG. 1. Plot of the excess energy Δe divided by system side L as a function of the variable $x = L\epsilon = L(1 - \theta_c/\theta)$ for different values of L to check the scaling property of the excess free energy: $L = 16$, dotted line; $L = 24$, dashed line; $L = 32$, dashed-dotted line; and $L = 40$, dashed-triple-dotted line. In this plot, the value $\theta_c = 1.268$, consistent with the results of Ref. [12], is used. The lines have been obtained by extrapolation using the techniques in Ref. [13] using two independent simulations at two different values of θ for every value of L. The inset shows the raw data before scaling (including the data corresponding to the $L = 8$ continuum line).

$\Delta e = (E_C - E_{NC})/2$, where E_C and E_{NC} denote the mean energy of the conserved- and nonconserved-order-parameter systems, respectively. This excess energy is related to the interface tension F_S of the model by

$$\Delta e/L^{d-1} = \frac{d}{d\beta}(\beta F_S), \tag{12}$$

where $\beta = 1/(k_B T)$. For an infinite system, the interfacial tension vanishes at the critical point with a power law of exponent μ [14]:

$$F_S = F_0 \left(1 - \frac{\theta_c(\chi)}{\theta}\right)^{\mu}, \tag{13}$$

whereas for a finite system it depends on a finite-size scaling function $\Sigma(x)$:

$$F_S(L, \epsilon) = \epsilon^{\mu} \Sigma(L^{1/\nu} \epsilon), \tag{14}$$

where ν is the correlation length critical exponent and $\epsilon = 1 - \theta_c(\chi)/\theta$. From the last three equations it can be deduced [15] that for $\epsilon \approx 0$ and large L, $\Delta e(L, \epsilon)/L$ is expected to be a scaling function of the variable $x = L\epsilon$ (for the $d = 2$ case considered here we have used the known values [14] for the exponents $\nu = 1$ and $\mu = 1$). In Fig. 1 we have plotted $\Delta e(L, \epsilon)/L$ as a function of the variable x. A good collapse of the points is obtained using for θ_c the value 1.268, which lies inside the error bars of Ref. [12]. Although the scaling behavior for the interface free energy or the interface tension has previously been studied numerically for the Ising model [15, 16], this is, to our knowledge, the first verification of this scaling law for the ϕ^4 model.

In conclusion, we have derived a method to study numerically conserved-order-parameter systems. This method can be regarded as an "exact" integration of the CHC equation in the stationary (equilibrium) state. As an application we have computed the excess interface energy of the ϕ^4 model, reproducing the expected scaling behavior. Furthermore, it was shown that both the conserved-order-parameter and the nonconserved-order-parameter HMC algorithms are special cases of possible HMC algorithms generated by more general dynamics.

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