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Cluster Monte Carlo algorithm with a conserved order parameter

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We propose a cluster simulation algorithm for statistical ensembles with fixed order parameter. We use the tethered ensemble, which features Helmholtz's effective potential rather than Gibbs's free energy and in which canonical averages are recovered with arbitrary accuracy. For the $D=2,3$ Ising model our method's critical slowing down is comparable to that of canonical cluster algorithms. Yet, we can do more than merely reproduce canonical values. As an example, we obtain a competitive value for the 3D Ising anomalous dimension from the maxima of the effective potential.

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Monte Carlo simulations [1] constitute one of the most important modern tools of theoretical physics. In situations that defy an analytical treatment, a Monte Carlo computation succeeds by wandering randomly across the system's configuration space. Over the years many methods have been proposed in order to optimize this sampling process. Here we combine two: fixing some global parameter in order to guide the exploration of phase space and the use of cluster update algorithms.

Cluster methods appear in the 1980s [2] as an answer to the problem of critical slowing down [3], the drastic deceleration of the dynamics in the neighborhood of the critical point. For a system of linear size L, the characteristic times are $\tau \propto L^z$ (typically $z \approx 2$). Only in very few situations can one define an efficient cluster method capable of achieving $z<1$.

Beyond the canonical ensemble setting, considering global conservation laws is often useful (as in micromagnetic [4] or microcanonical [5] ensembles). It is known that $z=4-\eta$ for locally conserved order parameter dynamics in Ising models [6] (η is the anomalous dimension). For nonlocal conservation laws z is smaller [7,8]. Despite continued research on cluster methods [9], the development of an efficient cluster method in this situation has long been considered somewhat of a challenge [8].

Here we present a working cluster algorithm with a globally conserved order parameter. We employ the tethered Monte Carlo (TMC) framework [10], which we briefly review. TMC is a general approach to reconstruct the effective potential [3,11]. We demonstrate our cluster method in the standard benchmark of the $D=2,3$ Ising model. In the first case it outperforms the Metropolis version of [10], while in the second it exhibits a dynamic critical exponent compatible with that of the canonical Swendsen-Wang algorithm.

The tethered ensemble is similar to the micromagnetic one, but instead of fixing the magnetization we couple it to a Gaussian "magnetostat" in order to define a new parameter, $\hat{m}$. This ensemble arises from the canonical one through a Legendre transformation that replaces the magnetic field h by $\hat{m}$. Thus, Helmholtz's effective potential takes the place of Gibbs's free energy. The main observable is the tethered magnetic field $\hat{h}$ considered as a function of $\hat{m}$.

We shall work on the Ising model in a cubic lattice of size $N=L^D$ and periodic boundary conditions with partition function ($\langle\cdot,\cdot\rangle$: nearest neighbors)

$$Z=\sum_{\{\sigma_x\}} \exp\left[\beta \sum_{\langle x,y\rangle} \sigma_x\sigma_y\right], \quad \sigma_x = \pm 1. \tag{1}$$

We shall consider its energy and magnetization,

$$E=Ne=-\frac{1}{D}\sum_{\langle x,y\rangle}\sigma_x\sigma_y, \quad M=Nm=\sum_x \sigma_x. \tag{2}$$

We use lowercase for densities so that, for instance, e is the energy per bond. Canonical averages are denoted by $\langle\cdot\rangle_\beta$ as in the specific heat and susceptibility:

$$C=N[\langle e^2\rangle_\beta - \langle e\rangle_\beta^2], \quad \chi=N[\langle m^2\rangle_\beta - \langle m\rangle_\beta^2]. \tag{3}$$

Note that the probability density (pdf) $p_1(m)$ is the sum of $N+1$ Dirac deltas. We smooth it by coupling m to N Gaussian demons to build the tethered ensemble

$$\hat{M}=N\hat{m}=M+\frac{1}{2}\sum_i \phi_i^2. \tag{4}$$

As the ϕ_i are independent, $\hat{m}\simeq m+1/2$. The definitions of the pdf $p(\hat{m})$ for $\hat{m}$ and of the effective potential $\Omega_N(\hat{m},\beta)$ are straightforward

$$p(\hat{m})=e^{N\Omega_N(\hat{m},\beta)} = \frac{1}{Z}\int_{-\infty}^{\infty}\prod_{i=1}^{N} d\phi_i \sum_{\{\sigma_x\}} e^{-\beta E+M-\hat{M}}\delta\left(\hat{m}-m-\sum_i \phi_i^2/(2N)\right). \tag{5}$$

Our use of demons is reminiscent of Creutz's microcanonical algorithm [12], but we shall integrate the ϕ_i out in order to define our *tethered averages*,

$$\langle O\rangle_{\hat{m},\beta}=\frac{\sum_{\{\sigma_x\}} O(\hat{m};\{\sigma_x\})\omega_N(\beta,\hat{m};\{\sigma_x\})}{\sum_{\{\sigma_x\}}\omega_N(\beta,\hat{m};\{\sigma_x\})}, \tag{6}$$

where O represents a generic observable and

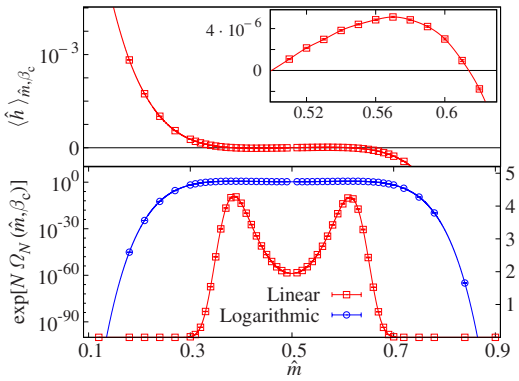

FIG. 1. (Color online) Computation of the effective potential $\Omega_N(\hat{m},\beta_c)$ [Eq. (5)] for an $L=128$ Ising 3D lattice. Top: we simulate each point independently to measure $\langle \hat{h} \rangle_{\hat{m},\beta_c}$ [Eq. (8)] (the lines are cubic splines and the errors are much smaller than the points). Bottom: this curve is then integrated to yield $p(\hat{m})$, which we show in a linear (□) and in a logarithmic (○) scale. Inset: $\langle \hat{h} \rangle_{\hat{m},\beta_c}$ for $\hat{m} \simeq m + 1/2 > 1/2$.

$$\omega_N(\beta,\hat{m};\{\sigma_x\}) = e^{-\beta E + M - \hat{M}} (\hat{m} - m)^{(N-2)/2} \theta(\hat{m} - m) \tag{7}$$

(θ is Heaviside's step function). Then we find that

$$\hat{h} \equiv -1 + \frac{N/2 - 1}{\hat{M} - M}, \quad \langle \hat{h} \rangle_{\hat{m},\beta} = \frac{\partial \Omega_N(\hat{m},\beta)}{\partial \hat{m}}. \tag{8}$$

Therefore, we can construct the effective potential by integrating $\langle \hat{h} \rangle_{\hat{m},\beta}$ on $\hat{m}$. Once we have $\Omega_N(\hat{m},\beta)$ we can compute canonical averages for any given value of the external magnetic field h with the formula

$$\langle O \rangle_\beta(h) = \frac{\int d\hat{m} e^{N[\Omega_N(\hat{m},\beta) + h\hat{m}]} \langle O \rangle_{\hat{m},\beta}}{\int d\hat{m} e^{N[\Omega_N(\hat{m},\beta) + h\hat{m}]}}. \tag{9}$$

The TMC simulation algorithm consists of four steps: (1) select an appropriate sampling $\hat{m}_i$, $i=1,\ldots,N_{\hat{m}}$ for $\hat{m}$, keeping in mind that $\hat{m} \simeq m + 1/2$. (2) Run independent simulations for each $\hat{m}_i$, measuring the tethered averages $\langle O \rangle_{\hat{m},\beta}$. (3) Integrate (a smooth interpolation of) $\langle \hat{h} \rangle_{\hat{m},\beta}$ to obtain $\Omega_N(\hat{m},\beta)$. (4) Use Eq. (9) to recover the canonical averages. Figure 1 illustrates this process for the 3D Ising model. Let us remark that this is the algorithm for reproducing canonical averages. However, see below, one can also obtain physically relevant results directly from the tethered averages.

In [10] we implemented this algorithm, using Metropolis dynamics for step (2). Surprisingly enough, magnetic observables such as $\hat{h}$ or m presented no critical slowing down (other quantities such as the energy presented the $z \approx 2$ behavior typical of a local update [7]).

Our cluster algorithm, a tethered version of Swendsen-Wang, is best explained using the bond-occupation variables n_{xy} (=0,1) and the conditional probability distributions of [13]. The lattice bond joining neighboring sites $\boldsymbol{x}$ and $\boldsymbol{y}$ is *occupied* if $n_{xy}=1$. The occupied bonds partition the lattice in

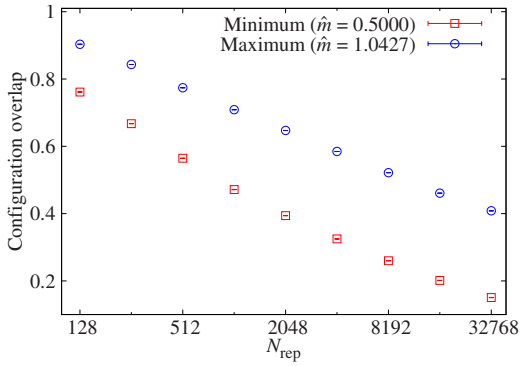

FIG. 2. (Color online) Spin overlap [Eq. (12)] in a 2D critical $L=512$ Ising model at the central minimum (□) and right maximum (○) of the effective potential [Eq. (5)].

connected clusters of size N_i, $i=1,\ldots,N_c$. Plugging in Eq. (7) the identity

$$e^{\beta(\sigma_x\sigma_y - 1)} = \sum_{n_{xy}=0,1} [(1-p)\delta_{n_{xy},0} + p\,\delta_{\sigma_x,\sigma_y}\delta_{n_{xy},1}], \tag{10}$$

where $p = 1 - e^{-2\beta}$, we immediately read the conditional probabilities of the spins given the bonds and vice versa: (a) as in a canonical case, given the $\{\sigma_x\}$, bonds are independent and n_{xy} is 1 with probability $p\,\delta_{\sigma_x,\sigma_y}$. (b) Given the n_{xy} the N_i spins within cluster i are equal to $S_i = \pm 1$. The probability of the 2^{N_c} configuration of the $\{S_i\}$ depends on $M = \Sigma_{i=1}^{N_c} S_i N_i$ through Eq. (7):

$$p(\{S_i\}) \propto e^{M - \hat{M}} (\hat{M} - M)^{(N-2)/2} \theta(\hat{M} - M). \tag{11}$$

Our cluster update will consist, then, in a cluster tracing using conditioned probability (a) and in a cluster flipping using (b). For this last step we perform a dynamical Monte Carlo, taking the S_i at $t=0$ from the initial spin configuration. At each t we select $N_c' \ll N_c$ clusters ($N_c' \approx 5$ works just fine). We randomly pick lattice sites, selecting the cluster to which they belong, until we find N_c' different clusters. We then use Eq. (11) to perform a heat bath among the $2^{N_c'}$ configurations with the remaining $N_c - N_c'$ clusters fixed [14]. We take N_{rep} such steps.

Taking $N_{rep} > 1$ steps is advantageous because over a large number of repetitions many of the S_i will eventually be flipped, decorrelating the system. Furthermore, it takes much longer to trace the clusters than to flip them once so N_{rep} can be made relatively large without noticeably increasing the simulation time. In Fig. 2 we represent the overlap

$$o = \frac{\left\langle \sum_x [\sigma_x^{t=0} \sigma_x^{t=N_{rep}} - \langle m \rangle_{\hat{m},\beta}^2] \right\rangle_{\hat{m},\beta}}{N(1 - \langle m \rangle_{\hat{m},\beta}^2)}, \tag{12}$$

which vanishes for completely uncorrelated configurations. Clearly, the configuration can significantly evolve for a fixed distribution of the bonds. A major error reduction (a factor 25 in our largest lattices) is achieved by measuring $\hat{h}$ at *each* of the N_{rep} steps.

TABLE I. Integrated autocorrelation times for the energy at $\hat{m}=0.5$ and $\beta=\beta_c$ for the $D=2,3$ Ising model. We compare the cluster and mixed versions of our TMC algorithm. We also include the results of [17] for canonical Swendsen-Wang. Our values for z_E are fits to $\tau_E=AL^{z_E}$, where the smallest lattice in range is $L_{\min}=128$(2D) and $L_{\min}=32$(3D). dof is the degrees of freedom of the fit.

$D=2$			$D=3$			
L	Cluster	Met.+Cluster	L	Cluster	Met.+Cluster	Swendsen-Wang
16	2.310(14)	0.775(3)	16	2.135(13)	0.782(3)	5.459(3)
24	2.440(26)	0.920(4)	32	2.80(3)	1.134(5)	7.963(9)
32	2.758(20)	1.055(5)	48	3.467(28)	1.427(8)	9.831(9)
64	3.347(22)	1.417(7)	64	3.88(3)	1.700(10)	11.337(12)
128	4.11(5)	1.861(12)	96	4.79(5)	2.152(14)	13.90(3)
256	4.87(4)	2.391(16)	128	5.46(6)	2.566(17)	15.90(5)
512	5.79(8)	3.040(24)	192	6.54(11)	3.32(4)	19.10(9)
1024	6.78(8)	3.70(4)	256	7.51(13)	3.85(5)	21.83(10)
z_E	0.241(7)		z_E	0.472(8)	0.591(4)	0.460(5)
χ^2/dof	0.36/2		χ^2/dof	5.85/5	4.61/5	

Naturally, one must eventually refresh the bond configuration. A simulation at fixed $\hat{m}$ then consists of N_{MC} steps where one traces the clusters and performs N_{rep} iterations of the random walk in the S_i space. We have empirically found that an N_{rep} that equilibrates the cluster-tracing and cluster-flipping times is close to optimal and very easy to find [one only has to scale N_{rep} with N, as the tracing of clusters is an $\mathcal{O}(N \ln N)$ operation]. For $N=256^3$ spins, this results in $N_{\mathrm{rep}} \approx 5\times 10^5$.

The efficiency of a MC method is best assessed through the equilibrium autocorrelation function [15] for an observable O, $C_O(t) \equiv \langle [O(0)-\langle O\rangle][O(t)-\langle O\rangle]\rangle$. The slowness of the dynamics can be quantified with the integrated autocorrelation time τ_O. Defining $\rho_O(t)=C_O(t)/C_O(0)$, τ_O is just the time integral of $\rho_O(t)$ in $(0,\infty)$. We estimate it with the self-consistent window method [15] for our numerical estimate $\bar{\rho}_O$ of ρ_O,

$$\tau_O = \frac{1}{2} + \sum_{t=1}^{\Lambda} \bar{\rho}_O(t), \quad \Lambda = W\tau_O. \tag{13}$$

We typically use $W=6$ but have checked that the results are consistent for several Ws. Since $\tau_O \propto L^{z_O}$, one is interested in the observable with largest z_O (E in our case as is typical for cluster methods).

We have used τ_E to assess our algorithm's performance for the Ising model in two [at $\beta=\beta_c=\ln(1+\sqrt{2})/2$] and three dimensions (at $\beta=0.221\,654\,59 \approx \beta_c$ [16]). For both D's, we find that the τ_E are largest at $\hat{m}=0.5$ [the central minimum of $p(\hat{m})$], so we report their values at that point in Table I. In 2D we obtain $z_E=0.241(7)$, while in 3D our dynamic exponent is $z_E=0.472(8)$, compatible with the Swendsen-Wang value of $z_E=0.460(5)$ [17]. We also include our results with a slightly modified algorithm, where we take two Metropolis steps each cluster step. This mixed algorithm has significantly smaller τ'_E in both dimensions. Paradoxically, in 3D, $z'_E > z_E$ (z'_E is immeasurable in 2D), which probably means that larger L would be needed to compute it properly. Since for our lattice sizes the mixed algorithm fares better, we shall use it hereafter.

As a proof of TMC's accuracy, we have reproduced some of the critical Swendsen-Wang simulations of [17] for the 3D Ising model (Table II). In accordance with our τ_E analysis, the errors with both algorithms are comparable. In 2D, the new cluster algorithm outperforms Metropolis. For instance, for an $L=1024$ lattice, taking ten times fewer steps than in [10] and the same $\hat{m}$ grid, cluster errors are eight times smaller for E, six times smaller for C, and ten times smaller for χ and ξ.

Yet TMC can do more than reproduce canonical averages. Let us compute the anomalous dimension η. Finite-size scaling [10,11] tells us that the right maximum of $p(\hat{m};L)$ at β_c (Fig. 1) scales as

$$\hat{m}_{\mathrm{peak}} - \frac{1}{2} = AL^{-(\eta+D-2)/2} + \cdots \quad (A=\text{const.}), \tag{14}$$

where the dots stand for scaling corrections.

Unlike in a canonical simulation, we locate $\hat{m}_{\mathrm{peak}}$ through $\langle \hat{h} \rangle_{\hat{m}_{\mathrm{peak}},\beta}=0$. We simulate two very close values of $\hat{m}$ at either side of the peak and use a linear interpolation. Our 3D results are in Table III.

We have found that Eq. (14) yields remarkably good fits for $L_{\min}=48$. Furthermore, increasing $L_{\min}$ results in compat-

TABLE II. Comparison of canonical Swendsen-Wang (data from [17]) with TMC for an $N=128^3$ lattice at β_c. We take 10^6 MC steps at each of the 50 points of our $\hat{m}$ grid (Fig. 1). This results in a similar number of MCS for both simulations. (ξ: second-moment correlation length [11,18]).

	MCS	$-\langle e\rangle_\beta$	C	χ	ξ
SW	48×10^6	0.3309822(16)	22.155(18)	21193(13)	82.20(3)
TMC	50×10^6	0.3309831(15)	22.174(13)	21202(13)	82.20(6)

TABLE III. Position of the peak of $p(\hat{m};L)$ for the $D=3$ Ising model at β_c. In each row we report the result of a fit to Eq. (14) (the first column is also the fit's $L_{\min}$).

$L\|L_{\min}$	MCS	$\hat{m}_{\text{peak}}-\frac{1}{2}$	η	χ^2/dof
16	1.0×10^8	0.33421(5)	0.03392(21)	42.6/6
32	1.0×10^8	0.23377(4)	0.03526(30)	8.79/5
48	1.0×10^8	0.18956(4)	0.0360(5)	4.24/4
64	1.0×10^8	0.16341(4)	0.0368(7)	1.02/3
96	1.0×10^8	0.13240(4)	0.0363(12)	0.78/2
128	1.0×10^8	0.114083(24)	0.0373(19)	0.31/1
192	6.0×10^7	0.09246(4)		
256	8.2×10^6	0.07959(12)		

ible values of η, with growing errors. Our preferred estimate is $\eta=0.0360(7)$, where we took the central value from $L_{\min}=48$ and the error from $L_{\min}=64$ to account for systematic effects. This estimate compares favorably with the best Monte Carlo computation known to us, $\eta=0.0362(8)$ [19], and is compatible with a high-temperature expansion value of $\eta=0.036\,39(15)$ [20] (however, both quoted values [19,20] were computed with a perfect action not in the Ising model).

In summary, we have shown how models with conserved order parameter can be efficiently simulated with a cluster method. We work in the tethered ensemble framework, which allows us to compute the Helmholtz effective potential. The method is tested in the $D=2,3$ Ising model. For the computation of canonical expectation values in large lattices, our cluster algorithm is no less efficient than a canonical one in 3D (in 2D the dynamical exponent $z\approx0.24$ is larger than that for the canonical algorithm but still very small). The tethered ensemble permits a very efficient computation of quantities such as the maxima of the effective potential, which would be extremely costly to reproduce in a canonical setting. Our estimate for the anomalous dimension of the 3D Ising model compares favorably with all previous Monte Carlo computations known to us. We plan to further develop this algorithm to study disordered systems [21] and the condensation transition [22].

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