Probability-Changing Cluster Algorithm for Potts Models

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We propose a new effective cluster algorithm of tuning the critical point automatically, which is an extended version of the Swendsen-Wang algorithm. We change the probability of connecting spins of the same type, $p = 1 - e^{-J/k_BT}$, in the process of the Monte Carlo spin update. Since we approach the canonical ensemble asymptotically, we can use the finite-size scaling analysis for physical quantities near the critical point. Simulating the two-dimensional Potts models to demonstrate the validity of the algorithm, we have obtained the critical temperatures and critical exponents which are consistent with the exact values; the comparison has been made with the invaded cluster algorithm.

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Cluster algorithms [1,2] have been successfully used to overcome slow dynamics in the Monte Carlo simulation. Swendsen and Wang (SW) [1] applied the Kasteleyn-Fortuin (KF) [3] representation to identify clusters of spins. The problem of the thermal phase transition is mapped onto the geometric percolation problem in the cluster formalism [3–5]. Quite recently, based on the cluster formalism, the multiple-percolating clusters of the Ising system with large aspect ratio have been studied [6].

Machta *et al.* [7] proposed another type of cluster algorithm, which is called the invaded cluster (IC) algorithm; this algorithm samples the critical point of a spin system without *a priori* knowledge of the critical temperature. It is in contrast with the usual procedure that one makes simulations for various parameters to determine the critical point. The IC algorithm has been shown to be efficient in studying various physical quantities in the critical region, but the ensemble is not necessarily clear. Moreover, it has a problem of "bottlenecks," which causes the broad tail in the distribution of the fraction of the accepted satisfied bonds [7].

In this Letter, extending the SW algorithm [1], we propose a new algorithm of tuning the critical point automatically. The basic idea of our algorithm is that we change the probability of connecting spins of the same type, $p = 1 - e^{-J/k_BT}$, in the process of the Monte Carlo spin update, where J is the exchange coupling. We decrease or increase p depending on the observation whether the KF clusters are percolating or not percolating. This simple negative feedback mechanism together with the finite-size scaling (FSS) property of the existence probability (also called the crossing probability) E_p, the probability that the system percolates, leads to the determination of the critical point. Since our ensemble is asymptotically canonical as Δp, the amount of the change of p, becomes 0, the distribution functions of physical quantities obey the FSS; as a result, we can determine critical exponents using the FSS analysis.

Let us explain the procedure for our probability-changing cluster (PCC) algorithm in detail. As an example, we consider the ferromagnetic q-state Potts model [8] whose Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (\delta_{\sigma_i,\sigma_j} - 1), \qquad \sigma_i = 1, 2, \ldots, q, \quad (1)$$

and for $q = 2$ this corresponds to an Ising model. The procedure of Monte Carlo spin update is as follows: (i) Start from some spin configuration and some value of p. (ii) Construct the KF clusters using the probability p and check whether the system is percolating or not. Update spins following the same rule as the SW algorithm; that is, flip all the spins on any KF cluster to one of q states. (iii) If the system is percolating (not percolating) in the previous test, decrease (increase) p by Δp (>0). (iv) Go back to the process ii.

After repeating the above processes, the distribution of p for our Monte Carlo samples approaches the Gaussian distribution of which mean value is $p_c(L)$; $p_c(L)$ is the probability of connecting spins, such that the existence probability E_p becomes $1/2$. The width of the distribution depends on the choice of Δp in process iii and becomes 0 in the limit of $\Delta p \to 0$. We should note that $p_c(L)$ depends on the system size L, and E_p follows the FSS near the critical point,

$$E_p(p, L) \sim X(tL^{1/\nu}), \qquad t = (p_c - p)/p_c, \quad (2)$$

where p_c is the critical value of p for the infinite system ($L \to \infty$) and ν is the correlation-length critical exponent. (As for the FSS of E_p, see Ref. [9], for example.) We can estimate p_c from the size dependence of $p_c(L)$ using Eq. (2) and, in turn, estimate T_c through the relation $p_c = 1 - e^{-J/k_BT_c}$. We have chosen the value of E_p which gives $p_c(L)$ as $1/2$ because it is the simplest. We may modify the update process such that this value is different from $1/2$.

A comment should be made here on the choice of criterion to determine percolating. Machta *et al.* [7] used both the extension rule and the topological rule for their stopping condition. The former rule is that some cluster has maximum extent L in at least one of the d directions in d-dimensional systems. The latter rule is that some cluster

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winds around the system in at least one of the d directions. We can use any rule to determine percolating, but FSS functions for physical quantities, therefore $p_c(L)$, depend on the rule.

There is one free parameter in our algorithm; we may choose the difference Δp in process iii. In the limit of small Δp we obtain the canonical ensemble, but it takes a long time to equilibrate for small Δp. Practically, we may start with rather large Δp and switch to smaller Δp with monitoring the trail of the values of p. Small steps of preparation are enough for equilibration.

In order to show the validity of the present method, we have made simulations for the 2D ferromagnetic two-state Potts model (Ising model) and three-state Potts model. We have treated the systems with linear sizes $L = 64$, 128, 256, and 512. We start with $\Delta p = 0.01$ and gradually decrease Δp to the final value. We have chosen this final value of Δp as $1/(20 \times L^2)$; the steps for preparation are 10 000 for the largest size ($L = 512$). After reaching the final small value of Δp, we have taken 100 000 (200 000) Monte Carlo samples in the case of $q = 2$ ($q = 3$) with keeping Δp as constant. From each bond configuration, we have made 5 (10) spin configurations in order to get better statistics for magnetization in the case of $q = 2$ ($q = 3$). We have performed several runs for each size and have checked the statistical errors.

Let us show the results of the 2D Ising model ($q = 2$). In Fig. 1, we plot the size dependence of $T_c(L)$ for both rules in units of J/k_B. We have determined $p_c(L)$ from the average of p, and calculated $T_c(L)$ through the relation $p_c(L) = 1 - e^{-J/k_B T_c(L)}$. In this plot, as an illustration, we have used the known value of ν for the 2D Ising model ($\nu = 1$). Using the least squares method, we estimate T_c as 1.1344(2) [1.1346(2)] for the extension (topological) rule, which is consistent with the exact value, $[\ln(1 + \sqrt{2})]^{-1} = 1.1346$. Here, the number in the parentheses denotes the uncertainty in the last digit. We have used the known value of ν but we may treat ν as an unknown parameter to be determined. Assuming the FSS relation, $T_c(L) = T_c + aL^{-1/\nu}$, which is derived from Eq. (2), we may follow the three-parameter $(T_c, 1/\nu, a)$ nonlinear fitting procedure. Then, we have obtained $(T_c, 1/\nu) = [1.1345(2), 1.00(4)]$ for the extension rule and [1.1344(2), 1.04(4)] for the topological rule. Both estimates of T_c and ν are consistent with the exact values.

We plot the distribution of p, $f(p)$, for $L = 64$ with the topological rule, as an example, in the inset in Fig. 1, which shows that the distribution of p is sharply peaked at 0.581 96 with the standard deviation of 0.0004 for our choice of the final Δp. For comparison, we also show $f(p)$ for the IC algorithm of the same size with the same rule; different scales are used for the vertical axis in the inset to express two quite different data. We notice that the distribution of p for the IC algorithm is far broader. A simple linear analysis yields that the width of the distribution for the PCC algorithm is proportional to $\sqrt{\Delta p/a}$, where a is the value of dE_p/dp at $p_c(L)$; using the FSS we expect $a \propto L^{1/\nu}$. It should be noted that we have obtained the expected Δp and L dependence for the width of the distribution of p. We use the average value of p for the estimate of $p_c(L)$. Performing ten runs, we have estimated $p_c(64)$ as 0.581 954 ± 0.000 013; the statistical errors are very small.

The resulting energy histogram, $f(E)$, of our PCC algorithm for $L = 64$ with the topological rule is given in Fig. 2. The energy histogram obtained by the constant-temperature calculation using the SW algorithm is shown by a solid curve in Fig. 2; the temperature has been chosen

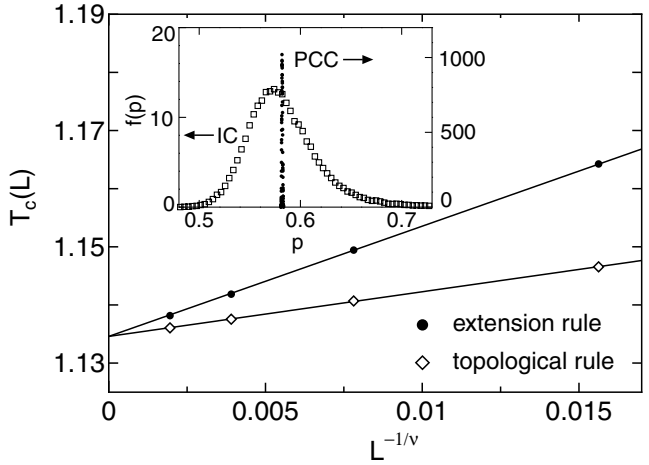

FIG. 1. Plot of $T_c(L)$ (in units of J/k_B) as a function of $L^{-1/\nu}$ for the 2D Ising model ($q = 2$), where $\nu = 1$. The system sizes are $L = 64$, 128, 256, and 512. In the inset, the distribution of p, $f(p)$, for $L = 64$ with the topological rule is shown for both the PCC and IC algorithms. Different scales are used for the vertical axis in the inset to express two quite different data.

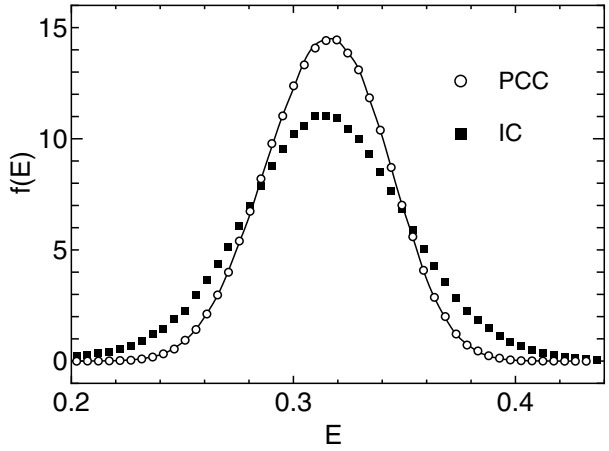

FIG. 2. The energy histogram, $f(E)$, of both the PCC and IC algorithms for $L = 64$ with the topological rule for the 2D Ising model ($q = 2$). The energy is measured in units of J. The energy histogram obtained by the constant-temperature calculation using the SW algorithm is also shown by a solid curve; the temperature has been chosen as $T_c(L)$ determined by the PCC algorithm.

as $T_c(L)$ determined by the PCC algorithm. The energy histogram of the PCC algorithm is indistinguishable from that by the constant-temperature calculation because of the sharp distribution of p. Thus, we may say that our ensemble is actually canonical for small enough Δp. The energy histogram of the IC algorithm, which is also given in Fig. 2, has broad tails for both high-energy and low-energy sides. Although our ensemble is almost canonical, there are deviations in physical quantities, in principle; the variance of energy, $\langle E^2\rangle - \langle E\rangle^2$, becomes larger with nonzero Δp, for example. We have checked the Δp dependence of the systematic deviation for large Δp. However, the deviation of the variance of energy is smaller than the statistical error, 2% for $L = 64$, with our choice of Δp.

In order to estimate another critical exponent β, the magnetization exponent, we plot the average of the squared magnetization $\langle m^2\rangle$ as a function of L in logarithmic scale in Fig. 3. Since our Monte Carlo samples are sharply peaked at $p = p_c(L)$, in other words, at $T = T_c(L)$, we can use the FSS relation,

$$\langle m^2\rangle_{T=T_c(L)} \sim L^{-2\beta/\nu}, \tag{3}$$

for the estimate of β/ν. From the slopes of the data for both rules, we have $\beta/\nu = 0.125(2)$ [0.126(2)] for the extension (topological) rule, which is consistent with the exact value, $1/8$ ($= 0.125$).

It is quite interesting to study the distribution function of physical quantities. We show the FSS plot of the distribution function $p(m)$ in Fig. 4, based on the FSS relation,

$$p(m)_{T=T_c(L)} \sim L^{\beta/\nu} f(mL^{\beta/\nu}). \tag{4}$$

The scaling plot for the extension rule (a) and that for the topological rule (b) are given there. The data for various sizes are collapsed on a single curve. We have very good FSS behavior for both rules. Two rules give different $tL^{1/\nu}$ in Eq. (2) for $E_p = 1/2$. It is easier to percolate for the extension rule compared with the topological rule. Therefore, $T_c(L)$ of the extension rule is higher than that of the topological rule, which results in the difference in the FSS functions for $p(m)$ between two rules.

Next turn to the case of the three-state Potts model. The size dependence of $T_c(L)$ for both rules is shown in Fig. 5. We have used the known value of ν for this plot; the exponent ν for the 2D three-state Potts model conjectured by the conformal field theory [10] is $5/6$. We estimate the extrapolated value of T_c as 0.994 90(6) [0.994 94(6)] for the extension (topological) rule from Fig. 5. This value is consistent with the exact value, $[\ln(1 + \sqrt{3})]^{-1} = 0.994\,97$. The convergence is very good for the three-state Potts model. It is in contrast with the situation of the IC algorithm [7], where the convergence is not good enough maybe due to the problem of bottlenecks.

We can estimate the critical exponent β/ν for the three-state Potts model from the size dependence of $\langle m^2\rangle$ as in the case of the Ising model. For the order parameter of the three-state Potts model, we use the vector order parameter (m_x, m_y). The x and y components of the vector order parameter are obtained from the three components m_1, m_2, and m_3, as $m_x = m_1 - (1/2)(m_2 + m_3)$ and $m_y = (\sqrt{3}/2)(m_2 - m_3)$. Using the FSS relation (3) for the three-state Potts model, we have $\beta/\nu = 0.131(2)$ [0.134(2)] for the extension (topological) rule, which is again consistent with the conjectured value, $2/15$ ($= 0.1333$) [10]. We have also found nice FSS behavior for the order-parameter distribution functions $p(m)$ of the three-state Potts model as in the case of the Ising model. Here, m stands for the absolute value of the vector order parameter. The details will be given in a separate paper.

Here we may remark on the computation time. We need only to modify the code of the SW algorithm slightly in order to change p. The typical computation time to get 10^5 Monte Carlo samples for $L = 64$ is 471 s using the Alpha 21164A (533 MHz) machine, which is about 30% longer than that for the SW algorithm, 361 s. The most

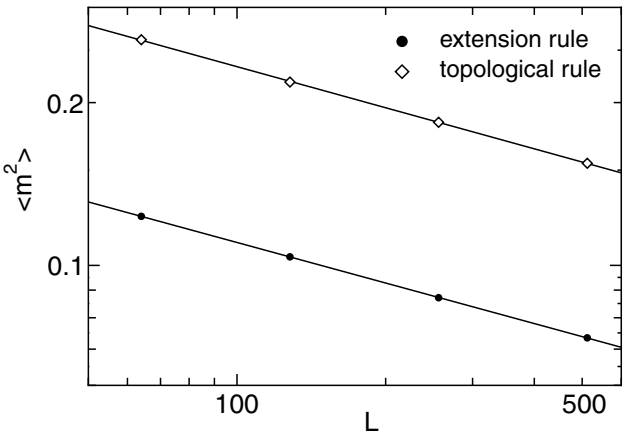

FIG. 3. Plot of $\langle m^2\rangle$ as a function of L for the 2D Ising model ($q = 2$) in logarithmic scale.

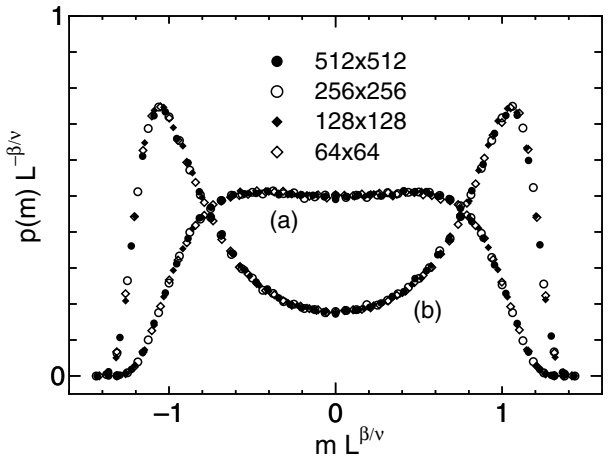

FIG. 4. FSS plot of $p(m)$ for the 2D Ising model ($q = 2$), where $\beta/\nu = 1/8$. The rules to determine percolating are the extension rule (a) and the topological rule (b).

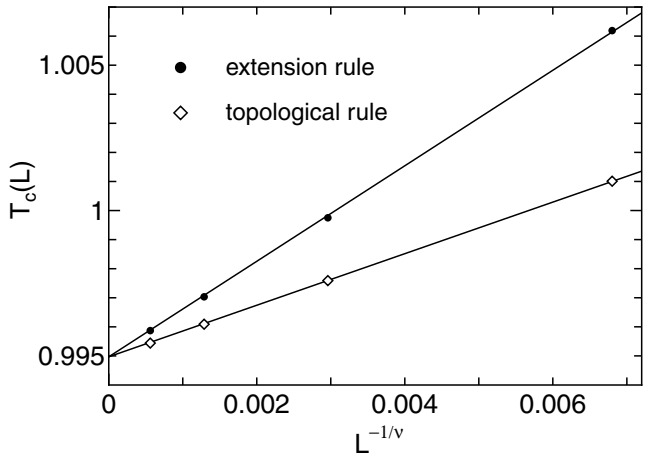

FIG. 5. Plot of $T_c(L)$ (in units of J/k_B) as a function of $L^{-1/\nu}$ for the 2D three-state Potts model, where $\nu = 5/6$. The system sizes are $L = 64$, 128, 256, and 512.

time is spent on the usual procedure of the SW algorithm, that is, the assignment of the cluster and the cluster spin update. With a small cost of computation time, we can determine the critical point automatically without making simulations for various parameters. In contrast, it takes 958 s in the case of the IC algorithm to get 10^5 samples for $L = 64$ because one should check whether the system is percolating several times before getting one Monte Carlo sample.

To summarize, we have proposed a new cluster algorithm of tuning the critical point automatically. Our algorithm is the extension of the SW algorithm [1], but we change the probability of connecting spins p in the process of Monte Carlo spin update. The resulting distribution of p is sharply peaked at $p_c(L)$. We approach the canonical ensemble in the limit of small Δp, which has been explicitly checked by the energy histogram. This is in contrast with the histogram of the IC algorithm [7], which has broad tails for both high-energy and low-energy sides. Thus, we can use the FSS analysis for the physical quantities. The estimated values of the critical temperatures and the critical exponents for the 2D Potts models are consistent with the exact values. In order to get a more accurate estimate of the critical point and critical exponents, the FSS analysis employed by Ferrenberg and Landau [11] in a high-resolution Monte Carlo study is useful for the data obtained by the PCC algorithm; we extract ν first, and with ν determined quite accurately we can estimate T_c. Since the main purpose of the present Letter is to present a new and simple idea of the cluster algorithm, the refined data analysis including the corrections to FSS will be left to a subsequent study.

In the present study, we have shown the application of the PCC algorithm to the thermal phase transition of Potts models, but the idea is based only on the property of a percolation problem. Thus, of course, we can use this algorithm in the study of the geometric percolation problem, that is, the $q = 1$ Potts model, to get the percolation threshold, p_c, and various critical properties.

Moreover, we can apply the PCC algorithm to any problem where the mapping to the cluster formalism exists. It is straightforward to apply this algorithm to the diluted Ising (Potts) model. The lack of self-averaging has been recently discussed for the three-dimensional diluted Ising model [12,13]. The PCC algorithm is quite useful for the problem with the lack of self-averaging, where the distribution of T_c due to the randomness is important, because we can tune the critical point of each random sample automatically. Another direction of application is the cluster quantum Monte Carlo simulation [14,15], and this problem is left to a future study.

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