Broad histogram relation for the bond number and its applications

Chiaki Yamaguchi, Naoki Kawashima, and Yutaka Okabe
Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan
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We discuss Monte Carlo methods based on the cluster (graph) representation for spin models. We derive a rigorous broad histogram relation (BHR) for the bond number; a counterpart for the energy was derived by Oliveira previously. A Monte Carlo dynamics based on the number of potential moves for the bond number is proposed. We show the efficiency of the BHR for the bond number in calculating the density of states and other physical quantities.

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I. INTRODUCTION

The development of new algorithms for the Monte Carlo simulation is important to overcome the problem of slow dynamics. We may classify such attempts into two categories. The first category is the extended ensemble method; one uses an ensemble different from the ordinary canonical ensemble with a fixed temperature. The multicanonical method [1,2], the simulated tempering [3], the exchange Monte Carlo method [4], the broad histogram method [5], the flat histogram method [6,7], and the Wang-Landau algorithm [8] are examples of the first category. The second category includes the cluster algorithm; one flips a large number of spins in a correlated cluster at a time instead of a single-spin flip, which helps the relaxation time decrease drastically. Examples of the second category are the Swendsen-Wang algorithm [9] and the Wolff algorithm [10]. Recently Tomita and Okabe [11] proposed an effective cluster algorithm, which is called the probability-changing cluster algorithm, of tuning the critical point automatically.

The combination of the approaches of two categories is a challenging problem to explore an efficient algorithm. Janke and Kappler [12] proposed a trial to combine the multicanonical method and the cluster algorithm; their method is called the multibondic ensemble method. Quite recently, Yamaguchi and Kawashima [13] have improved the multibondic ensemble method; they have also shown that the combination of the Wang-Landau algorithm and the improved multibondic ensemble method yields much better statistics compared to the original multibondic ensemble method by Janke and Kappler [12].

One calculates the energy density of states (DOS) $g(E)$ in the multicanonical method [1,2] and the Wang-Landau method [8]; the energy histogram $H(E)$ is checked during the Monte Carlo process. In contrast, the DOS for bond number n_b, $\Omega(n_b)$, is calculated in the multibondic ensemble method [12] or the improved multibondic ensemble method by Yamaguchi and Kawashima [13]; the histogram for bond number, $H(n_b)$, is checked in the Monte Carlo process.

In proposing the broad histogram method, Oliveira *et al.* [5] paid attention to the number of potential moves, or the number of the possible energy change, $N(S,E\rightarrow E')$, for a given state S. The total number of moves is

$$\sum_{\Delta E} N(S,E\rightarrow E+\Delta E)=N$$

for a single-spin-flip process, where N is the number of spins. The energy DOS is related to the number of potential moves as

$$g(E)\ \langle N(S,E\rightarrow E')\rangle_E = g(E')\ \langle N(S',E'\rightarrow E)\rangle_{E'}, \tag{1}$$

where $\langle\cdots\rangle_E$ denotes the microcanonical average with fixed E. This relation is shown to be valid on general grounds [14], and hereafter we call Eq. (1) as the broad histogram relation (BHR) for the energy. One may use the number of potential moves $N(S,E\rightarrow E')$ for the probability of updating states. While the original dynamics [5] was criticized to be not entirely correct [6,15], a refined dynamics is employed in the flat histogram method [7]. Alternatively, one may employ other dynamics which has no relation to $N(S,E\rightarrow E')$, but Eq. (1) is used when calculating the energy DOS [16,17]. It was stressed [16,17] that $N(S,E\rightarrow E')$ is a macroscopic quantity, which is the advantage of using the number of potential moves. We do not have to care about the relative number of visits for different energy levels E. It is contrary to the case of the multicanonical method [1,2] or the Wang-Landau method [8]. The only crucial point is the uniformity of visits within the same energy level [16].

It is quite interesting to ask whether there is a relation similar to the BHR, Eq. (1), for the bond number. In this paper, using the cluster (graph) representation, we derive the BHR for the bond number. We propose a dynamics based on the number of potential moves for the bond number. Using the DOS for the bond number thus obtained, we calculate the specific heat for model spin systems. We also employ other dynamics, that is, the multibondic ensemble method [12] and its improvement [13], and calculate the bond-number DOS, based on the BHR for the bond number. Comparing the efficiency of several methods, we show that the calculation of the bond-number DOS through the BHR gives much better statistics compared to the direct calculation of the DOS.

The rest of the paper is organized as follows. In Sec. II, we briefly review the cluster (graph) representation for the Q-state Potts model. In Sec. III, we derive the BHR for the bond number. A dynamics based on the number of potential moves for the bond number is discussed in Sec. IV. In Sec. V, calculating the accuracy of the specific heat for the two-dimensional (2D) Ising model, we compare the efficiency of several methods. The summary and discussions are given in Sec. VI.

II. CLUSTER FORMALISM

We briefly review the cluster (graph) formalism for the Q-state Potts model. We are concerned with the Hamiltonian

$$\mathcal{H}=-J\sum_{\langle i,j\rangle}\delta_{\sigma_i,\sigma_j},\quad \sigma_i=\{1,\ldots,Q\},$$

where J is the exchange coupling constant and the summation is taken over the nearest-neighbor pairs $\langle i,j\rangle$. From now on, we represent the energy in units of J, and the Boltzmann constant is set to be 1.

The partition function for a given temperature T is expressed as

$$Z(T)\equiv\sum_S W_0(S)=\sum_E g(E)W_0(E(S),T)$$

with the Boltzmann weight of state S having the energy E,

$$W_0(S)=W_0(E(S),T)=e^{-E(S)/T},$$

and the energy DOS,

$$g(E)\equiv\sum_{\{S|E(S)=E\}}1.$$

With the framework of the dual algorithm [18,19], the partition function is also expressed in the double summation over state S and graph G as

$$Z(T)=\sum_{S,G}V_0(G)\ \ \Delta(S,G),$$

where $\Delta(S,G)$ is a function that takes the value one when S is compatible to G and takes the value zero otherwise. A graph consists of a set of bonds. The weight for graph G, $V_0(G)$, is defined as

$$V_0(G)=V_0(n_b(G),T)=(e^{1/T}-1)^{n_b(G)}$$

for the Q-state Potts model, where $n_b(G)$ is the number of ''active'' bonds in G. This is nothing but the Fortuin-Kasteleyn representation [20] for the Q-state Potts model. We say a pair (i,j) is satisfied if $\sigma_i=\sigma_j$, and unsatisfied otherwise. Satisfied pairs become active with a probability $p=1-e^{-1/T}$ for given T.

By taking the summation over S with G with fixing the number of bonds n_b, the expression for the partition function becomes

$$Z(T)=\sum_{n_b=0}^{N_B}\Omega(n_b)V_0(n_b,T),$$

where N_B is the total number of nearest-neighbor pairs in the whole system. Here, $\Omega(n_b)$ is the DOS for the bond number, defined as the number of consistent combinations of graphs and states such that the graph consists of n_b bonds,

$$\Omega(n_b)\equiv\sum_{\{G|n_b(G)=n_b\}}\sum_S\ \ \Delta(S,G).$$

Then, the canonical average of a quantity A is calculated by

$$\langle A\rangle_T=\frac{\sum_{n_b}\langle A\rangle_{n_b}\Omega(n_b)V_0(n_b,T)}{Z(T)},\tag{2}$$

where $\langle A\rangle_{n_b}$ is the microcanonical average with the fixed bond number n_b for the quantity A defined as

$$\langle A\rangle_{n_b}\equiv\frac{\sum_{\{G|n_b(G)=n_b\}}\sum_S A(S,G)\Delta(S,G)}{\Omega(n_b)}.\tag{3}$$

Thus, if we obtain $\Omega(n_b)$ and $\langle\cdots\rangle_{n_b}$ during the simulation process, we can calculate the canonical average of any quantity at any temperature.

We should note that for the calculation of the energy E, it is convenient to use the relation

$$\langle E\rangle_T=T^2\frac{d}{dT}\ln Z(T)=-\frac{e^{1/T}}{e^{1/T}-1}\ \langle n_b\rangle_T.\tag{4}$$

Similarly, the specific heat per one site C is given by

$$CNT^2=-\frac{e^{1/T}}{(e^{1/T}-1)^2}\langle n_b\rangle_T+\left(\frac{e^{1/T}}{e^{1/T}-1}\right)^2(\langle n_b^2\rangle_T-\langle n_b\rangle_T^2).\tag{5}$$

The above equations (4) and (5) were derived by Janke and Kappler [12].

III. BHR FOR THE BOND NUMBER

The relation between the energy DOS and the number of potential moves for energy, the BHR for the energy, was rigorously derived by Oliveira [14]. Here we follow a method similar to that used by Oliveira to derive the BHR for the bond number. Instead of using the relation between states, we consider the relation between graphs.

The number of potential moves from the graph with the bond number n_b to the graph with n_b+1, $N(S,G,n_b\rightarrow n_b+1)$, for fixed S is equal to that of the number of potential moves from the graph with n_b+1 to that with n_b, $N(S,G',n_b+1\rightarrow n_b)$. That is, the following relation is satisfied:

$$\sum_{\{G|n_b(G)=n_b\}}N(S,G,n_b\rightarrow n_b+1)$$

$$=\sum_{\{G'|n_b(G')=n_b+1\}}N(S,G',n_b+1\rightarrow n_b).\tag{6}$$

Taking a summation over states S and using the definition of the microcanonical average with the fixed bond number n_b, Eq. (3), we rewrite Eq. (6) as

$$\Omega(n_b)\langle N(G,n_b\to n_b+1)\rangle_{n_b} = \Omega(n_b+1)\ \langle N(G',n_b+1\to n_b)\rangle_{n_b+1}. \quad (7)$$

This is the BHR for the bond number. It should be noted that $N(G,n_b\to n_b+1)$ is a possible number of bonds to add, and related to the number of satisfied pairs for the given state S,

$$n_p(S)=\sum_{\langle i,j\rangle}\delta_{\sigma_i(S),\sigma_j(S)},$$

by

$$N(G,n_b\to n_b+1)=n_p(S)-n_b.$$

With use of the microcanonical average with fixed bond number for n_p, we have the relation

$$\langle N(G,n_b\to n_b+1)\rangle_{n_b}=\langle n_p\rangle_{n_b}-n_b. \quad (8)$$

On the other hand, the possible number of bonds to delete, $N(G',n_b+1\to n_b)$, is simply given by n_b+1, that is,

$$\langle N(G',n_b+1\to n_b)\rangle_{n_b+1}=n_b+1. \quad (9)$$

From the BHR for the bond number, Eq. (7), we have

$$\frac{\Omega(n_b)}{\Omega(0)}=\prod_{l=0}^{n_b-1}\frac{\Omega(l+1)}{\Omega(l)}=\prod_{l=0}^{n_b-1}\frac{\langle N(G,l\to l+1)\rangle_{n_b=l}}{\langle N(G,l+1\to l)\rangle_{n_b=l+1}}. \quad (10)$$

Then, substituting Eqs. (8) and (9) into Eq. (10), we obtain the bond-number DOS, $\Omega(n_b)$, as

$$\ln\Omega(n_b)=\ln\Omega(0)+\sum_{l=0}^{n_b-1}\ln\left(\frac{\langle n_p\rangle_{n_b=l}-l}{l+1}\right). \quad (11)$$

When calculating the bond-number DOS from the BHR for the bond number, we only need the information on $\langle n_p\rangle_{n_b}$, the microcanonical average with fixed n_b of the number of satisfied pairs n_p. It is much simpler than the case of the BHR formulation for the energy DOS.

Moreover, in the computation of n_p, we can use an improved estimator. If a pair of sites (i,j) belong to the different cluster, this pair is satisfied with a probability of $1/Q$. If a pair of sites belong to the same cluster, this pair is always satisfied. Then, we can employ an improved estimator $\tilde{n}_p$ as

$$\tilde{n}_p(G)=\left(1-\frac{1}{Q}\right)\sum_{\langle i,j\rangle}\delta_{c_i(G),c_j(G)}+\frac{N_B}{Q}, \quad (12)$$

where $c_i(G)$ represent a cluster that a site i belongs to. Only the information on graph is needed. By definition, $\langle\tilde{n}_p\rangle_{n_b}=\langle n_p\rangle_{n_b}$. We employ the improved estimator in the whole calculation below. Inserting Eq. (12) into Eq. (11), we have

$$\frac{\Omega(n_b)}{Q^N}=\frac{1}{n_b!}\prod_{l=0}^{n_b-1}\left[\left(1-\frac{1}{Q}\right)\langle\delta_{c_i(G),c_j(G)}\rangle_{n_b=l}+\frac{N_B}{Q}-l\right]. \quad (13)$$

Here we have used the relation

$$\Omega(0)=Z(T\to\infty)=Q^N.$$

It is interesting to check Eq. (13) for a special case. The $Q\to 1$ limit of the Q-state Potts model is the bond percolation problem. If we substitute $Q=1$ into Eq. (13), we obtain

$$\Omega(n_b)=\binom{N_B}{n_b},$$

which is the expected relation for the bond percolation problem.

IV. FLAT HISTOGRAM METHOD FOR THE BOND NUMBER

Let us consider the update process for the Monte Carlo simulation. In the multibondic ensemble method, a graph is updated by adding or deleting a bond for a satisfied pair of sites [12]. The histogram $H(n_b)$ becomes flat if we use the following rule. If there is a bond already on the chosen pair, we delete it with a probability

$$P(n_b\to n_b-1)=\frac{\Omega(n_b)}{\Omega(n_b-1)+\Omega(n_b)}, \quad (14)$$

On the other hand, if there is no bond and if the pair is satisfied, we add a bond with a probability

$$P(n_b\to n_b+1)=\frac{\Omega(n_b)}{\Omega(n_{b+1})+\Omega(n_b)}. \quad (15)$$

Since the exact form of the bond-number DOS $\Omega(n_b)$ is not known *a priori*, we renew $\Omega(n_b)$ iteratively in the Monte Carlo process by several ways [12,13].

We may use the number of potential moves for the bond number, $\langle N(G,\cdots)\rangle_{n_b}$, for the probability of update. Inserting Eqs. (7), (8), and (9) into Eqs. (14) and (15), we get the probability to delete a bond,

$$P(n_b\to n_b-1)=\frac{\langle n_p\rangle_{n_b-1}+1-n_b}{\langle n_p\rangle_{n_b}-1+1}, \quad (16)$$

and the probability to add a bond,

$$P(n_b\to n_b+1)=\frac{n_b+1}{\langle n_p\rangle_{n_b}+1}, \quad (17)$$

respectively.

The actual Monte Carlo procedure is as follows. We start from some state (spin configuration) S, and an arbitrary graph G consistent with it. We add or delete a bond of satisfied pairs with the probability (16) or (17). After making such a process as many as the number of total pairs, N_B, we

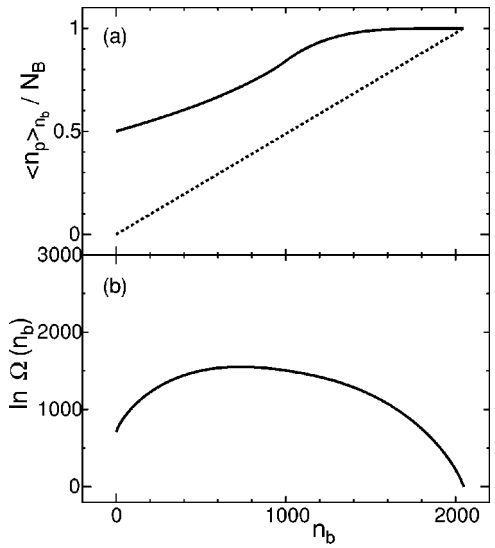

FIG. 1. (a) $\langle n_p \rangle_{n_b}/N_B$ and (b) $\ln \Omega(n_b)$ of the 32×32 Ising model obtained by the cluster-flip flat histogram method. The dotted line in (a) denotes n_b/N_B.

flip every cluster with the probability 1/2. And we repeat the process. Since we do not know the exact form of $\langle n_p \rangle_{n_b}$, we use the accumulated average for $\langle n_p \rangle_{n_b}$. The dynamics proposed here can be regarded as the flat histogram method for the bond number, which we call the cluster-flip flat histogram method. The conventional flat histogram method for the energy [7] will be referred to as the single-spin-flip flat histogram method hereafter. As $\langle n_p \rangle_{n_b}$ converges to the exact value, the histogram $H(n_b)$ becomes flat. We calculate the bond-number DOS by using Eq. (13), and then calculate various quantities by Eq. (2), or Eqs. (4) and (5).

Here, we have described the procedure for the multiple cluster update of the Swendsen-Wang type [9], but we can also employ the single cluster update of the Wolff type [10].

V. RESULTS

First, we simulate the $L\times L$ Ising model on the square lattice with the periodic boundary conditions by using the cluster-flip flat histogram method. We show $\langle n_p \rangle_{n_b}/N_B$ as a function of n_b for $L=32$ by the solid line in Fig. 1(a); we give n_b/N_B by the dotted line. The number of Monte Carlo sweeps (MCS) is 5×10^7. The difference between the solid and dotted lines represents the number of potential moves $\langle N(n_b\rightarrow n_b+1)\rangle/N_B$, whereas the difference between the dotted line and the horizontal axis represents $\langle N(n_b\rightarrow n_b-1)\rangle/N_B$. We should note that $\langle n_p \rangle_{n_b=0}/N_B=1/2$, which is expected from Eq. (12). The logarithm of the bond-number DOS, $\ln \Omega(n_b)$, obtained by $\langle n_p \rangle_{n_b}$ is shown in Fig. 1(b) as a function of n_b. The temperature dependence of the specific heat calculated using Eq. (5) is shown in Fig. 2; the deviation from the exact result obtained by Beale [21] is not visible in this scale.

Let us compare the performance of the cluster-flip flat histogram method proposed in this paper with that of the single-spin-flip flat histogram method [7]. To do this, we check the number of MCS to satisfy the flatness condition for the histogram $H(n_b)$ or $H(E)$; we state that the flatness condition is fulfilled if the histogram $H(n_b)$ or $H(E)$ for all possible n_b or E is equal to or larger than 80% of the average histogram $\overline{H}$. In Fig. 3, we show the size dependence of the number of MCS to satisfy the flatness condition, which we call the flatness time $t_{\rm flat}$ hereafter, for both the cluster-flip flat histogram method and the single-spin-flip flat histogram method in logarithmic scale. The linear system sizes L are 4, 8, 12, 16, 20, 24, and 32. The average is taken over many samples. The number of samples ranges from 20 for the largest system to 1000 for the smallest. We see from Fig. 3 that for the single-spin-flip flat histogram method the flatness time increases more rapidly as the system size increases. The least-squares fitting of the data gives

$$\ln t_{\rm flat} \sim 4.04(2) + 1.75(1)\ \ln N$$

for the cluster flat histogram method, and

$$\ln t_{\rm flat} \sim 1.28(7) + 2.46(1)\ \ln N$$

for the single-spin-flip flat histogram method.

As another example, we simulate the 2D ten-state Potts model on the square lattice. A strong first-order phase transition occurs in this model. We show $\langle n_p \rangle_{n_b}/N_B$ for the 32×32 lattice by the solid line in Fig. 4(a); we give n_b/N_B by the dotted line. The number of MCS is 5×10^7. The number of potential moves $\langle N(n_b\rightarrow n_b+1)\rangle/N_B$ and $\langle N(n_b\rightarrow n_b$

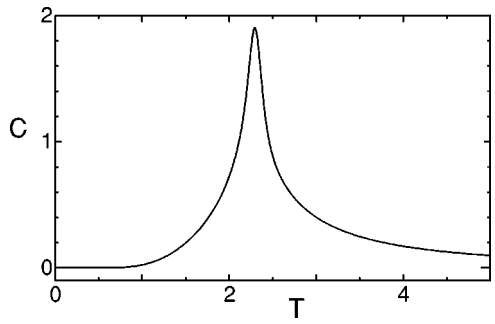

FIG. 2. Specific heat per site of the 2D Ising model for $L=32$ obtained by the cluster-flip flat histogram method.

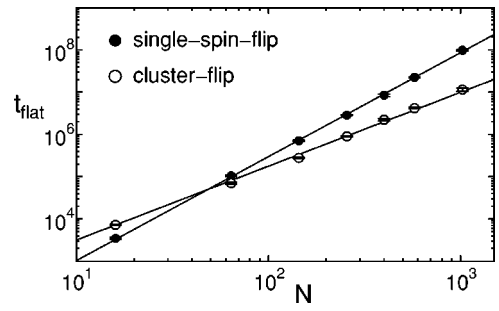

FIG. 3. Size dependence of the flatness time for the 2D Ising model. The linear system sizes L are 4, 8, 12, 16, 20, 24, and 32; $N=L^2$. The cluster-flip flat histogram method and the single-spin-flip flat histogram method are compared.

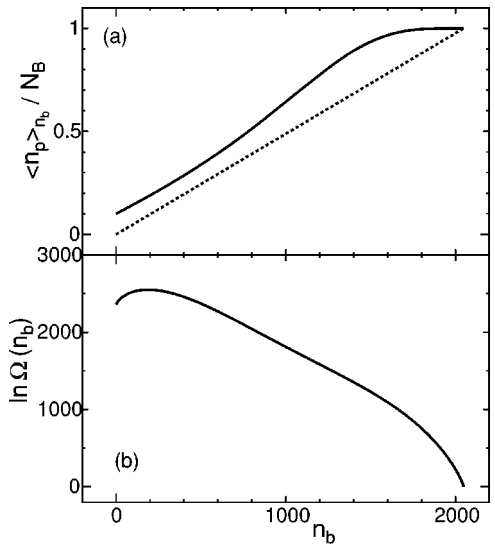

FIG. 4. (a) $\langle n_p \rangle_{n_b} / N_B$ and (b) $\ln \Omega(n_b)$ of the 32×32 ten-state Potts model obtained by the cluster-flip flat histogram method. The dotted line in (a) denotes n_b / N_B.

$-1)\rangle / N_B$ are given in the same manner as in the case of the Ising model. It is to be noted that $\langle n_p \rangle_{n_b=0} / N_B = 1/10$ for the ten-state Potts model. The logarithm of the bond-number DOS, $\ln \Omega(n_b)$, obtained by $\langle n_p \rangle_{n_b}$ is shown in Fig. 4(b). The temperature dependence of the energy obtained by Eq. (4) is given in Fig. 5. The latent heat ΔQ is shown in the figure. The comparison of the flatness time for the 2D ten-state Potts model is shown in Fig. 6. The linear system sizes L are 4, 8, 12, 16, 20, and 24. The number of samples to take the average ranges from 5 for the largest system to 1000 for the smallest. The flatness time of the single-spin-flip flat histogram method increases more rapidly with size than that of the cluster-flip flat histogram method, although it is not clear whether the size dependence is linear or not in logarithmic scale. It again shows the superiority of the cluster-flip flat histogram method over the single-spin-flip flat histogram method.

In the calculations presented above, we have used the number of potential moves both for the dynamics and the estimator of $\Omega(n_b)$ or $\langle n_p \rangle_{n_b}$. However, our procedure to calculate the bond-number DOS $\Omega(n_b)$ using the number of potential moves, or more explicitly, using $\langle n_p \rangle_{n_b}$, Eq. (11) or

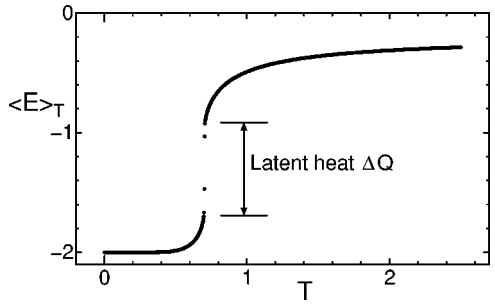

FIG. 5. Energy of the 2D ten-state Potts model for $L = 32$ obtained by the cluster-flip flat histogram method.

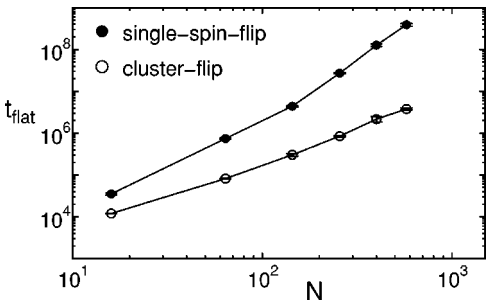

FIG. 6. Size dependence of the flatness time for the 2D ten-state Potts model. The linear system sizes L are 4, 8, 12, 16, 20, and 24; $N = L^2$. The cluster-flip flat histogram method and the single-spin-flip flat histogram method are compared.

(13), is independent of the dynamics. We may use the multibondic ensemble method [12] or its improvement [13], and monitor $\langle n_p \rangle_{n_b}$ to compute $\Omega(n_b)$, although $\Omega(n_b)$ is directly used for the probability to update and renewed with the help of the histogram $H(n_b)$, such as $\Omega^{\text{old}}(n_b) H(n_b) \rightarrow \Omega^{\text{new}}(n_b)$. We compare the accuracy of the calculation for several dynamics and the procedure to calculate $\Omega(n_b)$. For that purpose, we study the errors of the specific heat for the 2D Ising model. The energy DOS is exactly calculated by Beale [21]. As already shown in Fig. 2, the errors of our calculation are very small; we treat the relative error, which is defined as

$$\epsilon(T) \equiv \left| \frac{C_{\text{simulation}}(T) - C_{\text{exact}}(T)}{C_{\text{exact}}(T)} \right|$$

for the specific heat C. The relative errors $\epsilon(T)$ of the 32×32 Ising model in the case of the cluster-flip flat histogram method are shown in Fig. 7(a). The number of MCS is 20 000 N_B. The average value of $\epsilon(T)$ in the range of $1.0 \leqslant T \leqslant 4.0$, which will be denoted by $\overline{\epsilon(T)}$, is as small as 0.0002.

In the case of the multibondic ensemble method, we can calculate $\Omega(n_b)$ either through the number of potential moves or by the direct calculation with the help of the histogram $H(n_b)$. The errors $\epsilon(T)$ of the 32×32 Ising model in the case of the multibondic ensemble method are plotted in Fig. 7(b). The number of MCS is 20 000 N_B; we renew $\Omega(n_b)$ for the probability of graph update by every 100 N_B MCS. The solid line denotes the data for the calculation using the number of potential moves, and dotted lines denotes those for the direct calculation using $H(n_b)$. We see that the calculation of $\Omega(n_b)$ through the number of potential moves gives much smaller errors. The average value $\overline{\epsilon(T)}$ is 0.0002 for the calculation using the number of potential moves, whereas that for the direct calculation with $H(n_b)$ is 0.043. We also show the results of the improved multibondic method in Fig. 7(c). The conditions are the same as those for the multibondic method. The average value $\overline{\epsilon(T)}$ for the calculation using the number of potential moves is 0.0002, whereas that for the direct calculation with $H(n_b)$ is 0.0087. The calculation of $\Omega(n_b)$ through the number of potential moves again gives much smaller errors compared to the di-

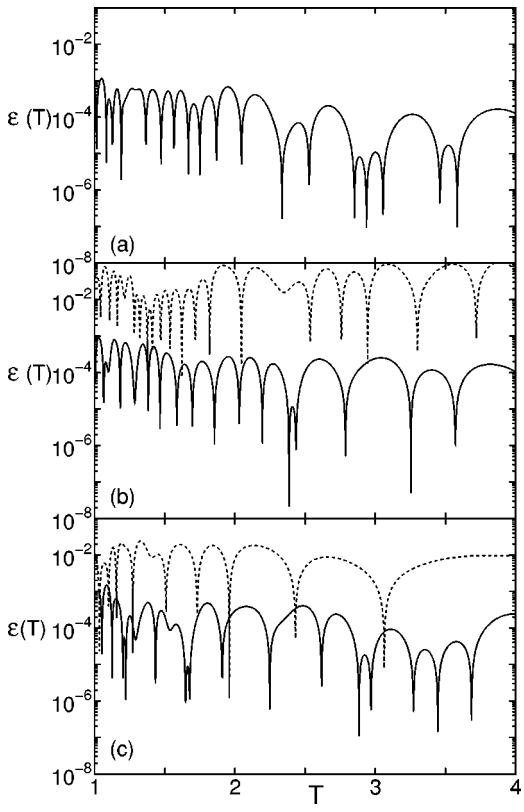

FIG. 7. Relative errors of the specific heat for the 32×32 Ising model; (a) the cluster-flip flat histogram method, (b) the multibondic ensemble method, and (c) the improved multibondic ensemble method. The number of MCS is 20 000 N_B. The solid line denotes the data obtained by the calculation using the number of potential moves, and dotted line denotes those obtained by the direct calculation with $H(n_b)$.

rect calculation with $H(n_b)$. It is interesting to notice that $\overline{\epsilon(T)}$ take almost the same value for several methods if we follow the procedure to calculate $\Omega(n_b)$ through $\langle n_p\rangle_{n_b}$. The data of $\overline{\epsilon(T)}$ for several methods are tabulated in Table I for convenience.

VI. SUMMARY AND DISCUSSIONS

To summarize, we have derived the rigorous BHR for the bond number, investigating the cluster (graph) representation of the spin models. We have shown that the bond-number DOS $\Omega(n_b)$ can be calculated in terms of $\langle n_p\rangle_{n_b}$. We have proposed a Monte Carlo dynamics based on the number of potential moves for the bond number, which is regarded as the flat histogram method for the bond number. We have shown the efficiency of the BHR for the bond number in calculating the bond-number DOS and other physical quantities.

TABLE I. Average relative error of the specific heat $\overline{\epsilon(T)}$ for the 2D 32×32 Ising model. We compare the data for several Monte Carlo methods and the procedure to calculate $\Omega(n_b)$, the calculation using the number of potential moves (potential move) and the direct calculation with $H(n_b)$ (direct).

$\overline{\epsilon(T)}$	Potential move	Direct
Cluster-flip flat histogram	0.0002	
Multibondic	0.0002	0.043
Improve multibondic	0.0002	0.0087

For the dynamics, the combination of the Wang-Landau idea [8] and the cluster algorithms is useful in accelerating the diffusion of the random walker, as was pointed out before [13]. However, here we have made more emphasis on the use of the BHR for the estimator of $\Omega(n_b)$. The advantage of using the BHR may be attributed to the fact that the number of potential moves is a macroscopic quantity, which is the same situation as the BHR for the energy [16,17]. Moreover, the use of the improved estimator for calculating the number of potential moves, Eq. (13), gives much better statistics for the calculation.

The number of potential moves for the energy, $N(S,E\rightarrow E\pm\Delta E)$, has several possibilities for ΔE. On the contrary, in the case of the number of potential moves for the bond number, $N(G,n_b\rightarrow n_b\pm1)$, the change of the bond number is limited to one, which makes the calculation of the bond-number DOS through the number of potential moves much simpler than that of the energy DOS.

Recently, a cluster Monte Carlo algorithm to simulate the Q-state Potts model for any real $Q(>0)$ was proposed by Gliozzi [22]. It is interesting to apply the BHR to that method. Since only the information on graph is used in that Monte Carlo algorithm, Eq. (12) is useful for calculating $\langle n_p\rangle_{n_b}$.

In this paper, we argued the BHR for the bond number. We can extend the present idea to the relation including two variables, for example, the bond number and the cluster number. The extension to more general cases, such as the loop algorithm of the quantum Monte Carlo simulation, may attract much attention, which will be studied in near future.

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[1] B. A. Berg and T. Neuhaus, Phys. Rev. Lett. **68**, 9 (1992); B.A. Berg and T. Celik, *ibid.* **69**, 2292 (1992).
[2] J. Lee, Phys. Rev. Lett. **71**, 211 (1993).
[3] E. Marinari and G. Parisi, Europhys. Lett. **19**, 451 (1992).
[4] K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996).
[5] P. M. C. de Oliveira, T. J. P. Penna, and H. J. Herrmann, Braz. J. Phys. **26**, 677 (1996); Eur. Phys. J. B **1**, 205 (1998).

[6] J. S. Wang, Eur. Phys. J. B **8**, 287 (1998).
[7] J. S. Wang and L. W. Lee, Comput. Phys. Commun. **127**, 131 (2000); J. S. Wang, Physica A **281**, 147 (2000).
[8] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001).
[9] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58**, 86 (1987).
[10] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
[11] Y. Tomita and Y. Okabe, Phys. Rev. Lett. **86**, 572 (2001); J. Phys. Soc. Jpn. **71**, 1570 (2002).
[12] W. Janke and S. Kappler, Phys. Rev. Lett. **74**, 212 (1995).
[13] C. Yamaguchi and N. Kawashima, Phys. Rev. E **65**, 056710 (2002).
[14] P. M. C. de Oliveira, Eur. Phys. J. B **6**, 111 (1998).
[15] B. A. Berg and U. H. E. Hansmann, Eur. Phys. J. B **6**, 395 (1998).
[16] P. M. C. de Oliveira, Braz. J. Phys. **30**, 195 (2000); **30**, 766 (2000).
[17] A. R. Lima, P. M. C. de Oliveira, and T. J. P. Penna, J. Stat. Phys. **99**, 691 (2000).
[18] D. Kandel and E. Domany, Phys. Rev. B **43**, 8539 (1991).
[19] N. Kawashima and J. E. Gubernatis, Phys. Rev. E **51**, 1547 (1995).
[20] P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn. **26**, Suppl. p. 11 (1969); C. M. Fortuin and P. W. Kasteleyn, Physica (Utrecht) **57**, 536 (1972).
[21] P. D. Beale, Phys. Rev. Lett. **76**, 78 (1996).
[22] F. Gliozzi, Phys. Rev. E **66**, 016115 (2002).