Determining the density of states for classical statistical models: A random walk algorithm to produce a flat histogram

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We describe an efficient Monte Carlo algorithm using a random walk in energy space to obtain a very accurate estimate of the density of states for classical statistical models. The density of states is modified at each step when the energy level is visited to produce a flat histogram. By carefully controlling the modification factor, we allow the density of states to converge to the true value very quickly, even for large systems. From the density of states at the end of the random walk, we can estimate thermodynamic quantities such as internal energy and specific heat capacity by calculating canonical averages at any temperature. Using this method, we not only can avoid repeating simulations at multiple temperatures, but we can also estimate the free energy and entropy, quantities that are not directly accessible by conventional Monte Carlo simulations. This algorithm is especially useful for complex systems with a rough landscape since all possible energy levels are visited with the same probability. As with the multicanonical Monte Carlo technique, our method overcomes the tunneling barrier between coexisting phases at first-order phase transitions. In this paper, we apply our algorithm to both first- and second-order phase transitions to demonstrate its efficiency and accuracy. We obtained direct simulational estimates for the density of states for two-dimensional ten-state Potts models on lattices up to 200×200 and Ising models on lattices up to 256×256. Our simulational results are compared to both exact solutions and existing numerical data obtained using other methods. Applying this approach to a three-dimensional $\pm J$ spin-glass model, we estimate the internal energy and entropy at zero temperature; and, using a two-dimensional random walk in energy and order-parameter space, we obtain the (rough) canonical distribution and energy landscape in order-parameter space. Preliminary data suggest that the glass transition temperature is about 1.2 and that better estimates can be obtained with more extensive application of the method. This simulational method is not restricted to energy space and can be used to calculate the density of states for any parameter by a random walk in the corresponding space.

I. INTRODUCTION

Computer simulation now plays a major role in statistical physics [1], particularly for the study of phase transitions and critical phenomena. One of the most important quantities in statistical physics is the density of states $g(E)$, i.e., the number of all possible states (or configurations) for an energy level E of the system, but direct estimation of this quantity has not been the goal of simulations. Instead, most conventional Monte Carlo algorithms [1] such as Metropolis importance sampling [2], Swendsen-Wang cluster flipping [3,4], etc., generate a canonical distribution $g(E)e^{-E/k_BT}$ at a given temperature. Such distributions are so narrow that, with conventional Monte Carlo simulations, multiple runs are required if we want to know thermodynamic quantities over a significant range of temperatures. In the canonical distribution, the density of states does not depend on the temperature at all. If we can estimate the density of states $g(E)$ with high accuracy for all energies, we can then construct canonical distributions at any temperature. For a given model in statistical physics, once the density of states is known, we can calculate the partition function as $Z = \Sigma_E g(E) e^{-\beta E}$, and the model is essentially ''solved'' since most thermodynamic quantities can be calculated from it. Though computer simulation is already a very powerful method in statistical physics [1], it seems that there is no efficient algorithm to calculate the density of states very accurately for large systems. Even

for exactly solvable models such as the two-dimensional (2D) Ising model, $g(E)$ is impossible to calculate exactly for a large system [5].

The multicanonical ensemble method [6–9] proposed by Berg *et al.* has been proved to be very efficient in studying first-order phase transitions where simple canonical simulations have difficulty overcoming the tunneling barrier between coexisting phases at the transition temperature [6,9–16]. In the multicanonical method, we have to estimate the density of states $g(E)$ first, then perform a random walk with a flat histogram in the desired region in the phase space, such as between two peaks of the canonical distribution at the first-order transition temperature. In a multicanonical simulation, the density of states need not necessarily be very accurate, as long as the simulation generates a relatively flat histogram and overcomes the tunneling barrier in energy space. This is because the subsequent re-weighting [6,8], does not depend on the accuracy of the density of the states as long as the histogram can cover all important energy levels with sufficient statistics. (If the density of states could be calculated very accurately, then the problem would have been solved in the first place and we need not perform any further simulation such as with the multicanonical simulational method.)

Lee [17] independently proposed the entropic sampling method, which is basically equivalent to multicanonical ensemble sampling. He used an iteration process to calculate the microcanonical entropy at E which is defined by $S(E)$

$=\ln[g(E)]$ where $g(E)$ is the density of states. He also applied his method to the 2D ten-state ($Q=10$) Potts model and the 3D Ising model; however, just as for other simple iteration methods, it works well only for small systems. He obtained a good result with his method for the 24×24 2D $Q=10$ Potts model and the $4\times4\times4$ 3D Ising model.

de Oliveira *et al.* [18–20] proposed the broad histogram method with which they calculated the density of states by estimating the probabilities of possible transitions between all possible states of a random walk in energy space. Using simple canonical average formulas in statistical physics, they then calculated thermodynamic quantities for any temperature. Though the authors believed that the broad histogram relation is exact, their simulational results have systematic errors even for the Ising model on a 32×32 lattice in references [18,21]. They believed that the error was due to the particular dynamics adopted within the broad histogram method [22]. Very recently, they have reduced the error near T_c to a small value for $L=32$ [23].

It is thus an extremely difficult task to calculate density of states directly with high accuracy for large systems. All methods based on accumulation of histogram entries, such as the histogram method of Ferrenberg and Swendsen [24], Lee's version of multicanonical method (entropic sampling) [17], broad histogram method [18,21,25], and flat histogram method [21] have the problem of scalability for large systems. These methods suffer from systematic errors when systems are large, so we need a superior algorithm to calculate the density of states for large systems.

Very recently, we introduced a new, general, efficient Monte Carlo algorithm that offers substantial advantages over existing approaches [26]. In this paper, we will explain the algorithm in detail, including our implementation, and describe its application not only to first- and Second-order phase transitions, but also to a 3D spin glass model that has a rough energy landscape.

The remainder of this paper is arranged as follows. In Sec. II, we present our general algorithm in detail. In Sec. III, we apply our method to the 2D $Q=10$ Potts model that has a first-order phase transition. In Sec. IV, we apply our method to a model with a second-order phase transition to test the accuracy of the algorithm. In Sec. V, we consider the 3D $\pm J$ spin glass model, a system with rough landscapes. Discussion and the conclusion are presented in Sec. VI.

II. A GENERAL AND EFFICIENT ALGORITHM TO ESTIMATE THE DENSITY OF STATES WITH A FLAT HISTOGRAM

Our algorithm is based on the observation that if we perform a random walk in energy space by flipping spins randomly for a spin system, and the probability to visit a given energy level E is proportional to the reciprocal of the density of states $1/g(E)$, then a flat histogram is generated for the energy distribution. This is accomplished by modifying the estimated density of states in a systematic way to produce a ''flat'' histogram over the allowed range of energy and simultaneously making the density of states converge to the true value. We modify the density of states constantly during

each step of the random walk and use the updated density of states to perform a further random walk in energy space. The modification factor of the density of states is controlled carefully, and at the end of simulation the modification factor should be very close to one which is the ideal case of the random walk with the true density of states.

At the very beginning of our simulation, the density of states is *a priori* unknown, so we simply set all entries to $g(E)=1$ for all possible energies E. Then we begin our random walk in energy space by flipping spins randomly and the probability at a given energy level is proportional to $1/g(E)$. In general, if E_1 and E_2 are energies before and after a spin is flipped, the transition probability from energy level E_1 to E_2 is

$$p(E_1\rightarrow E_2)=\min\left[\frac{g(E_1)}{g(E_2)},1\right]. \tag{1}$$

Each time an energy level E is visited, we modify the existing density of states by a modification factor $f>1$, i.e. $g(E)\rightarrow g(E)f$. (In practice, we use the formula $\ln[g(E)]\rightarrow\ln[g(E)]+\ln(f)$ in order to fit all possible $g(E)$ into double precision numbers for the systems we will discuss in this paper.) If the random walk rejects a possible move and stays at the same energy level, we also modify the existing density of states with the same modification factor. Throughout this paper we have used an initial modification factor of $f=f_0=e^1\simeq2.71828,\ldots,$ which allows us to reach all possible energy levels very quickly even for a very large system. If f_0 is too small, the random walk will spend an extremely long time to reach all possible energies. However, too large a choice of f_0 will lead to large statistical errors. In our simulations, the histograms are generally checked about each 10000 Monte Carlo (MC) sweeps. A reasonable choice is to make $(f_0)^{10000}$ have the same order of magnitude as the total number of states (Q^N for a Potts model). During the random walk, we also accumulate the histogram $H(E)$ (the number of visits at each energy level E) in the energy space. When the histogram is ''flat'' in the energy range of the random walk, we know that the density of states converges to the true value with an accuracy proportional to that modification factor $\ln(f)$. Then we reduce the modification factor to a finer one using a function like $f_1=\sqrt{f_0}$, reset the histogram, and begin the next level random walk during which we modify the density of states with a finer modification factor f_1 during each step. We continue doing so until the histogram is ''flat'' again and then reduce the modification factor $f_{i+1}=\sqrt{f_i}$ and restart. We stop the random walk when the modification factor is smaller than a predefined value [such as $f_{\text{final}}=\exp(10^{-8})\simeq1.00000001$]. It is very clear that the modification factor acts as a most important control parameter for the accuracy of the density of states during the simulation and also determines how many MC sweeps are necessary for the whole simulation. The accuracy of the density of states depends on not only f_{final}, but also many other factors, such as the complexity and size of the system, criterion of the flat histogram, and other details of the implementation of the algorithm.

It is impossible to obtain a perfectly flat histogram and the phrase ''flat histogram'' in this paper means that histogram $H(E)$ for all possible E is not less than $x\%$ of the average histogram $\langle H(E) \rangle$, where $x\%$ is chosen according to the size and complexity of the system and the desired accuracy of the density of states. For the $L=32$, 2D Ising model with only nearest-neighbor couplings, this percentage can be chosen as high as 95%, but for large systems, the criterion for ''flatness'' may never be satisfied if we choose too high a percentage and the program may run forever.

One essential constraint on the implementation of the algorithm is that the density of states during the random walk converges to the true value. The algorithm proposed in this paper has this property. The accuracy of the density of states is proportional to $\ln(f)$ at that iteration; however, $\ln(f_{\mathrm{final}})$ cannot be chosen arbitrary small or the modified $\ln[g(E)]$ will not differ from the unmodified one to within the number of digits in the double precision numbers used in the calculation. If this happens, the algorithm no longer converges to the true value, and the program may run forever. Even if f_{final} is within range but too small, the calculation might take excessively long to finish.

We have chosen to reduce the modification factor by a square-root function, and f approaches one as the number of iterations approaches infinity. In fact, any function may be used as long as it decreases f monotonically to one. A simple and efficient formula is $f_{i+1}=f_i^{1/n}$, where $n>1$. The value of n can be chosen according to the available CPU time and expected accuracy of the simulation. For the systems that we have studied, the choice of $n=2$ yielded good accuracy in a relatively short time, even for large systems. When the modification factor is almost one and the random walk generates a uniform distribution in energy space, the density of states should converge to the true value for the system.

Procedures for allowing $f \to 1$ have been examined by Hüller [27] who used data from two densities of states for two different values of f to extrapolate to $f=1$. However, his data for a small Ising system yield larger errors than our direct approach. The applicability of his method to large systems also needs a more detailed study.

The method can be further enhanced by performing multiple random walks, each for a different range of energy, either serially or in parallel fashion. We restrict the random walk to remain in the range by rejecting any move out of that range. The resultant pieces of the density of states can then be joined together and used to produce canonical averages for the calculation of thermodynamic quantities at any temperature.

Almost all recursive methods update the density of states by using the histogram data directly only after enough histogram entries are accumulated [6,7,11,13–16,28–30]. Because of the exponential growth of the density of states in energy space, this process is not efficient because the histogram is accumulated linearly. In our algorithm, we modify the density of states at each step of the random walk, and this allows us to approach the true density of states much faster than conventional methods especially for large systems. (We also accumulate histogram entries during the random walk,

but we only use it to check whether the histogram is flat enough to go to the next level random walk with a finer modification factor.)

We should point out here that the total number of configurations increases exponentially with the size of the system; however, the total number of possible energy levels increases linearly with the size of system. It is thus easy to calculate the density of states with a random walk in energy space for a large system. In this paper, for example, we consider the Potts model on an $L \times L$ lattice with nearest-neighbor interactions [31]. For $Q \geqslant 3$, the number of possible energy levels is about $2N$, where $N=L^2$ is the total number of the lattice site. However, the average number of possible states (or configurations) on each energy level is as large as $Q^N/2N$, where Q is the number of possible states of a Potts spin and Q^N is the total number of possible configurations of the system. This is the reason why most models in statistical physics are well defined, but we cannot simply use our computers to realize all possible states to calculate any thermodynamic quantities, this is also the reason why efficient and fast simulational algorithms are required in the numerical investigations.

By the end of simulation, we only obtain relative density, since the density of states can be modified at each time it is visited. We can apply the condition that the total number of possible states for the Q state Potts model is $\Sigma_E g(E)=Q^N$ or the number of ground state is Q to get the absolute density of states.

III. APPLICATION TO A FIRST-ORDER PHASE TRANSITION

A. Potts model and its canonical distribution

In this section, we apply our algorithm to a model with a first-order phase transition [32,33]. We choose the 2D ten state Potts model [31] since it serves as an ideal laboratory for temperature-driven first-order phase transitions. Since some exact solutions and extensive simulational data are available, we have ample opportunity to compare our results with other values.

We consider the two-dimensional $Q=10$ Potts model on $L \times L$ square lattice with nearest-neighbor interactions and periodic boundary conditions. The Hamiltonian for this model can be written as

$$\mathcal{H}=-\sum_{\langle ij \rangle} \delta(q_i,q_j) \qquad (2)$$

and $q=1,2,\ldots,Q$. The Hamiltonian (or energy) is in the unit of the nearest coupling J. We assume $J=1$ for simplicity in this paper. During the simulation, we select lattice sites randomly and choose integers between $[1:Q]$ randomly for new Potts spin values. The modification factor f_i changes from $f_0=e^1=2.718\,28$ at the very beginning to $f_{\mathrm{final}}=\exp(10^{-8}) \simeq 1.000\,000\,01$ by the end of the random walk. To guarantee the accuracy of thermodynamic quantities at low temperatures in further calculations, in this paper we use the condition that the number of the ground states is Q to normalize the density of states. The densities of states for
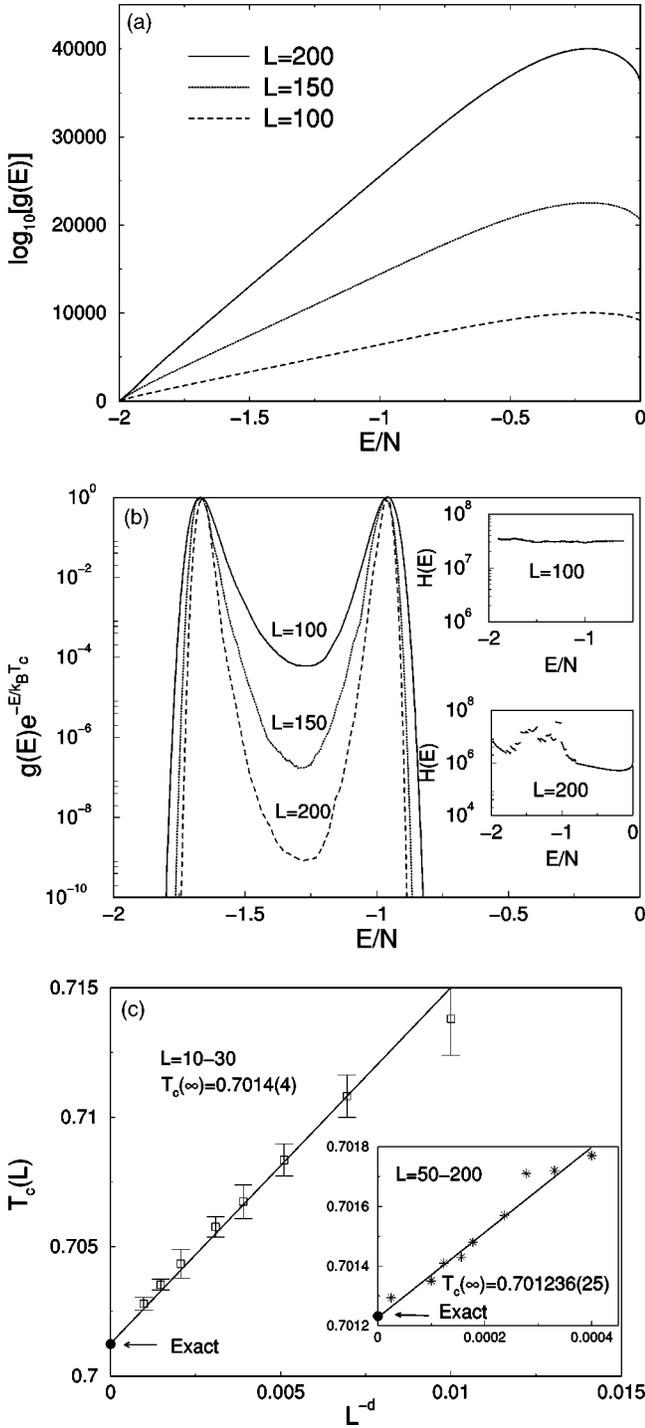
FIG. 1. (a) Density of states $g(E)$ for the 2D $Q=10$ Potts model. (b) The canonical distributions at T_c. (c) Extrapolation of finite lattice ''transition temperatures.''

$$P(E,T) = g(E)e^{-E/k_B T}. \qquad (3)$$

The temperature is defined in the unit of J/k_B with $J=1$. From the simulational result for the density of states $g(E)$, we can calculate the canonical distribution by the above formula at any temperature without performing multiple simulations. In Fig. 1(b), we show the resultant double-peaked canonical distribution [33], at the transition temperature T_c for the first-order transition of the $Q=10$ Potts model. The ''transition temperatures'' are determined by the temperatures where the double peaks are of the same height. Note that the peaks of the distributions are normalized to one in this figure. The valley between two peaks is quite deep, e.g., is 7×10^{-5} for $L=100$. The latent heat for this temperature-driven first-order phase transition can be estimated from the energy difference between the double peaks. Our results for the locations of the peaks are listed in the Table I. They are consistent with the results obtained by multicanonical method [6] and multibondic cluster algorithm [9] for those lattice sizes for which these other methods are able to generate estimates. As the table shows, our method produces results for substantially larger systems than have been studied by these other approaches.

Because of the double peak structure at a first-order phase transition, conventional Monte Carlo simulations are not efficient since an extremely long time is required for the system to travel from one peak to the other in energy space. With the algorithm proposed in this paper, all possible energy levels are visited with equal probability, so it overcomes the tunneling barrier between the coexisting phases in the conventional Monte Carlo simulations. The histogram for $L=100$ is shown in an inset of the Fig. 1(b). The histogram in the figure is the overall histogram defined by the total number of visits to each energy level for the random walk. Here, too, we choose the initial modification factor $f_0 = e^1$, and the final one as $\exp(10^{-8}) \simeq 1.00000001$; and the total number of iterations is 27. In our simulation, we do not set a predetermined number of MC sweeps for each iteration, but rather give the criterion that the program checks periodically. Generally, the number of MC sweeps needed to satisfy the criterion increases as we reduce the modification factor to a finer one, but we cannot predict the exact number of MC sweeps needed for each iteration before the simulation. We believe that it is preferable to allow the program to decide how great a simulational effort is needed for a given modification factor f_i. This also guarantees a sufficiently flat histogram resulting from a random walk that in turn determines the accuracy of the density of states at the end of the simulation. We nonetheless need to perform some test runs to make sure that the program will finish within a given time. The entire simulational effort used was about 3.3×10^7 visits (6.6×10^7 MC sweeps) for $L=100$. With the program we implemented, the simulation for $L=100$ can be completed within two weeks in a single 600 MHz Pentium III processor.

To speed up the simulation, we need not constrain ourselves to performing a single random walk over the entire energy range with high accuracy. If we are only interested in a specific temperature range, such as near T_c, we could first

100×100, 150×150, and 200×200 are shown in Fig. 1(a). It is very clear from the figure that the maximum density of states for $L=200$ is very close to 10^{40000} which is actually about 5.75×10^{39997} from our simulational data.

Conventional Monte Carlo simulation (such as Metropolis sampling [1,2]) realizes a canonical distribution $P(E,T)$ by generating a random walk Markov chain at a given temperature

TABLE I. Estimates of ''transition temperature'' T_c and positions of double peaks E_1^{max}, E_2^{max} for the $Q=10$ Potts model with our method, the multicanonical (MUCA) ensemble [6], and the multibondic (MUBO) cluster algorithm [9]. E_1^{max} and E_2^{max} are the energy per lattice site at the two peaks of canonical distribution at T_c.

Size		Our method		MUCA			MUBO		
L	T_c	E_1^{max}	E_2^{max}	T_c	E_1^{max}	E_2^{max}	T_c	E_1^{max}	E_2^{max}
12	0.709 91	0.8402	1.7013	0.710 540	0.806	1.688	0.710 540 2	0.833	1.72
16	0.706 53	0.8694	1.6967	0.706 544	0.844	1.676	0.706 514 4	0.867	1.71
20	0.705 11	0.8925	1.6875				0.704 789 1	0.883	1.69
24	0.703 62	0.8940	1.6765	0.703 730	0.908	1.698			
26	0.703 17	0.9002	1.6805				0.703 412 0	0.908	1.682
30	0.702 89	0.9233	1.6888						
34	0.702 58	0.9343	1.6732	0.702 553	0.927	1.683	0.702 553 0	0.921	1.676
40	0.702 39	0.9337	1.6731						
50	0.701 77	0.9416	1.6776				0.701 876 5	0.940	1.674
60	0.701 71	0.9522	1.6733						
70	0.701 53	0.9519	1.6717	0.701 562	0.9511	1.670			
80	0.701 43	0.9576	1.6701						
90	0.701 41	0.9551	1.6727						
100	0.701 35	0.9615	1.6699	0.701 378	0.9594	1.6699			
120	0.701 31	0.9803	1.6543						
150	0.701 27	0.9674	1.6738						
200	0.701 24	0.9647	1.6710						
∞	0.701 236 ± 0.000 025								
exact	0.701 232 . . .								

perform a low-precision unrestricted random walk, i.e., over all energies, to estimate the required energy range, and then carry out a very accurate random walk for the corresponding energy region. The inset of Fig. 1(b) for $L=100$ only shows the histograms for the extensive random walks in the energy range between $E/N=-1.90$ and -0.6. If we need to know the density of states more accurately for some energies, we also can perform separate simulations, one for low-energy levels, one for high-energy levels, the other for middle energy, which includes double peaks of the canonical distribution at T_c. This scheme not only speeds up the simulation, but also increases the probability of accessing the energy levels for which both maximum and minimum values of the distributions occur by performing the random walk in a relatively small energy range. If we perform a single random walk over all possible energies, it will take a long time to generate rare spin configurations. Such rare energy levels include the ground-energy level or low-energy levels with only a few spins with different values and high energy levels where all, or most, adjacent Potts spins have different values.

With the algorithm in this paper, if the system is not larger than 100×100, the random walk on important energy regions (such as that which includes the two peaks of the canonical distribution at T_c) can be carried out with a single processor and will give an accurate density of states within about 10^7 visits per energy level. However, for a larger system, we can use a parallelized algorithm by performing random walks in different energy regions, each using a different processor. We have implemented this approach using PVM (parallel virtual machine) with a simple master-slave model

and can then obtain an accurate estimate for the density of states with relatively short runs on each processor. The densities of states for 150×150 and 200×200, shown in Fig. 1(b), were obtained by joining together the estimates obtained from 21 independent random walks, each constrained within a different region of energy. The histograms from the individual random walks are shown in the second inset of Fig. 1(b) for 200×200 lattice. In this case, we only require that the histogram of the random walk in the corresponding energy segment is sufficiently flat without regard to the relative flatness over the entire energy range. In Fig. 1(b), the results for large lattices show clear double peaks for the canonical distributions at temperatures $T_c(L)=0.701\,27$ for $L=150$ and $T_c(L)=0.701\,243$ for $L=200$. The exact result is $T_c=0.701\,232,\ldots$, for the infinite system. Considering the valley which we find for $L=200$ is as deep as 9×10^{-10}, we can understand why it is impossible for conventional Monte Carlo algorithms to overcome the tunneling barrier with available computational resources.

If we compare the histogram for $L=100$ with that for $L=200$ in Fig. 1(b), we see very clearly that the simulation effort for $L=200$ (9.8×10^6 visits per energy level) is even less than the effort for $L=100$ (3.3×10^7 visits per energy level.). It is more efficient to perform random walks in relatively small energy segments than a single random walk over all energies. The reason is very simple, the random walk is a local walk, which means for a given E_1, the energy level for the next step only can be one of nine levels in the energy range $[E_1-4,E_1+4]$ (for the Potts model discussed in this

section). The algorithm itself only requires that the histogram on such local transitions is flat. (A single random walk, subject to the requirement of a flat histogram for all energy levels, will take quite long.) For random walks in small energy segments, we should be very careful to make sure that all spin configurations with energies in the desired range can be equally accessed so we restart the random walk periodically from independent spin configurations.

An important question that must be addressed is the ultimate accuracy of the algorithm. One simple check is to estimate the transition temperature of the 2D $Q=10$ Potts model for $L=\infty$ since the exact solution is known. According to the finite-size scaling theory, the ''effective'' transition temperature for finite systems behaves as

$$T_c(L) = T_c(\infty) + \frac{c}{L^d}, \qquad (4)$$

where $T_c(L)$ and $T_c(\infty)$ are the transition temperatures for finite- and infinite-size systems, respectively, L is the linear size of the system and d is dimension of the lattice.

In Fig. 1(c), the transition temperature is plotted as a function of L^{-d}. The data in the main portion of the figure are obtained from small systems ($L=10\sim30$), and the error bars are estimated by results from multiple independent runs. Clearly the transition temperature extrapolated from our simulational data is $T_c(\infty) = 0.7014 \pm 0.0004$, which is consistent with the exact solution ($T_c = 0.701\,232, \ldots,$) for the infinite system. To get an even more accurate estimate, and also test the accuracy of the density of states from single runs for large systems, we performed a single, long random walk on large lattices ($L=50\sim200$). The results, plotted as a function of lattice size in the inset of the figure, show that the transition temperature extrapolated from the finite systems is $T_c(\infty) = 0.701\,236 \pm 0.000\,025$, which is still consistent with the exact solution.

We also compare our simulational result for the $Q=10$ Potts model with the existing numerical data such as estimates of transition temperatures and double peak locations obtained with the multicanonical simulational method by Berg and Neuhaus [6] and the multibondic cluster algorithm by Janke and Kappler [9]. All results are shown in Table I. With our random walk simulational algorithm, we can calculate the density of states up to 200×200 within 10^7 visits per energy level to obtain a good estimate of the transition temperature and locations of the double peaks. Using the multicanonical method and a finite scaling guess for the density of states, Berg *et al.* only obtained results for lattices as large as 100×100 [6], and multibondic cluster algorithm data [9] were not given for systems larger than 50×50.

In Sec. IV, the accuracy of our algorithm will be further tested by comparing thermodynamic quantities obtained for 2D Ising model with exact solutions.

B. Thermodynamic properties of the $Q=10$ Potts model

One of the advantages of the our method is that the density of states does not depend on temperature; indeed with

the density of states, we can calculate thermodynamic quantities at any temperature. For example, the internal energy can be calculated by

$$U(T) = \frac{\sum_E E g(E) e^{-\beta E}}{\sum_E g(E) e^{-\beta E}} \equiv \langle E \rangle_T. \qquad (5)$$

To study the behavior of the internal energy near T_c more carefully, we calculate the internal energy for $L=60$, 100, and 200 near T_c as presented in Fig. 2(a). A very sharp ''jump'' in the internal energy at transition temperature T_c is visible, and the magnitude of this jump is equal to the latent heat for the (first-order) phase transition. Such behavior is related to the double peak distribution of the first-order phase transition. When T is slightly away from T_c, one of the double peaks increases dramatically in magnitude and the other decreases.

Since we only perform simulations on finite lattices, and use a continuum function to calculate thermodynamic quantities, all our quantities for finite-size systems will appear to be continuous if we use a very small scale. In the inset of Fig. 2(a), we use the same density of states again to calculate the internal energy for temperatures very close to T_c. On this scale, the ''discontinuity'' at the first-order phase transition disappears and a smooth curve can be seen instead of a sharp ''jump'' in the main portion of Fig. 2(a). The discontinuity in Fig. 2(a) is simply due to the coarse scale, but when the system size goes to infinity, the discontinuity will be real.

From the density of states we can also estimate the specific heat from the fluctuations in the internal energy

$$C(T) = \frac{\partial U(T)}{\partial T} = \frac{\langle E^2 \rangle_T - \langle E \rangle_T^2}{T^2}. \qquad (6)$$

In Fig. 2(b), the specific heat so obtained is shown as a function of temperature. We calculate the specific heat in the vicinity of the transition temperature T_c. The finite-size dependence of the specific heat is clearly evident. We find that specific heat has a finite maximum value for a given lattice size L that, according to the finite-size scaling theory for first-order transitions should vary as

$$c(L,T) L^{-d} \propto f([T - T_c(\infty)] L^d), \qquad (7)$$

where $c(L,T) = C(L,T)/N$ is the specific heat per lattice site, L is the linear lattice size, $d=2$ is the dimension of the lattice. $T(L=\infty) = 0.701\,23, \ldots,$ is the exact solution for the $Q=10$ Potts model [31]. In the inset of Fig. 2(b), our simulational data for systems with $L=60$, 100, and 200 can be well fitted by a single scaling function, moreover, this function is completely consistent with the one obtained from lattice sizes from $L=18$ to $L=50$ by standard Monte Carlo [33].

With the density of states, we not only can calculate most thermodynamic quantities for all temperatures without multiple simulations but we can also access some quantities,
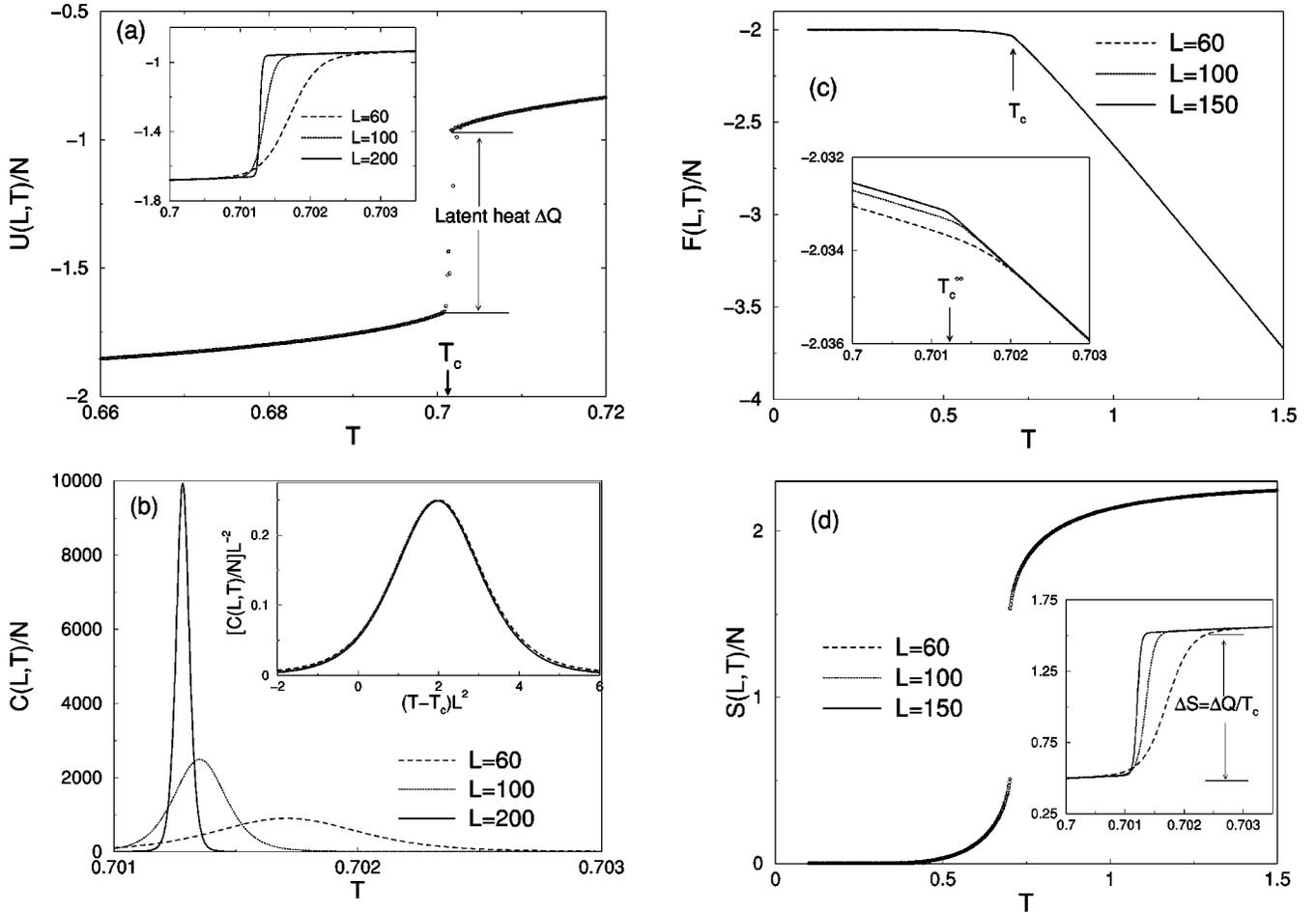
FIG. 2. Thermodynamic quantities calculated from the density of states for the $Q=10$ Potts model: (a) internal energy, (b) specific heat and the finite-size scaling function, (c) free energy, and (d) entropy.

such as the free energy and entropy, which are not directly available from conventional Monte Carlo simulations.The free energy is calculated using

$$Z=\sum_{\{config.\}} e^{-\beta E}=\sum_E g(E)e^{-\beta E}$$

$$F=-kT\log(Z). \qquad (8)$$

Our results for the free energy-per-lattice site is shown in Fig. 2(c) as a function of temperature. Since the transition is first-order, the free energy appears to have a "discontinuity" in the first derivative at T_c. This is typical behavior for a first-order phase transition, and even with the fine scale used in the inset of Fig. 2(c), this property is still apparent even though the system is finite. The transition temperature T_c is determined by the point where the first derivative appears to be discontinuous. With a coarse temperature scale we can not distinguish the finite-size behavior of our model; however, we can see a very clear size dependence when we view the free energy on a very fine scale as in the inset of Fig. 2(c).

The entropy is another very important thermodynamic quantity that cannot be calculated directly in conventional Monte Carlo simulations. It can be estimated by integrating

over other thermodynamic quantities, such as specific heat, but the result is not always reliable since the specific heat itself is not easy to determine accurately, particularly considering the "divergence" at the first-order transition. With an accurate density of states estimated by our method, we already know the free energy and internal energy for the system, so the entropy can be calculated easily

$$S(T)=\frac{U(T)-F(T)}{T}. \qquad (9)$$

It is very clear that the entropy is very small at low temperature and at $T=0$ is given by the density of states for the ground state. We show the entropy as a function of temperature in a wide region in Fig. 2(d).

The entropy has a very sharp "jump" at T_c, just as does the internal energy and such behavior can be seen very clearly in the inset of Fig. 2(d), when we recalculate the entropy near T_c. The change of the entropy at T_c shown in the figure can be obtained by the latent heat divided by the transition temperature, and the latent heat can be obtained by the jump in internal energy at T_c in Fig. 2(a).

With the histogram method proposed by Ferrenberg and Swendsen [24], it is possible to use simulational data at spe-

cific temperatures to obtain complete thermodynamic information near, or between, those temperatures. Unfortunately, it is usually quite hard to get accurate information in the region far away from the simulated temperature due to difficulties in obtaining good statistics, especially for large systems where the canonical distributions are very narrow. With the algorithm proposed in this paper, the histogram is ''flat'' for the random walk and we always have essentially the same statistics for all energy levels. Since the output of our simulation is the density of states, which does not depend on the temperature at all, we can then calculate most thermodynamic quantities at any temperature without repeating the simulation. We also believe the algorithm is especially useful for obtaining thermodynamic information at low temperature or at the transition temperature for the systems where the conventional Monte Carlo algorithm is not so efficient.

C. The tunneling time for the $Q=10$ Potts model at T_c

To study the efficiency of our algorithm, we measure the tunneling time τ, defined as the average number of sweeps needed to travel from one peak to the other and return to the starting peak in energy space. Since the histogram that our random walk produces is flat in energy space, we expect the tunneling time will be the same as for the ideal case of a simple random walk in real space, i.e., $\tau(N_E) \sim N_E$, where N_E is the total number of energy levels. To compare our simulational results to those for the ideal case, we also perform a random walk in real space. We always use a fixed $g(x_i)=1$ in one-dimensional real space, where x_i is a discrete coordinate of position that can be chosen simply as $1,2,3,4,\ldots,N_E$. The random walk is a local random walk with transition probability $p(x_i \rightarrow x_j)=1/2$, where $x_j=x_{i\pm1}$. We use the same definition of the tunneling time to measure the behavior of this quantity. The tunneling time for the ideal case satisfies the simple power law as $\tau(N_E) \sim N_E^\alpha$ and the exponent α is equal to 1. (τ is defined using the unit of sweep of N_E sites.) Our simulational data for random walks in energy space yield a tunneling time that is well described by the power law $\tau \sim N^\alpha$ as shown in Fig. 3. The solid lines in the graph have the simple power law as $\tau(N_E) \sim N_E$, and we see that our simulation result is very close to the ideal case. Since our method needs an extra effort to update the density of states to produce a flat histogram during the random walk in energy space, the tunneling time is much longer than the real space case. Also, because the tunneling time depends on the accuracy of the density of states, which is constantly modified during the random walk in energy space, it is not a well-defined quantity in our algorithm. The tunneling time, shown in Fig. 3 is the overall tunneling time, which includes all iterations with the modification factors from $f_0=e^1 \simeq 2.71828,\ldots$, to the final modification factor $f_{\text{final}}=\exp(10^{-8}) \simeq 1.00000001$.

We should point out that the two processes are not exactly the same, since the random walk in real space uses the exact density of states $[g(x_i)=1]$. However, the random walk in energy space requires knowledge of the density of states, which is *a priori* unknown. The algorithm we propose in this paper is a random walk with the density of states that is
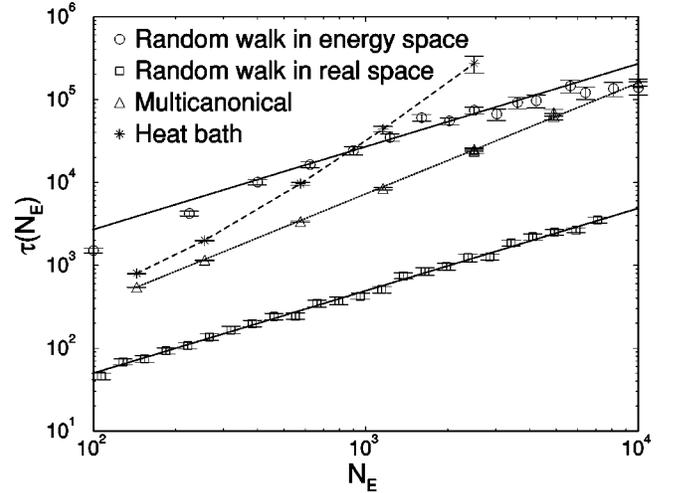

FIG. 3. Tunneling times τ for the $Q=10$ Potts model for our random walk algorithm in energy space, and for an ideal random walk in real space, for the multicanonical ensemble method, and for the heat bath algorithm. The solid lines show the ideal case with $\tau(N_E) \sim N_E$.

modified at each step during the walk in energy space. At the end of our random walk, the modification factor approaches one, and the estimated density of states approaches the true value. The two processes are then almost identical.

Conventional Monte Carlo algorithms (such as the heat-bath algorithm) have an exponentially fast growing tunneling time. According to Berg's study in Ref. [7], the tunneling time obeys the exponential law $\tau(L)=1.46L^{2.15}e^{0.080L}$. The multicanonical simulational method has reduced the tunneling time from an exponential law to a power law as $\tau(N_E) \sim N_E^\alpha$. However, the exponent α is as large as $\simeq 1.33$ [6], which is far away from the ideal case $\alpha=1$. Very recently, Janke and Kappler introduced the multibondic cluster algorithm, the exponent α is reduced to as small as 1.05 for 2D ten-state Potts model [9]. In Fig. 3, we also show the result obtained with the multicanonical method and the heat bath algorithm in Ref. [6]. We should point out that just like the multicanonical simulational method, our algorithm has a power increasing tunneling time with a smaller exponent α. For small systems, our algorithm offers less advantage because of the effort needed to modify the density of states during the random walk. Very recently, Neuhaus has generalized this algorithm to estimate the canonical distribution for $T<T_c$, in magnetization space for the Ising model [34]. He found that for small systems, the exponent for CPU time versus L for our algorithm and multicanonical ensemble simulations are almost identical. Our results in Fig. 3 are only for single-range random walks, and multiple-range random walks have been proven more efficient for larger systems.

IV. APPLICATION TO A SECOND-ORDER PHASE TRANSITION

The algorithm we proposed in this paper is very efficient for the study of any order phase transitions. Since our method is independent of temperature, it reduces the critical
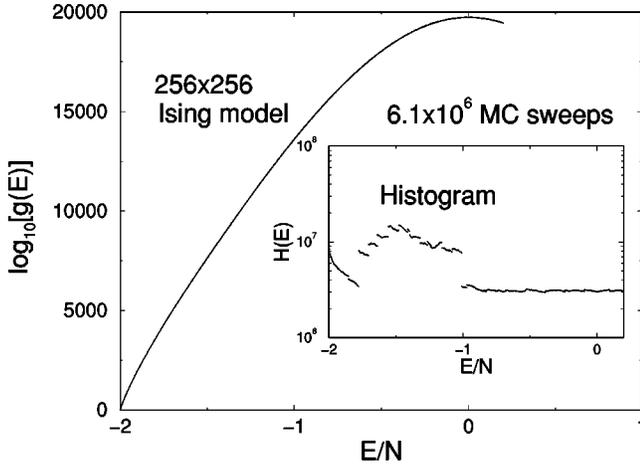
FIG. 4. Density of states ($\log_{10}[g(E)]$) of the 2D Ising model for $L=256$ (multiple range random walks). The overall histogram of the random walk is shown in the inset.
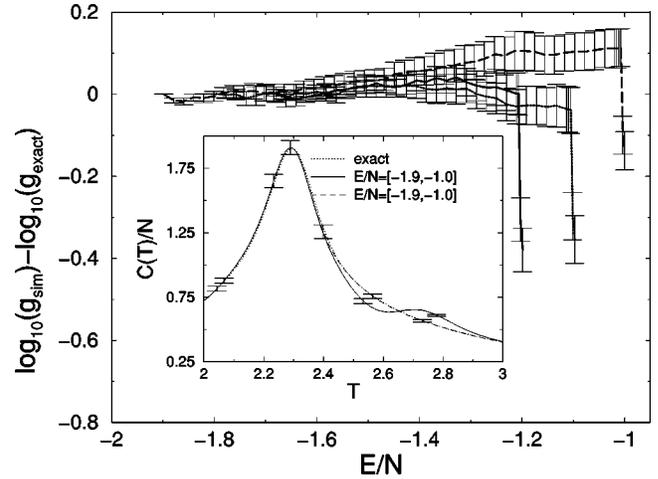

FIG. 5. The errors in the density of states for random walks in different energy ranges for the 2D Ising model. In the inset, we show the specific heats calculated from the density of states for the random walk in the ranges $E/N=[-1.9,-1.0]$ (solid line), the exact density (dotted line), and the density of states that the two highest energy entries are deleted for $E/N=[-1.9,-1.0]$ (dashed line).

slowing down at the second-order phase transition T_c and slow dynamics at low temperature. We estimate the density of states very accurately with a flat histogram, the algorithm will be very efficient for general simulational problems by avoiding the need for multiple simulations at multiple temperatures.

To check the accuracy and convergence of our method, we apply it to the 2D Ising model with nearest neighbor interactions on a $L \times L$ square lattice. This model provides an ideal benchmark for new algorithms [24,35,36] and is also an ideal laboratory for testing theory [5,37]. This model can be solved exactly, therefore we can compare our simulational results with exact solutions.

In Fig. 4, we show our estimation of the density of states of Ising model on 256×256 lattice. Since the density of states for $E>0$ has almost no contribution to the canonical average at finite positive temperature, we only estimate the density of states in the region $E/N \in [-2,0.2]$ out of the whole energy $[-2,2]$. To speed up our calculation, we divide the desired energy region $[-2,0.2]$ into 15 energy segments, and estimate the density of states for each segment with independent random walks. The modification factor changes from $f_0=e^1 \simeq 2.718\,28\ldots$ to $f_{\text{final}}=\exp(10^{-7}) \simeq 1.000\,000\,1,\ldots,$. The resultant density of states can be joined from adjacent energy segments. To reduce the boundary effects of the random walk on each segment, we keep about several hundred overlapping energy levels for random walks on two adjacent energy segments. The histograms of random walks are shown in the inset of this figure. We only require a flat histogram for each energy segment. To reduce the error of the density of states relevant to the accuracy of the thermodynamic quantities near T_c we optimize the parameter and perform additional multiple random walks for the energy range $E/N \in [-1.8,-1]$ with the same number of processors. For this we use the density of states obtained from the first simulations as starting points and continue the random walk with modification factors changing from $\exp(10^{-6}) \simeq 1.000\,001$ to $\exp(10^{-9}) \simeq 1.000\,000\,001$. The total computational effort is about 9.2×10^6 visits on each energy level. Note that the total number of possible energy

levels is $N-1$ and we perform random walks only on $[-2,0.2]$ out of $[-2,2]$. The real simulational effort is about 6.1×10^6 MC sweeps for the Ising model with $L=256$. With the program we implemented, it took about 240 CPU hours on a single IBM SP Power3 processor.

The density of states in Fig. 4 is obtained by the condition that the number of ground states is two for the 2D Ising model (all up or down). This condition guarantees the accuracy of the density of states at low energy levels that are very important in the calculation of thermodynamic quantities at low temperature. With this condition, when $T=0$, we can get exact solutions for internal energy, entropy, and free energy when we calculate such quantities from the density of states. If we apply the condition that the total number of states is 2^N for the ferromagnetic Ising model, we cannot guarantee the accuracy of the energy levels at or near ground states because the rescaled factor is dominated by the maximum density of states.

For $L=256$, we perform multiple random walks on different energy ranges, and one problem arises, that is the error of the density of states due to the random walk in a restricted energy range. We perform three independent random walks in the ranges $E/N=[-1.7,-1.2]$, $E/N=[-1.8,-1.1]$, and $E/N=[-1.9,-1.0]$ to calculate the densities of states on these ranges. In Fig. 5, we show the errors of our simulation results from the exact values. We make our simulational densities of states match up with the exact results at the left edges. It is very clear that the width of the energy range of the random walks is almost not relevant to the errors of the density of states. The reason is that the random walks only require the local histogram to be flat as we discussed in the previous section.

To study the influence of the errors of the densities of states on the thermodynamic quantities calculated from them, in the energy range that we perform random walks, we replace the exact density of states with the simulational density of states. In the inset of Fig. 5, the specific heat calcu-

lated from such density of states is shown as a function of temperature. We also show the exact value with the simulational data, the difference is obvious. To reduce the boundary effect, we delete the last two density entries, and insert them into the exact density of states again, then the difference between exact (dotted line) and simulational date (long dashed line) is not visible with the resolution of the figure. With our test in the three different ranges of energy, it is quite safe to conclude that the boundary effect will not be present in our multiply random walks if we have a couple of energy levels overlap for adjacent energy ranges. In our real simulations for large systems, we have hundreds of overlapping energy levels.

Since the exact density of states is only available on small systems, it is not so interesting to compare the simulational density of states itself. The most important thing is the accuracy of estimations for thermodynamic quantities calculated from such density of states on large systems. With the density of states on large systems, we apply canonical average formulas to calculate internal energy, specific heat, free energy, and entropy. Ferdinand and Fisher [38] obtained the exact solutions of above quantities for the 2D Ising model on finite-size lattices. Our simulational results on finite-size lattice can be compared with those exact solutions.

The internal energy is estimated from the canonical average over energy of the system as Eq. (5). The exact and simulational data perfectly overlap with each other in a wide temperature region from $T=0$ to $T=8$. A stringent test of the accuracy is provided by the inset of Fig. 6, which shows the relative errors $\varepsilon(U)$. Here, the relative error is generally defined for any quantity X by

$$\varepsilon(X) \equiv \frac{|X_{\text{sim}} - X_{\text{exact}}|}{X_{\text{exact}}}. \tag{10}$$

With the density of states obtained with our algorithm, the relative error of simulational internal energy for $L=256$ is smaller than 0.09% for the temperature region from $T=0$ to 8. From Eq. (5), it is very clear that the canonical distribution serves as a weighting factor, and since the distribution is very narrow, $U(T)$ is only determined by a small portion of the density of states. (For the $L=50$ 2D Ising model at T_c, only the density of states for $E/N \in [-1.6,-1.2]$ contributes in a major way to the calculation.) Therefore the error $\varepsilon(U)$ is also determined by the errors of the density of states in the same narrow energy range.

The entropy of the 2D Ising model can be calculated with Eq. (9). In Fig. 6(b), the simulational data and exact results are presented in the same figure. With the scale in the figure, the difference between our simulational data and exact solutions are not visible. In the inset of Fig. 6(b), the relative errors of our simulational data are plotted as a function of temperature. For the Ising model on a 256×256 lattice, the relative errors are smaller than 1.2% for all temperature range. Very recently, with the flat histogram method [39] and the broad histogram method [18–20], the entropy was estimated with 10^7 MC sweeps for the same model on 32×32 lattice; however, the errors in Ref. [21] are bigger than our errors for 256×256.
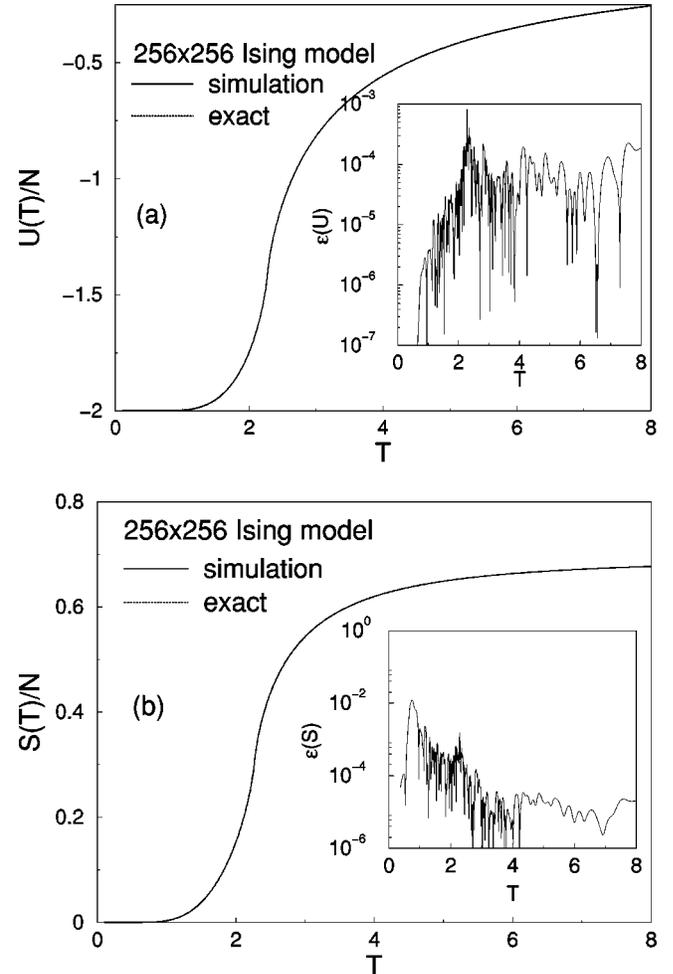

FIG. 6. Thermodynamic quantities for the 2D Ising model calculated from the density of states. Relative errors with respect to the exact solutions by Ferdinand and Fisher are shown in (a) for internal energy U, (b) for entropy S.

V. APPLICATION TO THE 3D $\pm J$ EA MODEL

Spin glasses [40] are magnetic systems in which the interactions between the magnetic moments produce frustration because of some structural disorder. One of the simplest theoretical models for such systems is the Edwards-Anderson model (EA model) [41] proposed twenty five years ago. For such disordered systems, analytical methods can provide only very limited information, so computer simulations play a particularly important role. However, because of the rough energy landscape of such disordered systems, the relaxation times of the conventional Monte Carlo simulations are very long. The dynamical critical exponent was estimated as large as $z \simeq 6$ [42–44]. Normally, simulations can be performed only on rather small systems, and many properties concerning the spin glasses are still left unclarified [45–52].

In this paper, we consider the three-dimensional $\pm J$ Ising spin glass EA model. The model is defined by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j, \tag{11}$$

TABLE II. Estimates of entropy (s_0) and internal energy (e_0) per lattice site at zero temperature for the 3D EA model by our method and the multicanonical method (MUCA) [15].

| Size | Our method | | MUCA | |
L	s_0	e_0	s_0	e_0
4	0.075±0.027	−1.734±0.006	0.0724±0.0047	−1.7403±0.0114
6	0.061±0.025	−1.767±0.024	0.0489±0.0049	−1.7741±0.0074
8	0.0493±0.0069	−1.779±0.016	0.0459±0.0030	−1.7822±0.0081
12	0.0534±0.0012	−1.780±0.012	0.0491±0.0023	−1.7843±0.0030
16	0.0575±0.0037	−1.7758±0.0041		
20	0.0556±0.0034	−1.7745±0.0043		

where σ is an Ising spin and the coupling J_{ij} is quenched to ± 1 randomly. The summation runs over the nearest-neighbors $\langle i,j \rangle$ on a simple cubic lattice.

One of the most important issues for a spin-glass model is the low-temperature behavior. Because of the slow dynamics and rough phase-space landscape of this model, it is also one of the most difficult problems in simulational physics. The algorithm proposed here is not only very efficient in estimating the density of states but also very aggressive in finding the ground states. From a random walk in energy space, we can estimate the ground-state energy and the density of states very easily. For a spin-glass system, after we finish the random walk, we can obtain the absolute density of states by the condition that the total number of states is 2^N. The entropy at zero temperature can be calculated from either $S_0 = \ln[g(E_0)]$ or $\lim_{T \to 0} U - F/T$, where E_0 is the energy at ground states. Both relations will give the same result since U and F are calculated from the same density of states. Our estimates for $s_0 = S_0/N$ and $e_0 = E_0/N$ per lattice site, listed in Table II, agree with the corresponding estimates made with the multicanonical method. With our algorithm, we can estimate the density of states up to $L=20$ by a random walk in energy space for few hours on a 400 MHz processor.

If we are only interested in the quantities directly related to the energy, such as free energy, entropy, internal energy, and specific heat, one-dimensional random walk in energy space will allow us to calculate these quantities with a high accuracy as we did in the 2D Ising model. However for spin-glass systems, one of the most important quantities is the order parameter that can be defined by [41]

$$q^{EA}(T) \equiv \lim_{t \to \infty} \lim_{N \to \infty} q(T,t), \quad q(T,t) \equiv \left\langle \sum_{i=1}^{N} \sigma_i(0)\sigma_i(t)/N \right\rangle.$$
(12)

Here, $N=L^3$ is the total number of the spins in the system, L is the linear size of the system, $q(T,t)$ is the autocorrelation function, which depends on the temperature T and the evolution time t, and $q(T,0)=1$. When $t \to \infty$, $q(T,t)$ becomes the order parameter of the spin glass. This parameter takes the following values:

$$q^{EA}(T) \begin{cases} =1 & \text{if} \quad T=0 \\ =0 & \text{if} \quad T \geq T_g \\ \neq 0 & \text{if} \quad 0 < T < T_g. \end{cases}$$
(13)

The value at $T=0$ can be different from one in the case where the ground state is highly degenerate.

In our simulation, there is no temperature introduced during the random walk. And it is more efficient to perform a random walk in single system than two replicas. So the order-parameter can be defined by

$$q \equiv \left\langle \sum_{i=1}^{N} \sigma_i^0 \sigma_i/N \right\rangle,$$
(14)

where $\{\sigma_i^0\}$ is one of spin configurations at ground states and $\{\sigma_i\}$ is any configuration during the random walk. The behavior of q we defined above is basically the same as the order parameter defined by Edwards and Anderson [41]. It is not exact same order-parameter defined by Edwards and Anderson, but was used in the early numerical simulations by Morgenstern and Binder [53,54].

After first generating a bond configuration, we perform a one-dimensional random walk in energy space to find a spin configuration $\{\sigma_i^0\}$ for the ground states. Since the order parameter is not directly related to the energy, to get a good estimate of this quantity we have to perform a two-dimensional random walk to obtain the density of states $G(E,q)$ with a flat histogram in E-q space. This also allows us to overcome the barriers in parameter space (or configuration space) for such a complex system. The rule for the 2D random walk is the same as the 1D random walk in the energy space.

With the density of states $G(E,q)$, we can calculate any quantities as we did in the previous sections. It is very interesting to study the roughness of this model. First, we study the canonical distribution as a function of the order parameter

$$P(q,T) = \sum_E G(E,q)e^{-E/k_B T}.$$
(15)

In Fig. 7(a), we show a 3D plot for the canonical distribution at different temperatures for one bond configuration of $L=6$ EA model. At low temperatures, there are four peaks, and the depth of the valleys between peaks depends upon temperature. When the temperature is high, the multiple peaks converge to a single central peak. Because we use the linear scale to show our result in Fig. 7(a), it is not clear how deep the dips among peaks are. In Fig. 7(b), we show
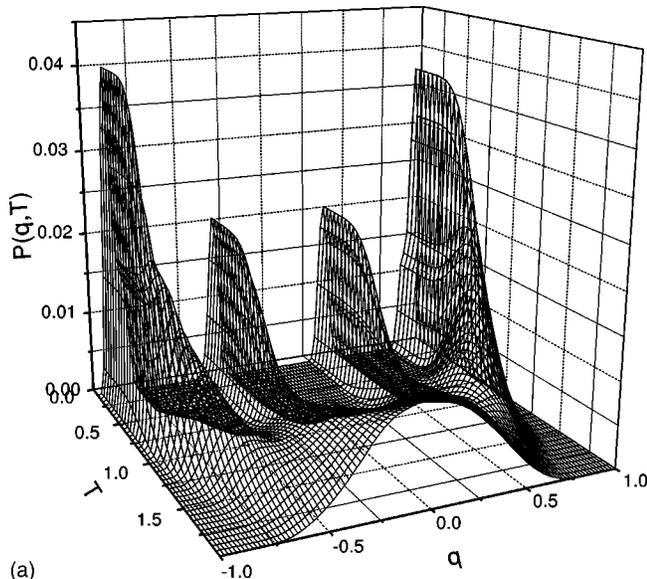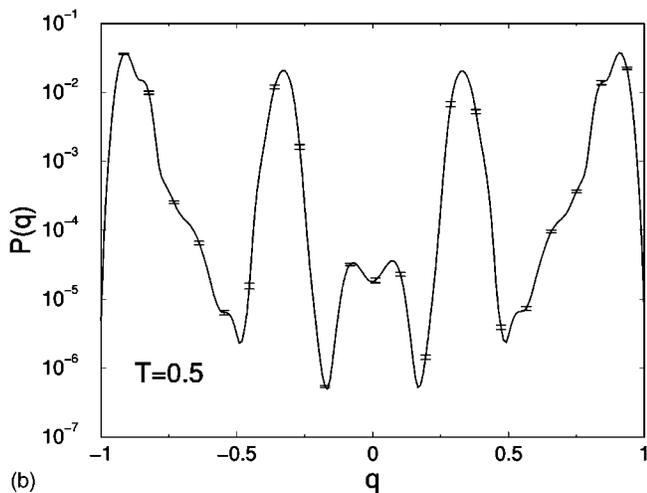
FIG. 7. (a) Overview of the rough topology of the canonical distribution in the order-parameter space for one bond configuration of the 3D EA model on an $L=6$ simple cubic lattice. (b) The logarithmic plot for the canonical distribution as a function of the order-parameter for the 3D EA model at the temperature $T=0.5$.

the canonical distribution using logarithmic scale for the same distribution but only at $T=0.5$, and we find that the dips are as deep as 10^{-4}. We also noted there actually are six peaks, but the plot with a linear scale does not show all of them because two are as small as 10^{-3} compared to other four peaks.

In Fig. 8(a), we show the roughness of the canonical distribution for another realization on an 8^3 lattice. Because of the wide variation in the distribution at low temperature, we used a logarithmic scale: the relative size of dips are as deep as 10^{-30} at $T=0.1$. There are several local minima even at high temperatures. With conventional Monte Carlo simulations, it is almost impossible to overcome the barriers at the low temperature, so the simulation will get trapped in one of the local minima as shown in the figure. With our algorithm,

all states will be visited with more or less the same probability and trapping is not a problem.

With the density of states $G(E,q)$, we also can calculate the energy landscape by

$$U(q,T) = \frac{\sum_{E,q} E G(E,q) e^{-\beta E}}{\sum_{E,q} G(E,q) e^{-\beta E}}. \qquad (16)$$

In Fig. 8(b), we show the internal energy as a function of order parameter for temperatures $T=0.1\sim2.0$. We find that the landscape is very rough at low temperatures. The roughness of the energy landscape agrees with the one for canonical distribution. But the maxima in energy landscape are corresponding to the minima approximately in the canonical distribution.

As we already noted in the previous paragraph, the roughness of the landscape of the spin-glass model makes the conventional Monte Carlo simulation extremely difficult to apply. Therefore, even a quarter of a century after the model was proposed, we even cannot conclude whether there is a finite phase transition between the glass phase and the disordered phase. With Monte Carlo simulations on a large system ($64^2\times128$) and a finite-size scaling analysis on a small lattice, Marinari *et al.* [55] expressed doubt about the existence of the ''well-established'' finite-temperature phase transition of the 3D Ising spin glass [42,45]. Their simulational data can be described equally well by a finite-temperature transition or by a $T=0$ singularity of an unusual type. Kawashima and Young's simulational data could not rule out the possibility of $T_g=0$ [46]. Thus, even the existence of the finite-temperature phase transition is still controversial, and thus, the nature of the spin-glass state is uncertain. Although the best available computer simulation results [13,50,56] have been interpreted as a mean-fieldlike behavior with replica-symmetry breaking (RSB) [57], Moore *et al.* showed evidence for the droplet picture [58] of spin glasses within the Migdal-Kadanoff approximation. They argued that the failure to see droplet model behavior in Monte Carlo simulations was due to the fact that all existing simulations are done at temperatures too close to transition temperature so that system sizes larger than the correlation length were not used. As discussed in the previous paragraph, the lower the temperature is, the rougher the canonical distribution and energy landscape are; hence, it is almost impossible for conventional Monte Carlo methods to overcome the barrier between local minima and globe minima. It is possible to heat the system up to increase the possibility of escape from local minima by simulated annealing and the more recent simulated tempering method [59] and parallel tempering method [60,61], but it is still very difficult to perform equilibrium simulations at low temperatures. Very recently, Hatano and Gubernatis proposed a bivariate multicanonical Monte Carlo method for the 3D $\pm J$ spin-glass model, and their result also favors the droplet picture [16,62]. Marinari, Parisi *et al.* argued, however, that the data were not thermalized [56]. The nature of spin glasses thus remains controversial [49].
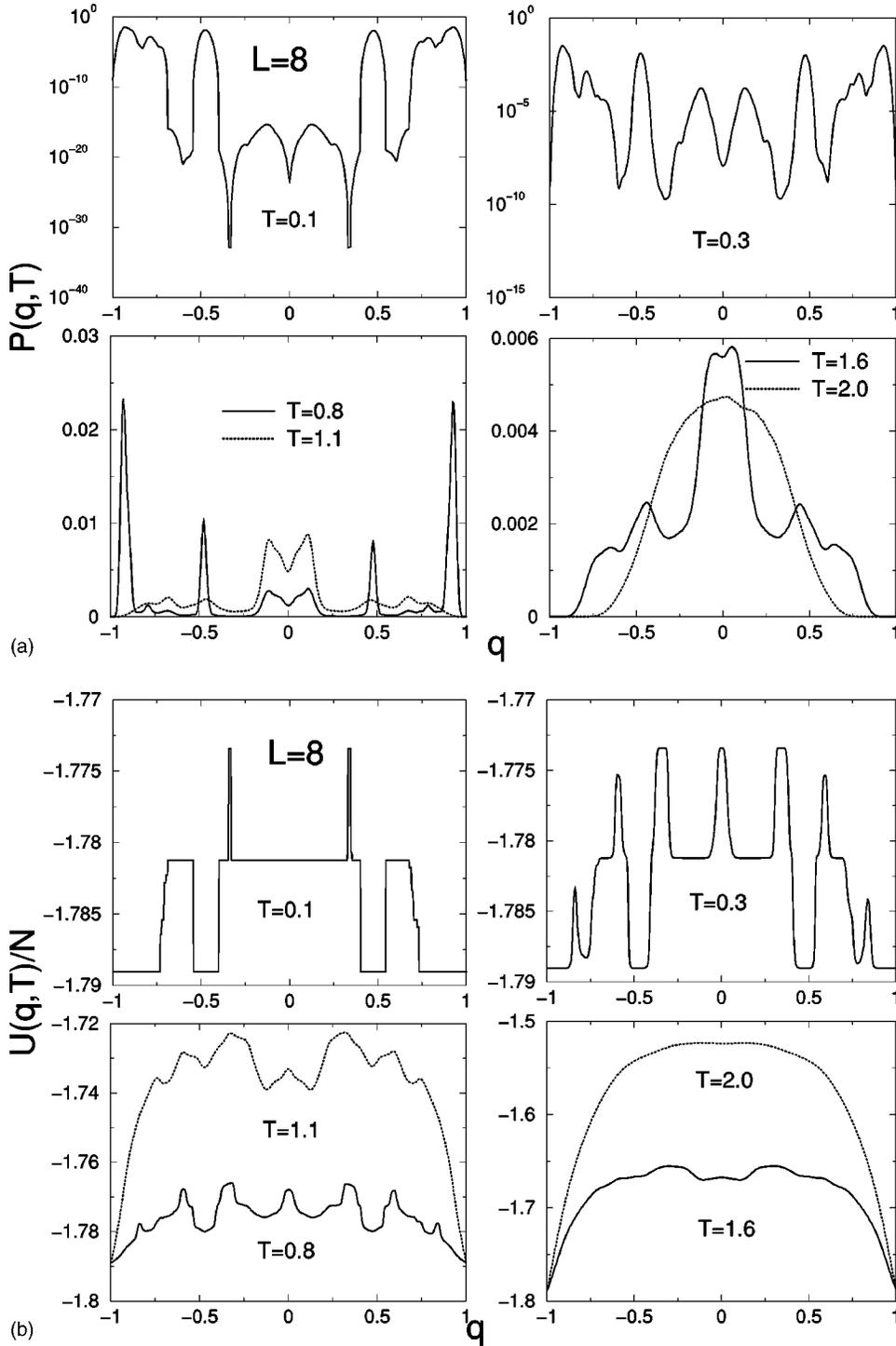
FIG. 8. (a) The canonical distribution $P(q)$ as a function of the order parameter for one bond configuration of the 3D EA model on an $L=8$ simple cubic lattice at the temperature $T=0.1 \sim 2.0$. (b) Corresponding energy landscapes $U(q,T)$ at different temperatures.

The algorithm proposed in this paper provides an alternative for the study of complex systems. Because we need to calculate the order parameter with high accuracy, and this quantity is not directly related to the energy, we need to perform a random walk in the two-dimensional energy-order parameter space. After we estimate the density of states in this 2D space, we can calculate the order parameter at any temperature from the canonical average. In Fig. 9(a), we show our results for the 3D EA model for $L=4$, 6, and 8. Because we need to perform a 2D random walk with a total

of about L^6 states, the simulation is only practical for a small system ($L \leq 8$). The results in the figure are the average over 100 realizations for $L=4$, 50 realizations for $L=6$, and 20 for $L=8$.

We notice that the behavior of $\langle q(T) \rangle$ is very similar to the magnetization (the order parameter for the Ising model), but the finite value at low temperature is not necessarily equal to one because of the high degeneracy of the ground state for the spin-glass model. The fluctuation of the order parameter at the different temperatures for $L=4$, 6, and 8 is
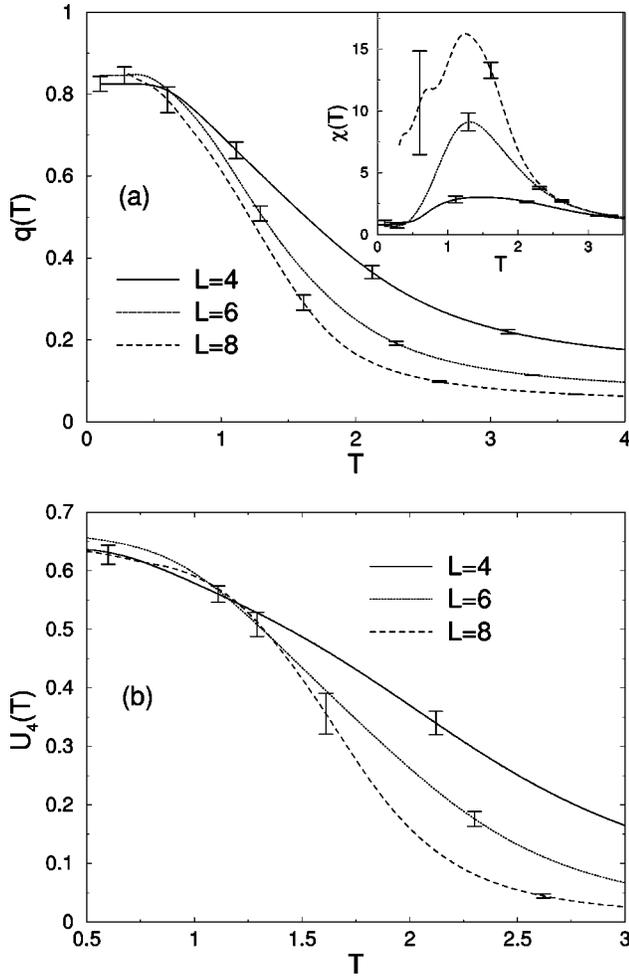
FIG. 9. Properties of the 3D EA spin glass model calculated from the density of states $G(E, q)$ resulting from a 2D random walk in energy-order parameter space: (a) The order parameter vs temperature. (b) The temperature dependence of the fourth order cumulant of the order parameter. The cumulants for different lattice sizes cross around $T_c = 1.2$.

shown in the inset of the figure.

To estimate the transition temperature of the spin-glass system, we calculated the fourth-order cumulant as a function of temperature. In Fig. 9(b), we show our simulational results for $L = 4$, 6, and 8. All curves clearly cross around $T_g = 1.2$. Below this temperature, the spin configurations are frozen into some disorder ground state and the order parameter assumes a finite value. Above this temperature T_g, the system is in a disordered state and the order parameter vanishes.

One complication for simulation of such random systems is the determination of the relative importance of the error due to the simulation algorithm and the error due to the finite sampling of bond distributions. From Figs. 9(a) and 9(b), we cannot tell what the origin of the error bars is so we also performed multiple independent simulations for the same bond configuration on an $L = 6$ 3D EA model. We found that the statistical errors for the order parameter and the fourth-order cumulant from these simulations were much smaller than the error bars shown in Figs. 9(a) and 9(b) for all

temperatures. We conclude that the error bars in the figure arise almost completely from the randomness of the system.

The computational resources devoted here to the EA model were not immense. All our simulations for one bond configuration ($L = 4$, 6, and 8) were performed within two days on (multiple) Linux machines ($200 - 800$ MHz) in the Center for Simulational Physics. This effort should thus be viewed as a feasibility study, and substantially more effort would be required to determine the nature of the spin-glass phase or to estimate the transition temperature with high accuracy. Nonetheless, we believe that these results show the applicability of our method to systems with a rough landscape. Because the number of states is about N^2 for 2D random walks, such calculations not only require huge memory during the simulation but also substantial disk space to store the density of states for the later calculation of thermodynamic quantities.

VI. DISCUSSION AND CONCLUSION

In this paper, we proposed an efficient algorithm to calculate the density of states directly for large systems. By modifying the estimate at each step of the random walk in energy space and carefully controlling the modification factor, we can determine the density of states very accurately. Using the density of states, we can then calculate thermodynamic quantities at any temperature by applying simple statistical physics formulas. An important advantage of this approach is that we can also calculate the free energy and entropy, quantities that are not directly available from conventional Monte Carlo simulations.

We applied our method to the 2D $Q = 10$ Potts model that demonstrates a typical first-order phase transition. By estimating the density of states with lattices as large as 200×200, we calculated the internal energy, specific heat, free energy, and entropy in a wide temperature region. We found a typical first-order phase transition with a ''discontinuity'' for the internal energy and entropy at T_c. The first derivative of the free energy also shows such a discontinuity at T_c. The transition temperature estimated from simulational data is consistent with the exact solution.

We also applied our algorithm to the 2D Ising model, which shows a second-order phase transition. It was also possible to calculate the density of states for a 256×256 lattice with a computational effort of 6.1×10^6 Monte Carlo sweeps. With the accurate density of states, we calculated the internal energy and entropy. For all temperatures between $T = 0$ and $T = 8$, the relative errors are smaller than 0.09% for internal energy, 1.2% for entropy.

The algorithm was also applied with success to the 3D $\pm J$ EA spin-glass model for which we could determine the roughness of the energy landscape and canonical distribution in the order-parameter space. The internal energy and entropy at zero temperature were estimated up to a lattice size 20^3, and the transition temperature was estimated at about $T_g = 1.2$.

In this paper, we only concentrated the random walk in energy space (and order-parameter space); however, the idea is very general and we can apply this algorithm to any pa-

rameters [11]. The energy levels of the models treated here are perfectly discrete and the total number of possible energy levels is known before simulation, but in a general model such information is not available. Since the histogram of the random walk with our algorithm tends to be flat, it is very easy to probe all possible energies and monitor the histogram entry at each energy level. For some models where all possible energy levels can not be fitted in the computer memory or the energy is continuous, e.g., the Heisenberg model, we may need to discretize the energy levels. According to our experience on discrete and continuous models, if the total number of possible energies is around the number of lattice sites N, the algorithm is very efficient for studying both first- or second-order phase transitions.

In this paper, we only applied our algorithm to simple models, but since the algorithm is very efficient even for large systems it should be very useful in the studies of general, complex systems with rough landscapes. It is clear, however, that more investigation is needed to better determine under which circumstances our method offers substantial advantage over other approaches and we wish to encourage the application of this approach to other models.

Note added in proof. Recently, we learned about Refs. [63,64] from the authors, who estimated the density of states from the histogram of microcanonical simulations. To get an accurate density of states over all the energy range, they performed independent simulations in multiple small windows in energy space. Their method is similar to our multiple-range random walk, but our random walk algorithm maintains a flat histogram even in small windows in energy space. They have successfully estimated the density states for the $L=10$, 3D Ising model with the nearest-neighbor interactions [63] and the $L=1000$, 1D Ising model with long-range interactions [64].

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