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Is the broad histogram random walk dynamics correct?

J.-S. Wang[a]

Department of Computational Science, National University of Singapore, Singapore 119260, Republic of Singapore

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Abstract. We show explicitly that the broad histogram single-spin-flip random walk dynamics does not give correct microcanonical average even in one dimension. The dynamics violates the detailed balance condition by an amount proportional to the inverse system size. As a result, in distribution different configurations with the same energy can have different probabilities. We propose a modified dynamics which ensures detailed balance and the histogram obtained from this dynamics is exactly flat. The broad histogram equation relating the average number of potential moves to density of states is generally valid.

PACS. 02.70.Lq Monte-Carlo and statistical methods – 05.50.+q Lattice theory and statistics; Ising problems

Two years ago, Oliveira *et al.* [1–4] proposed an interesting method for Monte-Carlo simulation of statistical mechanical systems. The number of degenerate states $n(E)$ is computed from equations relating $n(E)$ to the number of type of potential moves of a given dynamics. The Monte-Carlo computation is purely combinatorial (or geometrical) unrelated to thermodynamics. The temperature dependence enters only after simulation in the weighting formulas. It is indeed an efficient method in comparison with histogram [5,6], especially multiple histogram methods [6].

In the following, we use the Ising model to illustrate the method, but the idea generalizes easily to other models. One first chooses a protocol of Monte-Carlo moves, for example, the single-spin flips. For a given state σ with energy $E = E(\sigma)$ (σ without an index denotes the set of all spins), consider all possible single-spin flips. The single-spin flips change the current state into N possible new states, with new energy $E' = E(\sigma') = E + \Delta E$ taking a small set of values. We classify the N new states according to ΔE, and count the number of such moves $N(\sigma, \Delta E)$. We have $\sum_{\Delta E} N(\sigma, \Delta E) = N$. Then one can show rigorously that [3,7,8]

$$n(E)\big\langle N(\sigma, \Delta E)\big\rangle_E = n(E + \Delta E)\big\langle N(\sigma', -\Delta E)\big\rangle_{E+\Delta E} \tag{1}$$

as long as a set of moves and their reverse moves are both allowed. The average is a microcanonical average, *i.e.*, average over all configurations having a fixed energy with equal weight:

$$\big\langle A(\sigma)\big\rangle_E = \frac{1}{n(E)} \sum_{E(\sigma)=E} A(\sigma). \tag{2}$$

Equation (1) is the fundamental result of the broad histogram method. Once the quantity $\langle N(\sigma, \Delta E)\rangle_E$ is computed by any means, the density of states can be solved from equation (1). Since there are more equations than variables $n(E)$ in general, one can either discard part of the equations, solving $n(E)$ iteratively, or use least square method. In any case, once $n(E)$ is determined from the set of equations, the canonical average is computed by

$$\big\langle A(\sigma)\big\rangle_T = \frac{\sum_E n(E)\big\langle A(\sigma)\big\rangle_E \exp(-E/k_BT)}{\sum_E n(E)\exp(-E/k_BT)}\cdot \tag{3}$$

There is no controversy on this part of the theory. However, the specific dynamics proposed in reference [1] is problematic. The dynamics is a random walk in energy as follows: pick a site at random, and compute energy change $\Delta E = E' - E$ if the spin is flipped. If the new state has a lower energy, $E' < E$, flip the spin. If the new state has a higher energy, $\Delta E > 0$, flip the spin with a probability $\min\big(1, N(\sigma, -\Delta E)/N(\sigma, \Delta E)\big)$. If the energies are the same, $\Delta E = 0$, flip the spin with some fixed probability, say 1.

We believe that such a dynamics is wrong in the sense that it does not give correct microcanonical average with the finite samples generated in this dynamics. The stationary probability distribution of the dynamics depends not only on energy E but also on the partition $N(\sigma, \Delta E)$ as pointed out already by Berg and Hansmann [7]. We show that such a dynamics does not satisfy detailed balance conditions with respect to an unknown but energy-dependent-only probability distribution.

Let us first quote a mathematical theorem [9] in the theory of discrete-time Markov chain using notations familiar to physicists. As before the symbol σ

[a] e-mail: wangjs@cz3.nus.edu.sg

will be a complete specification of the state (*e.g.*, in Ising model, the set of all spins). Let $P_0(\sigma)$ be the probability distribution of the initial configurations. If we start from a unique configuration (for example, from a ground state), $P_0(\sigma)$ will be 1 for the particular state, and 0 for all other states. Let $W(\sigma'|\sigma)$ be the transition probability, *i.e.*, the probability that the system will be in state σ' given that the current state is σ; $W(\sigma'|\sigma) \geq 0$, $\sum_{\sigma'} W(\sigma'|\sigma) = 1$. Then the probability distribution after n steps of moves is

$$P_n(\sigma) = \sum_{\sigma'} W^n(\sigma|\sigma')P_0(\sigma'), \tag{4}$$

where $W^n = W \cdot W \cdot \ldots W$ (n times), viewing W as a matrix, and W^n is matrix power. The theorem says that a unique large-step limit distribution

$$P(\sigma) = \lim_{n\to\infty} P_n(\sigma) = \lim_{n\to\infty} W^n(\sigma|\sigma') \tag{5}$$

exists independent of the initial probability distribution, if

1. W is irreducible, *i.e.*, $W^k(\sigma'|\sigma) > 0$ for all states σ and σ' and some $k \geq 0$. In words, for any initial state σ and any final state σ', it is possible with nonzero probability to move from σ to σ' in k steps, k arbitrary (0, 1, 2, ...) but finite. This is usually referred as ergodicity in some physics literature.
2. W is aperiodic, *i.e.*, $W^k(\sigma|\sigma) > 0$ for all $k > k_{min}$, for all σ. In words, starting from state σ, the probability that it comes back to state σ in k steps is nonzero for all k greater than a threshold value k_{min}. This point is seldomly mentioned in physics textbooks. When this condition fails, one can have probability distributions that oscillate between two or more forms. There will be no unique $P(\sigma)$.

Conditions 1 and 2 can be combined into a single statement: $W^k(\sigma'|\sigma) > 0$ for all σ and σ' and for all k for sufficiently large k.

The theorem guarantees that an equilibrium limit exists and is unique. If our aim is to simulate a known distribution, *e.g.*, Boltzmann distribution, we also require that $P(\sigma)$ is that distribution. It is sufficient then, in addition to 1 and 2, W also satisfies 3 – detailed balance,

$$W(\sigma|\sigma')P(\sigma') = W(\sigma'|\sigma)P(\sigma), \quad \text{for all } \sigma \text{ and } \sigma'. \tag{6}$$

Example 1

The single-spin-flip Glauber rate with random selection of sites satisfies 1, 2, and 3 for temperature $T > 0$ (but not if $T = 0$). In this case

$$W(\sigma'|\sigma) = \begin{cases} 0, & \text{if } \sigma \text{ and } \sigma' \text{ are not related by a single spin flip, and } \sigma \neq \sigma'; \\ \dfrac{1}{2N}\Big(1 - \tanh\dfrac{\Delta E}{2k_BT}\Big), & \sigma' \text{ is obtained by a flip from } \sigma. \end{cases} \tag{7}$$

The diagonal elements $W(\sigma|\sigma)$ are fixed by normalization (sum of the column of matrix W is 1, because probability of going anywhere is 1).

Clearly condition 1 is satisfied – for arbitrary state σ and σ', we can move from σ to σ' by flipping one by one those sites which differ, we can do this in k steps where k is the number of spins which differ. Condition 2 is also satisfied. Clearly $W(\sigma|\sigma)$ is nonzero for all σ, so is the diagonal elements of all power of W. Condition 3 is satisfied with respect to the Boltzmann equilibrium distribution.

Example 2

Consider a system of one spin. In each step, we flip the spin with probability one. Then

$$W = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad W^{2k} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad W^{2k+1} = W. \tag{8}$$

This stochastic matrix violates condition 2. Thus, it does not have a unique limit distribution.

The broad histogram Monte-Carlo dynamics in the basic form (single-spin-flip protocol) is as follows:

$$W(\sigma'|\sigma) = \begin{cases} 0, & \text{if } \sigma \neq F\sigma' \text{ and } \sigma \neq \sigma'; \\ \frac{1}{N}, & \text{if } \Delta E \leq 0 \text{ and } \sigma = F\sigma'; \\ \frac{1}{N}\min\Big(1, \frac{N(\sigma,-\Delta E)}{N(\sigma,\Delta E)}\Big), & \text{if } \Delta E > 0 \text{ and } \sigma = F\sigma'. \end{cases} \tag{9}$$

F changes configuration into a new configuration by a single-spin flip, and $\Delta E = E(\sigma') - E(\sigma)$ is the energy increment. $W(\sigma|\sigma)$ is again fixed by normalization ($\sum_{\sigma'} W(\sigma'|\sigma) = 1$). The factor $(1/N)$ on all of the terms reflects the fact that a site is picked at random. N is the total number of spins.

The dynamics has a problem with respect to condition 1, as the ground states are absorbing states. We cannot go to high energy states once the system is in the ground state. This small problem can be fixed by an *ad hoc* rule, *e.g.*, if $N(\sigma, \Delta E) = 0$ and $\Delta E < 0$, reset it to infinity.

Now, we look at condition 3, the detailed balance. Since we do not know $P(\sigma)$ for the above dynamics, we assume it depends on the state only through E, *i.e.*, $P(\sigma) = f\big(E(\sigma)\big)$ for some unknown function $f(E)$. Then consider two arbitrary states σ and σ' related by a single-spin flip with energy E and E', $\Delta E = E' - E > 0$. From σ to σ', energy increases, $W(\sigma'|\sigma) = (1/N)\min\big(1, N(\sigma, -\Delta E)/N(\sigma, \Delta E)\big)$. From σ' to σ, energy decreases, $W(\sigma|\sigma') = 1/N$. Now is

$$f(E)\min\Big(1, N(\sigma, -\Delta E)/N(\sigma, \Delta E)\Big) = f(E') \tag{10}$$

for some function $f(E)$? Clearly, this is not possible in general unless the ratio $N(\sigma, -\Delta E)/N(\sigma, \Delta E)$ is a function of E and E' only, and is independent of the current state σ. Within the single-spin-flip protocol, the ratio does depend on σ explicitly. We can easily find examples.

$P(\sigma)$ can be computed in principle (and in practice for small systems) by solving $WP = P$, when the dynamics is precisely fixed. Since the configurations in a simulation appear with probability $P(\sigma)$, the average is ultimately related to average with the weight of $P(\sigma)$. Microcanonical average is restored as long as we have $P(\sigma) = f\big(E(\sigma)\big)$, *i.e.*, the probability should be the same for configurations with the same energy.

We present results of a simulation of a 5-spin chain with periodic boundary condition with the specific dynamics as discussed above. The data are presented in Table 1 together with exact results expected from true microcanonical average. Monte-Carlo steps (MCS) are 10^8 in the average, so we expect 4 digits of accuracy.

The cases for $E/J = -5$ and 3 agree. But deviations of order 5% occur for the case $E/J = -1$. This is precisely due to the anomaly in $P(\sigma)$ in the dynamics, since we compute $\langle N(\sigma, \Delta E)\rangle_E$ by an arithmetic average:

$$\langle N(\sigma,\Delta E)\rangle_E = \sum_{\sigma,\ \text{such that}\ E(\sigma)=E} N(\sigma,\Delta E)P(\sigma) \Big/ \sum_{\sigma',\ E(\sigma')=E} P(\sigma')$$
$$\approx \sum N(\sigma \text{ of energy } E, \Delta E)/\text{No. of samples}. \quad (11)$$

If $P(\sigma)$ is a constant for a given E, then $P(\sigma)$ has no effect. But if $P(\sigma)$ for $E(\sigma) = E$, depends on σ explicitly, then the above average is not the microcanonical average.

The specific unnormalized $P(\sigma)$s of the five-spin broad histogram random walk dynamics are (computed with Mathematica exactly, which also agree with the simulation), $P(+++++) = 1$, $P(-++++) = 1$, $P(--+++) = 7/8$, $P(+-+-+) = 5/8$. Other degenerate state probabilities are obtained by translation and spin up-down symmetry. We also have $N(-++++, 4J) = 2$, $N(--+++, 4J) = 1$, and $N(-++++, -4J) = 1$, $N(--+++, -4J) = 0$. From these numbers, we get (averages at $E/J = -1$)

$$\langle N(4J)\rangle = \frac{2\cdot 1 + 1\cdot(7/8)}{1+7/8} = \frac{23}{15} \approx 1.5333, \quad (12)$$

$$\langle N(-4J)\rangle = \frac{1\cdot 1 + 0\cdot(7/8)}{1+7/8} = \frac{8}{15} \approx 0.5333, \quad (13)$$

which are exactly what we get from Monte-Carlo average and they are wrong! Values for $E/J = -5$ and 3 are trivially correct. This feature is generic. Six and seven spin chains have the same problem.

In actual implementation, a cumulative average of $N(\sigma, \Delta E)$ is used instead of the instantaneous value for the transition rates [1]. We have objections to the procedure. (1) If one uses the accumulated average $\langle N(\dots)\rangle$ up to the current state, then the dynamics is no longer Markovian – the transition rates not only depend on the current state but also on all the previous states. Then the theory of Markov chains does not apply. (2) Even if one uses the exact microcanonical average for the flip rate, the dynamics is still not correct in general. In Table 2 we present Monte-Carlo computations of $\langle N(\sigma, \Delta E)\rangle$ on a 4×4 lattice

Table 1. The average value $\langle N(\sigma, \Delta E)\rangle$ for a system of five-spin chain in broad histogram random walk dynamics from Monte-Carlo simulation and exact results with true microcanonical average.

E/J	$\langle N(\sigma, \Delta E = -4J)\rangle_E$	$\langle N(\sigma, \Delta E = +4J)\rangle_E$
Random walk dynamics result		
-5	0	5
-1	0.53326	1.53326
3	3	0
Exact microcanonical results		
-5	0	5
-1	1/2	3/2
3	3	0

for (a) the original pure random walk dynamics, (b) the dynamics with the instantaneous value $N(\sigma, \Delta E)$ replaced by exact microcanonical average values for the transition rates, and (c) the true microcanonical average by exact enumerations. Clearly, both the original dynamics and the modified one do not give correct answers.

In a variation of the method [4], the dynamics is applied to an ensemble with energy limited to a small window. By the same argument above, we see that this is also not correct.

Detailed balance is a delicate matter. Since the detailed balance gives us more equations than the number of unknowns ($P(\sigma)$) in general, such equations are inconsistent unless the transition probabilities have some special properties. To illustrate this point, let us take

$$W(\sigma'|\sigma) = \frac{1}{N}\delta_{\sigma,F\sigma'} r\big(E(\sigma')|E(\sigma)\big) + \delta_{\sigma,\sigma'} r\big(E(\sigma)|E(\sigma)\big), \quad (14)$$

where $\delta_{\sigma,F\sigma'}$ is 1 if σ and σ' differ by a single spin, and 0 otherwise. This transition matrix corresponds to a single-spin-flip protocol with a transition rate $r(E'|E)$ which depends on energies as an arbitrary function. Does this transition matrix preserve microcanonical property $[P(\sigma) = f\big(E(\sigma)\big)]$? The answer is not necessarily yes, unless

$$r(E|E')f(E') = r(E'|E)f(E). \quad (15)$$

This can be shown as follows:

$$\begin{aligned} P_2(\sigma) &= \sum_{\sigma'} W(\sigma|\sigma')P(\sigma') \\ &= r\big(E(\sigma)|E(\sigma)\big) f\big(E(\sigma)\big) \\ &\quad + \sum_{E'} \frac{N\big(\sigma, E'-E(\sigma)\big)}{N} r\big(E(\sigma)|E'\big) f(E') \\ &= f\big(E(\sigma)\big) + \sum_{E'} \frac{N\big(\sigma, E'-E(\sigma)\big)}{N} \\ &\quad \times \Big[r\big(E(\sigma)|E'\big)f(E') - r\big(E'|E(\sigma)\big) f\big(E(\sigma)\big)\Big]. \end{aligned} \quad (16)$$

Table 2. Monte-Carlo random walk dynamics and exact results on a 4×4 square lattice with periodic boundary conditions: (a) pure broad histogram random walk dynamics, using instantaneous $N(\sigma, \Delta E)$, MCS $= 1.45 \times 10^9$; (b) broad histogram random walk dynamics with strictly E-dependent flip rates, using the exact $\langle N(\sigma, \Delta E)\rangle_E$, MCS $= 1.45 \times 10^{10}$; (c) true microcanonical average computed by exact numeration of all the states. Statistical/numerical error is on the last digit.

$E/(4J)$	$\langle N(\sigma,\Delta E=-8J)\rangle_E$	$\langle N(\sigma,\Delta E=-4J)\rangle_E$	$\langle N(\sigma,\Delta E=0)\rangle_E$
(a) Random walk dynamics, current $N(\sigma, \Delta E)$			
4	0.9878	0.7850	1.6194
5	0.4348	1.5815	3.0233
6	0.4077	1.7295	5.4252
7	0.5626	2.6570	5.9934
(b) Random walk using average $\langle N(\sigma, \Delta E)\rangle$			
4	0.86573	0.80220	1.6888
5	0.39313	1.5878	3.2620
6	0.47274	1.7930	5.3393
7	0.48124	2.9319	5.8429
(c) Exact microcanonical average			
4	0.83018868	0.90566038	1.81132075
5	0.29629630	1.55555556	3.55555556
6	0.38755981	1.81818182	5.51196172
7	0.45283019	2.94339623	5.88679245

The last step used the fact that sum of the column elements in W is one. The first term depends on σ through E implicitly as required. But there is no guarantee that the rest of the sum is a function of E only. However, when equation (15) is satisfied, the rest of the terms are zero.

We can eliminate the unknown function $f(E)$ in equation (15) to get conditions on the matrix elements themselves. For example, for three distinct energies E, E', and E'' with nonzero transition probabilities among them, we must have [8,10],

$$r(E|E'')r(E''|E')r(E'|E) = r(E|E')r(E'|E'')r(E''|E) > 0. \tag{17}$$

If there are four different energies with nonzero transition probabilities among them, we should have equations involving products of four of the transition probabilities. This would be the case in three-dimensional Ising model with single-spin flips. This equation is not satisfied in the random walk dynamics with E-dependent-only rates where different sizes of energy jumps ($|\Delta E| = 0, 4J, 8J$) are allowed.

From the results presented in references [1–4] the deviations for thermodynamic quantities for large systems are almost unnoticeable. Let us discuss in the context of equation (17) why this is so. For the two-dimensional Ising model, this equation is the only relevant constraint equation. We define

$$v(E) = \left| 1 - \frac{r(E|E'')r(E''|E')r(E'|E)}{r(E|E')r(E'|E'')r(E''|E)} \right| \tag{18}$$

as the detailed balance violation, where we take $E' = E+4J$, and $E'' = E+8J$. For the random walk dynamics,

$$r(E'|E) = \begin{cases} 1, & \text{if } E' \le E; \\ \min\left(1, \frac{\langle N(\sigma,E-E')\rangle_E}{\langle N(\sigma,E'-E)\rangle_E}\right), & \text{if } E' > E. \end{cases} \tag{19}$$

Substituting this expression into equation (18), we obtain (for $E < 0$)

$$v(E) = \left| 1 - \frac{\langle N(\sigma,-4J)\rangle_E \langle N(\sigma',-4J)\rangle_{E'} \langle N(\sigma,8J)\rangle_E}{\langle N(\sigma,4J)\rangle_E \langle N(\sigma',4J)\rangle_{E'} \langle N(\sigma,-8J)\rangle_E} \right|. \tag{20}$$

If we take the large-size limit, then the functions $\langle N(\cdots)\rangle$ are smooth functions in energy, and we approximate the discrete spectrum by continuous functions, $n_i(u) = \lim_{N\to\infty}(1/N)\langle N(\sigma, i4J)\rangle_{uN}$, $i = 0, \pm1, \pm2$, $u = E/N$. It was pointed out to us by Oliveira [11] that the functions $n_i(u)$ can be related to thermodynamics, see also reference [12]. Here we give a slightly different argument for it. Since $n_i(u)$ are large-size microcanonical average, using the equivalence between different ensembles in the thermodynamic limit, we can compute the same qualities by canonical ensemble. $n_i(u)$ is simply the probability that a site is surrounded by $i + 2$ spins of the same signs. Evoking Boltzmann distribution, we can show $n_i(u)/n_{-i}(u) = \exp\big(i4J\beta(u)\big)$, where $\beta(u) = 1/k_BT$, T is the temperature for system at an average energy u per spin. Using this result, equation (20) can be further simplified [11] neatly as

$$v(u) = \left| 1 - e^{4J\left(\beta(u) - \beta(u+4J/N)\right)} \right| \approx -\frac{d\beta}{du}\,\frac{16J^2}{N}\,. \tag{21}$$

This result suggests that the violation is of order $1/N$ in general. At the critical region, it becomes even better, by a factor of the inverse specific heat. For the two-dimensional Ising model at T_c (near $u = u_c = -\sqrt{2}$), we have $v(u_c) \propto 1/(N \log N)$. This indeed justifies the results obtained by computer simulation on large systems. If the instantaneous value $N(\sigma, \Delta E)$ is used, we expect errors of order $1/\sqrt{N}$.

Since detailed balance violation is a small perturbation to the transition rate, we expect the Monte-Carlo result for $\langle N(\cdots)\rangle$ also violates detailed balance by an amount proportional to $v(u)$. We check this, replacing $r(E'|E)$ by Monte-Carlo estimates of $\langle N(\sigma, E' - E)\rangle_E$ in equation (18). Let us call this quantity $\bar{v}(u)$. Numerically we found $\bar{v}(u_c) = 0.3, 0.12, 0.03, 0.008$ for two-dimensional square lattice systems of linear size $L = 4$, 8, 16, 32, respectively. The results are consistent with equation (21). It is likely that density of states and thermodynamic quantities can have less deviations.

We have shown that the broad histogram random walk dynamics is only an approximate algorithm. It is thus desirable to have exact algorithms with any lattice sizes. A remedy to the problem is to use a single function $f(E)$, similar to reference [13] (which uses $f(E) \propto 1/n(E)$). For example, let $f(E) = 1/\langle N(\sigma, \Delta E)\rangle_E$ for a *fixed* ΔE. Use a flip rate $r = \min\big[1, f(E(\sigma'))/f(E(\sigma))\big]$ for a move from σ to σ'. This will at least fulfill the detailed balance. The second possibility is to restrict energy changes to only three possible values $0, \pm 4J$. The flip rates can be any arbitrary function of E and $\Delta E = 0, \pm 4J$. When such a condition is imposed, we can always find a consistent solution $f(E)$ to the detailed balance equations. This may introduce an ergodicity problem, but the inconsistency to equations like (17) will not occur. This also explains why the dynamics works in one dimension if E-dependent-only flip rates are used.

The last and perhaps also the best recommendation is to take

$$r(E'|E) = \min\left(1, \frac{\langle N(\sigma', E - E')\rangle_{E'}}{\langle N(\sigma, E' - E)\rangle_E}\right), \qquad (22)$$

without restriction to energy changes. When this rate is used, equation (17) and similar constraint equations are satisfied automatically (as long as the quantities are exact microcanonical averages). This is so because $\langle N(\sigma, \Delta E)\rangle_E$ themselves are also transitions rates [8] and also satisfy equations similar to equation (17). Moreover, we know exactly what is the stationary distribution $f(E)$. It is just the inverse density of states, *i.e.*, $f(E) \propto 1/n(E)$. The detailed balance conditions for this new dynamics are simply equivalent to equation (1). The dynamics also gives an exactly flat histogram. The histogram in general is proportional to $n(E)f(E)$. Since $f(E) \propto 1/n(E)$, the energy histogram is a constant.

For actual implementation, we must determine the microcanonical average iteratively, using at first cumulative average of $N(\sigma, \Delta E)$ for transition rates. After a first approximation, we can either refine them further, or use the slightly incorrect one but reinforce equation (17) exactly on data. When this is done, the histogram will not be exactly flat, but the dynamics is correct. A preliminary test indicates that a straightforward single run with cumulative average already gives quite satisfactory result. A detailed study of this dynamics will be presented elsewhere.

In conclusion, while the basic equation of the broad histogram method, equation (1), is not questioned, we have shown that the original random walk dynamics is only an approximation. Although it gives good results for large systems, on small systems, the value for $\langle N(\cdots)\rangle$ can have systematic errors as large as 20%. We proposed new transition rates that satisfy detailed balance condition. In particular, instead of using the ratio of number of moves to states with energy $\pm\Delta E$ from the current state, we use the ratio of average number of moves from new states to the current energy states and from current state to the new states. This very small change to the original method plus the requirement that the average values should be used ensures detailed balance. In addition, the histogram obtained by this dynamics is exactly flat.

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