Irreversible simulated tempering

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An extended ensemble Monte Carlo algorithm is proposed by introducing a violation of the detailed balance condition to the update scheme of the inverse temperature in simulated tempering. Our method, irreversible simulated tempering, is constructed based on the framework of the skew detailed balance condition. By applying this method to the ferromagnetic Ising model in two dimensions on a square lattice as a benchmark, the dynamical behavior of the inverse temperature and an autocorrelation function of the magnetization are studied numerically. It is found that the relaxation dynamics of the inverse temperature changes qualitatively from diffusive to ballistic by violating the detailed balance condition. Consequently, the autocorrelation time of magnetization is several times smaller than that for the conventional algorithm satisfying the detailed balance condition.

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I. INTRODUCTION

Since Metropolis et al. invented a Markov-chain Monte Carlo (MCMC) method in 1953 [1], it has been widely implemented in various research fields to evaluate expectation values for a high-dimensional probability distribution. Meanwhile, some improvement and development of the MCMC method have been made for more efficient sampling. Among them, simulated tempering [2, 3], developed in the field of statistical physics, is categorized as an extended ensemble method. In simulated tempering, the inverse temperature in the Gibbs-Boltzmann distribution is treated as a random variable as well as the configurations and thus the state space of the system is extended by adding the temperature. A Markov chain on the extended state space is constructed with a detailed balance condition (DBC), which is a sufficient condition for MCMC. The simulated tempering has been eagerly used for various problems in statistical physics [4–8] and protein-folding problems [9, 10].

Recently, a lifting technique in which the detailed balance condition (DBC) in the Markov chain is broken with the global balance condition still holding has been extensively studied. Several studies have shown that diffusive relaxation dynamics in a one-dimensional random walk with DBC is qualitatively improved by using the lifting technique [11–14]. The transition graph of the inverse temperature under a fixed configuration in the simulated tempering is the same as that in the random walk. Thus, we expect that the violation of DBC makes the relaxation dynamics of the inverse temperature in simulated tempering change qualitatively.

In this study, we propose to apply the idea of a skew detailed balance condition (SDBC) [14, 15] to the update scheme of the inverse temperature in simulated tempering, thus conducting the simulated tempering algorithm without DBC. As a benchmark, we examine the efficiency of our proposed algorithm in a two-dimensional Ising model and show, numerically, that SDBC changes, qualitatively, the relaxation dynamics of the inverse temperature in simulated tempering. Furthermore, we observe that the autocorrelation time of the magnetization is also reduced by the violation of DBC.

This paper is organized as follows. Sec. II introduces the simulated tempering method satisfying DBC. In Sec. III a simulated tempering algorithm with SDBC is constructed. We apply the proposed algorithm to an Ising model in two dimensions as a benchmark and confirm the efficiency of our proposed algorithm in Sec. IV. Section V summarizes the present work.

II. SIMULATED TEMPERING

In this section, we explain the outline of simulated tempering [2, 3] in order to fix our notation.

A. Setup

Let \( X \) be a configuration to be sampled from a target distribution function in MCMC simulations. In statistical physics, the target distribution \( P_\beta(X) \) is often given by the Gibbs-Boltzmann distribution with an inverse temperature \( \beta \),

\[
P_\beta(X) = \frac{1}{Z(\beta)} \exp[-\beta E(X)],
\]

(1)
where \( E(\mathbf{X}) \) is a model Hamiltonian and \( Z(\beta) \) is the partition function of the model. In simulated tempering, the (inverse) temperature, as well as the configuration, is a random variable. More specifically, \( \beta \) takes \( R \) different values determined before the simulation, expressed as \( \beta_1, \ldots, \beta_R \). Thus, a state is specified by these values, denoted by \((\mathbf{X}, \beta_r)\). Then, an extended equilibrium distribution \( P_{\text{ST}}(\mathbf{X}, \beta_r) \) for finding a state \((\mathbf{X}, \beta_r)\) is given as

\[
P_{\text{ST}}(\mathbf{X}, \beta_r) = \frac{1}{Z_{\text{ST}}} \exp[-\beta_r E(\mathbf{X}) + g_r],
\]

where the weight factor \( g_r \) is a constant depending only on the inverse temperature and the extended partition function \( Z_{\text{ST}} \) is

\[
Z_{\text{ST}} = \sum_{r=1}^{R} \sum_{\mathbf{X}} \exp[-\beta_r E(\mathbf{X}) + g_r] = \sum_{r=1}^{R} Z(\beta_r) e^{g_r}. \tag{3}\]

For a given \( \beta_r \), the probability for finding a configuration \( \mathbf{X} \) in Eq. (2) is proportional to that in Eq. (1). The average over the sampled configurations conditioned with \( \beta_r \) is equivalent to the equilibrium average at that temperature. In contrast, the marginal probability for a given \( \beta_r \) is obtained by

\[
P_{\text{ST}}(\beta_r) = \sum_{\mathbf{X}} P_{\text{ST}}(\mathbf{X}, \beta_r) = \frac{Z(\beta_r) e^{g_r}}{Z_{\text{ST}}}. \tag{4}\]

The marginal probability is independent of \( r \) when \( g_r = -\ln Z(\beta_r) \), which is proportional to the bulk free energy at \( \beta_r \) of the model simulated. In general, it is hard to estimate the value of the free energy for a statistical-mechanical model. However, if it could be estimated a priori, even approximately, a uniform sampling for \( r \) from high to low temperatures can be put into practice. By considering an appropriate Markov chain, the state of \( \beta_r \) wanders on the temperature axis in a random-walk manner. One may expect that it is relatively easy to sample configurations at sufficiently high temperatures, which would help an efficient sampling at low temperatures through the random walk of \( \beta_r \). This is what we expect to perform in simulated tempering.

**B. Simulated tempering algorithm with detailed balance condition**

An explicit update scheme of the simulated tempering method consists of the following two steps: an update of a configuration \( \mathbf{X} \) for a fixed \( \beta_r \), and an update of \( \beta_r \) for a fixed \( \mathbf{X} \). In order to generate a Markov chain, the corresponding two transition-probability matrices are introduced. One is the transition matrix from a state \((\mathbf{X}, \beta_r)\) to \((\mathbf{X}', \beta_r)\) denoted as \( T(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) \). The other is one from \((\mathbf{X}, \beta_r)\) to \((\mathbf{X}, \beta_l)\) as \( T(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) \). They satisfy DBC for the stationary distribution of Eq. (2). In practice, the Metropolis-Hastings type [10] of the transition probabilities is often used. Here, we assume that the transition probabilities are decomposed into

\[
T(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) = q(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) W(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r), \tag{5}\]

and

\[
T(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) = q(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) W(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r), \tag{6}\]

where \( q \) denotes the proposal probability and \( W \) is the acceptance probability. Then, the explicit forms of the Metropolis-Hastings type of the acceptance probabilities for Eq. (5) and (6) are given by

\[
W(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) = \min \left[ 1, \frac{q(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) P_{\text{ST}}(\mathbf{X}', \beta_r)}{q(\mathbf{X}, \beta_r | \mathbf{X}, \beta_r) P_{\text{ST}}(\mathbf{X}, \beta_r)} \right], \tag{7}\]

and

\[
W(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) = \min \left[ 1, \frac{q(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) P_{\text{ST}}(\mathbf{X}, \beta_l)}{q(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) P_{\text{ST}}(\mathbf{X}, \beta_r)} \right], \tag{8}\]

respectively.

For simplicity, the set of inverse temperatures are ordered such that \( \beta_1 < \beta_2 < \cdots < \beta_R \). In addition, throughout this paper we use the proposal probability \( q_{r,t} \equiv q(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) \) given by \( q_{1,2} = q_{R,R-1} = 1 \) and \( q_{r,r+1} = 1/2 \) if \( 1 < r < R \) and zero otherwise (Fig. 1). Note that \( q_{r,t} \) is independent of the configuration \( \mathbf{X} \). Then, the procedure of the simulated tempering method is described as follows.

1. Arbitrarily chose an initial state \((\mathbf{X}^{(0)}, \beta^{(0)})\).

2. Iterate the update trials for an original configuration \( \mathbf{X} \) at a fixed \( \beta \) according to the conventional Metropolis-Hastings method:

   (a) Suppose that the current state is \((\mathbf{X}, \beta_r)\) and select a configuration \( \mathbf{X}' \) with the probability \( q(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) \).

   (b) Accept the new state \((\mathbf{X}', \beta_r)\) with the probability \( W(\mathbf{X}', \beta_r | \mathbf{X}, \beta_r) \). If it is rejected, set the current state as the next state.

3. Iterate the update trials for an inverse temperature \( \beta \) according to the following procedure:

   (a) Suppose that the current state is \((\mathbf{X}, \beta_r)\) and choose \( \beta_l \) with the probability \( q_{r,t} \) as a candidate for the next inverse temperature (Fig. 1).

   (b) Accept the next state \((\mathbf{X}, \beta_l)\) with the probability \( W(\mathbf{X}, \beta_l | \mathbf{X}, \beta_r) \). If it is rejected, set the current state as the next state.
Although any inverse temperature could be chosen as a candidate in step 3, in practice we only consider the nearest ones to increase the transition rate. By repeating steps 2 and 3, our desired Markov chain of the state \((X, \beta)\) is obtained.

Since the simulated tempering was invented, it has been widely applied to various problems \([4, 10]\). In addition, the improvement of simulated tempering has been continuously studied \([17, 22]\). In particular, an efficient simulated tempering in which DBC breaks and the rejection rate is decreased with the violation of DBC using the Suwa-Todo algorithm \([23]\) was proposed recently in Ref. \([22]\). Others authors keep DBC unbroken. The typical relaxation time of the algorithm is reduced by some factor, but its temperature dynamics does not change quantitatively from standard diffusive dynamics.

III. SIMULATED TEMPERING WITH SKEW DETAILED BALANCE CONDITIONS

In the conventional simulated tempering method explained in the previous section, the transition graph of the inverse temperature \(\beta\) under fixed \(X\) in Fig. I is the same as that of a one-dimensional simple random walk. Thus, \(\beta\) behaves as a random walker on the graph. It is known that a random walk satisfying DBC is essentially a diffusive process and its relaxation time is of order \(O(\Omega^2)\), where \(\Omega\) denotes the number of states in the random walk. Several studies have shown, numerically and analytically, that the \(\Omega\)-dependence of the relaxation time is improved by introducing the “lifting” technique to the random walk in one dimension \([11, 13]\). Here DBC is broken by adding a lifting parameter while preserving the global balance condition. This strongly suggests that the performance of simulated tempering is improved qualitatively by the lifting of the update of \(\beta\). In this section, we apply the methodology of SDBC \([14, 15]\) to simulated tempering, especially to the update scheme of the inverse temperature. The proposed method is called irreversible simulated tempering.

A. Setup

Let us reconsider the setup of conventional simulated tempering to extend it to an irreversible one. By introducing an auxiliary random variable \(\varepsilon \in \{+, -\}\) to the system as a lifting parameter, the state space is duplicated. A state in the duplicated state space is denoted \((X, \beta_r, \varepsilon)\). Then, the extended equilibrium distribution \(P_{ST}(X, \beta_r, \varepsilon)\) for finding a state \((X, \beta_r, \varepsilon)\) is given by

\[
P_{ST}(X, \beta_r, \varepsilon) = \frac{1}{2Z_{ST}} \exp[-\beta_r E(X) + g_r].
\]

Note that the marginal probability for a given configuration \(X\) and an inverse temperature \(\beta_r\) is exactly the same as \(P_{ST}(X, \beta_r)\) and that it is uniform for a given \(\varepsilon\).

In this study, we apply the methodology of SDBC to the update scheme of the inverse temperature. The skew detailed balance condition in this context is expressed as

\[
T(X, \beta_l, +|X, \beta_r, +)P_{ST}(X, \beta_r, +) = T(X, \beta_r, -|X, \beta_l, -)P_{ST}(X, \beta_l, -),
\]

where \(T(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon)\) denotes the transition probability from a state \((X, \beta_l, \varepsilon)\) to \((X, \beta_r, \varepsilon)\). Again, we decompose the transition probability \(T(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon)\) into the product of a proposal probability and an acceptance probability expressed as

\[
T(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon) = q(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon)W(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon).
\]

By using the proposal probability \(q(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon)\), the general form of the Metropolis-Hastings-type acceptance probability that satisfies SDBC is explicitly given by

\[
W(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon) = \min \left[1, \frac{q(X, \beta_r, -\varepsilon|X, \beta_l, -\varepsilon)P_{ST}(X, \beta_l)}{q(X, \beta_l, \varepsilon|X, \beta_r, \varepsilon)P_{ST}(X, \beta_r)} \right],
\]

In this study, we construct the proposal probability as \(q_{r,1}^{(\varepsilon)}\), which is independent of the configuration \(X\) as follows (Fig. II):

\[
q_{1,2}^{(\varepsilon)} = q_{R,R-1}^{(\varepsilon)} = 1,
\]

\[
q_{r,r+1}^{(\varepsilon)} = \frac{1 \pm \delta \varepsilon}{2},
\]

if \(1 < r < R\), and \(q_r^{(\varepsilon)} = 0\) otherwise. The parameter \(\delta\) controls the violation of DBC and satisfies \(|\delta| < 1\). DBC is restored when the parameter \(\delta\) is set to zero. One expects that a finite positive value of \(\delta\) enhances a clockwise flow in the dynamics of \(\beta\) in Fig. II.
B. Simulated tempering algorithm with skew detailed balance conditions

For simplicity, we rewrite the acceptance probability \( W(X, \beta_i, \varepsilon | X, \beta_r, \varepsilon) \) as \( W_{r,l}^{(\varepsilon)} \). Then, the update scheme of an inverse temperature \( \beta \) and an auxiliary variable \( \varepsilon \) is described as follows:

1. Iterate the update trials for an inverse temperature \( \beta \) according to the following procedure:
   (a) Suppose that the current state is \( (X, \beta_r, \varepsilon) \) and choose \( \beta_l \) with the probability \( q_{r,l}^{(\varepsilon)} \) as a candidate of the next inverse temperature.
   (b) Accept the next state \( (X, \beta_l, \varepsilon) \) with the probability \( W_{r,l}^{(\varepsilon)} \).
   (c) If the trial is rejected, flip \( \varepsilon \) and set \( (X, \beta_r, -\varepsilon) \) as the next state with the probability

\[
\lambda_{r,l}^{(\varepsilon)} = \frac{\Lambda_{r,l}^{(\varepsilon)}}{1 - \sum_{l \neq r} q_{r,l}^{(\varepsilon)} W_{r,l}^{(\varepsilon)}}, \quad (15)
\]

where

\[
\Lambda_{r,l}^{(\varepsilon)} = \max \left[ 0, -\varepsilon - \sum_{\varepsilon' = \pm 1} \sum_{l \neq r} \varepsilon q_{r,l}^{(-\varepsilon')} W_{r,l}^{(-\varepsilon')} \right]. \quad (16)
\]

If it is also rejected, set the current state as the next state.

2. Update the configuration \( X \) with the conventional Metropolis-Hastings method at the inverse temperature \( \beta_l \), as explained in Sec. [II].

It is straightforward to verify that the global balance condition is satisfied in the above procedure [14, 15].

IV. BENCHMARK

In this section, we apply the proposed algorithm to an Ising model in two dimensions on a square lattice as a benchmark and numerically evaluate the efficiency of the algorithm. Let \( L \) denotes the linear size of the Ising model and let \( N = L^2 \). The energy function of the model is given by

\[
E(S) = -\sum_{(ij)} S_i S_j, \quad (17)
\]

with \( S = \{S_i\}_{i=1}^N \) and \( S_i = \pm 1 \). The sum is taken over the nearest neighbor pairs, imposing a periodic boundary condition. The energy unit is set to unity. The set of inverse temperatures in the simulated tempering is prepared from \( \beta_1 = 0.2 \) and \( \beta_R = 0.5 \), with the intermediate values equally spaced between them. Note that the critical inverse temperature of the model is known as \( \beta_c = \ln(1 + \sqrt{2})/2 \approx 0.4407 \) [24], which is inside the temperature region in our simulations.

In the present work, we focus our attention on the performance of irreversible simulated tempering for an ideal weight parameter \( g \). Thus, the parameter \( g_r \), which should be given a priori, is evaluated by using an exact free energy numerical method with a polynomial time of \( N [25] \) available for finite-size Ising models in two dimensions.

The determination of the parameter, which is an important issue when actually applying the algorithm to some statistical-mechanics models, is discussed in a separate paper [29].

A. Relaxation dynamics of the inverse temperature

We study the dynamics of the inverse temperature in simulated tempering. In this work, a Monte Carlo step (MCS) is defined by the time unit where \( N \) spin trials and a trial of \( \beta \) are performed. Figure 3 illustrates the time evolution of the relaxation function of \( \beta \) defined as

\[
\phi_{\beta}^{(n)} = \frac{\langle \beta^{(n)} \rangle - \langle \beta \rangle_{\text{eq}}}{\langle \beta^{(0)} \rangle - \langle \beta \rangle_{\text{eq}}}, \quad (18)
\]

where \( \langle \beta^{(n)} \rangle \) denotes the sample average of the inverse temperature after \( n \) MCS. The expectation in respect to the target distribution in Eq. (2) is denoted by \( \langle \cdot \rangle_{\text{eq}} \).
The initial conditions of $\beta$ are set as $\beta^{(0)} = \beta_R$. The relaxation function monotonically decays to zero with relaxation time. Figure 3 indicates that the convergence of $\beta$ with $\delta \neq 0$ is more than 10 times faster than that with $\delta = 0$ and that the larger $\delta$ is, the more the relaxation of $\beta$ is accelerated.

In order to evaluate quantitatively the improvement of the relaxation dynamics of the inverse temperature, we measure the relaxation time defined as

$$
\tau_{\text{relax}}(\epsilon) \equiv \inf\{n > 0; |\phi^{(n)}_\beta| < \epsilon\}. \quad (19)
$$

Figure 4 represents the $R$-dependence of the relaxation time $\tau_{\text{relax}}(\epsilon)$ with $\epsilon = 0.2$. Although no difference between $\delta = 0$ and $\delta \neq 0$ is observed for small $R$ in Fig. 4, the asymptotic behavior of the relaxation time is quite different in each case. In the case of $\delta = 0$, the relaxation time is asymptotically of order $O(R^2)$, which indicates that the relaxation dynamics of the inverse temperature is diffusive. On the other hand, the relaxation time for $\delta \neq 0$ is asymptotically proportional to $R$, which indicates that the relaxation dynamics is ballistic. This difference in the asymptotic behavior is qualitatively consistent with previous works on the one-dimensional simple random walk [11,13]. This shows that the violation of DBC yields an acceleration of the relaxation of $\beta$.

**B. Empirical transition matrix of inverse temperature**

The dynamics of the inverse temperature is explored also through another quantity. In implementing the irreversible simulated tempering algorithm, one can easily measure the empirical transition probability with respect to the inverse temperature $\beta$ and the auxiliary random variable $\epsilon$. The empirical transition probability from the state $(\beta_r, \epsilon)$ to $(\beta_t, \epsilon')$ is defined as

$$
\tilde{T}(\beta_t, \epsilon'|\beta_r, \epsilon) \equiv \frac{\text{# of transitions from } (\beta_r, \epsilon) \text{ to } (\beta_t, \epsilon')}{\text{# of visit } (\beta_r, \epsilon)}. \quad (20)
$$

In this study, we apply the irreversible simulated tempering algorithm to the two-dimensional Ising model for $2 \times 10^5 \times R$ MCSs after equilibration and measure the empirical transition probabilities. In our algorithm, explained in the previous section, the non-zero component of the transition probability is $\tilde{T}(\beta_r, \epsilon|\beta_r, \epsilon)$, $\tilde{T}(\beta_{r+1}, \epsilon|\beta_r, \epsilon)$, and $\tilde{T}(\beta_r, -\epsilon|\beta_r, \epsilon)$ with $\epsilon = \pm$. Figures 5 and 6 illustrate the $\beta$-dependence of the empirical transition probabilities. In Fig. 5, $\tilde{T}(\beta_{r+1}, +|\beta_r, +)$ has a dip around the critical inverse temperature for smaller values of $R$. However, the dip vanishes with increasing number of inverse temperatures and the empirical transition probability becomes flat with respect to $\beta$. Thus, the empirical transition matrix can be approximated by that of the lifted simple random walk in one dimension discussed in Ref. [14]. In addition, Fig. 6 shows that the empirical transition probability for the $\epsilon$ flip is approx-
approximately proportional to $R^{-1}$. In Ref. \cite{14} it was shown analytically that the lifted simple random walk in one dimension with $O(R^{-1})$ $\varepsilon$-flip probability follows a ballistic process. Thus, these results imply the reduction of the convergence rate of the inverse temperature.

To evaluate the convergence rate from the empirical transition matrix, we define the relaxation time as follows. Let $\lambda_k \ (k = 1, 2, ..., 2R)$ denote the eigenvalues of the empirical transition matrix defined as $\tilde{T} = \left(\tilde{T}(\beta_l, \varepsilon' | \beta_r, \varepsilon)\right)_{1 \leq r, l \leq R; \varepsilon, \varepsilon' = \pm} \in \mathbb{R}^{2R \times 2R}$. Without loss of generality, the eigenvalues are aligned as $1 = \lambda_1 > |\lambda_2| \geq \cdots \geq |\lambda_{2R}|$. Then, the relaxation time of the inverse temperature is defined as

$$\tilde{\tau}_{\text{relax}} \equiv -\frac{1}{\ln |\lambda_2|}.$$  \hfill (21)

Figure 7 illustrates the $R$-dependence of the relaxation time $\tilde{\tau}_{\text{relax}}$ obtained by numerically diagonalizing the empirical transition matrix. As shown in Fig. 4, the asymptotic behavior of the relaxation time in both the reversible and irreversible cases is compatible with the results obtained in the previous subsection. Thus, the acceleration of the relaxation dynamics of the inverse temperature by the violation of DBC is numerically and theoretically confirmed.

### C. Autocorrelation function

The acceleration of the relaxation of $\beta$ is expected to promote the acceleration of the relaxation of the magnetization in the Ising model. In this subsection, we observe the time evolution of the autocorrelation function of the magnetization whose initial state is prepared as an equilibrium state at $\beta_R$, the lowest temperature in our simulations. Let $m = \sum_{i=1}^N S_i / N$ denote the averaged spin and let $\langle \cdots \rangle_{\beta}$ be the expectation value with respect to the Gibbs-Boltzmann distribution in Eq. (1). Then, we define the (normalized) autocorrelation function of the magnetization in simulated tempering as

$$C_m = \frac{(m(0)m(n) - \langle m \rangle_{\beta_R}(m)_{\text{eq}})}{(m^2)_{\beta_R} - \langle m \rangle_{\beta_R}(m)_{\text{eq}}},$$  \hfill (22)
where $\langle m^{(0)} m^{(n)} \rangle$ denotes the sample average of the correlation between the initial averaged spin and that after $n$ MCSs. Figure 7 illustrates the time evolution of $C_m^{(n)}$, which indicates that the violation of DBC reduces the relaxation rate in the autocorrelation function by a factor as large as ten (10). This reduction is affected by the acceleration of the relaxation of $β$.

In order to evaluate quantitatively the improvement of the relaxation dynamics of the autocorrelation, the autocorrelation time is defined as

$$\tau_{\text{corr}}(\epsilon) \equiv \inf\{n > 0; |C_m^{(n)}| < \epsilon\}, \quad (23)$$

and especially $\tau_{\text{corr}} = \tau_{\text{corr}}(\epsilon = 0.2)$. Figure 8 represents the $R$-dependence of the autocorrelation time $\tau_{\text{corr}}$. As shown in Fig. 8 while there is no difference observed between $δ = 0$ and $δ \neq 0$ for small $R$, the autocorrelation time is improved for relatively large $R$. The above results confirm that the violation of DBC improves the efficiency of the simulated tempering algorithm with respect to the sampling of both $β$ and $X$.

V. SUMMARY AND DISCUSSION

We have constructed an irreversible simulated tempering algorithm by introducing the lifting technique based on the methodology of SDBC to the update scheme of the inverse temperature. Benchmarks for the Ising model show that our algorithm accelerates the relaxation dynamics of inverse temperature and the autocorrelation function of the magnetization compared to the traditional simulated tempering algorithm based on DBC. These results show that the lifting technique can improve the efficiency of extended-ensemble methods. Furthermore, we consider the empirical transition probability with respect to the inverse temperature and the lifting parameter to investigate the relaxation dynamics of the inverse temperature in detail. It is easily measured during numerical simulations in the irreversible simulated
tempering algorithm. We found that the empirical transition matrix is approximately the same as the transition matrix of the lifted simple random walk in one dimension discussed in Ref. [14]. Thus, it is theoretically confirmed that the lifting technique accelerates the relaxation dynamics of the inverse temperature.

Although we used our proposed algorithm for the Ising model in two dimensions in this paper, our algorithm is, in principle, applicable to any other system such as Potts model, Heisenberg spin glass, and protein systems. It is also possible to combine other update schemes of the configuration of target systems, such as the Swendsen-Wang algorithm and the Wolff algorithm, instead of the Metropolis-Hastings algorithm. Our algorithm could take over these advantages from the traditional simulated tempering method. It is worth investigating whether the irreversible simulated tempering combined with such an update scheme works effectively in a system with a first-order phase transition and spin glasses.

In this study, all inverse temperatures were arranged at equal distances and the weight factor $r$ was estimated by an exact numerical method. The choice of the set of inverse temperatures $\{\beta_r\}$ and parameters $g_r$ affect the efficiency of simulated tempering. Several studies have proposed their efficient choices [18, 26–28]. A promising way for estimating the weight factor is to implement the irreversible simulated tempering algorithm which is our current work in progress [29].

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