Dynamics of the One-Dimensional Ising Model without Detailed Balance Condition

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We study an irreversible Markov chain Monte Carlo method based on a skewed detailed balance condition for an one-dimensional Ising model. Dynamical behavior of the magnetization density is analyzed in order to understand the properties of this method. As a result, it is found theoretically that the relaxation time of the magnetization density is reduced by using some transition probabilities satisfying the skewed detailed balance condition, in comparison to that with the corresponding transition probability with the detailed balance condition, and that one of the transition probabilities changes the dynamical critical exponent even with a local spin update.

KEYWORDS: Markov chain Monte Carlo, Ising model, Glauber dynamics, detailed balance condition

1. Introduction

Markov chain Monte Carlo (MCMC) methods have been widely used for sampling from a high-dimensional probability distribution and for estimating expectation values under the distribution. Since Metropolis et al. have proposed a MCMC method as a simulation tool for studying liquid,1) it has been applied to various problems in physics as well as other research fields. The conventional MCMC methods, such as Metropolis-Hastings algorithm2) and heat-bath algorithm, have developed within the framework of the detailed balance condition (DBC), which ensures the existence of stationary distribution in a Markov chain. It is, however, not always necessary to make the MCMC method work correctly. MCMC methods which are not based on DBC have been discussed for improving the performance and, in fact, some MCMC methods without DBC have recently been proposed.3–5)

In the MCMC method, the convergence to the target distribution is guaranteed by using an irreducible and aperiodic Markov chain, characterized by a transition matrix. It is known that the rate of convergence of the distribution depends on the second largest eigenvalue of the transition matrix of the Markov chain. Because all the eigenvalues are real if the transition matrix satisfies DBC, an estimator converges to its asymptotic value exponentially. On the other hand, if the transition matrix does not satisfy DBC, some eigenvalues could be complex in principle and then the estimator behaves like a damped oscillation. Such dynamics may affect the efficiency of performance of MCMC methods.

Let us consider the efficiency of the MCMC method. When one estimates the expectation value \( \langle O \rangle \) of an observable \( O \) precisely, Monte Carlo steps \( M \) should be sufficiently large, depending on an actual algorithm and a probabilistic model to be studied, so that the empirical distribution converges to the target distribution. Then, a MCMC method is considered to be efficient if an estimator rapidly converges to an exact expectation value and the variance of the estimator is sufficient small. The variance of the estimator is often enlarged by the correlation between samples in the Markov chain, which inevitably appears in return for overcoming the curse of dimensionality in MCMC methods. The correlation between samples is evaluated from an integrated autocorrelation time \( \tau_{\text{int},O} \) defined by the autocorrelation function \( C(t;O) \).

\[
\tau_{\text{int},O} = \sum_{t=1}^{\infty} C(t;O) = \sum_{t=1}^{\infty} \frac{\langle O_{i+t}O_i \rangle - \langle O_i \rangle^2}{\langle O_i^2 \rangle - \langle O_i \rangle^2}, \tag{1.1}
\]

where \( O_i \) is the value of \( O \) at \( i \)-th Monte Carlo step (MCS) and \( C(t;O) \) does not depend on \( i \) after the system reaches equilibrium. The effective variance of the estimator is given as \( \sigma_{\text{eff},O}^2 \simeq (1 + 2\tau_{\text{int},O})\sigma_O^2 \), where \( \sigma_O^2 \) is the variance in the case of independent sampling. The correlation time \( \tau_{\text{int},O} \) increases with increase of the correlation between samples. Consequently, the number of effective samples decreases as \( M_{\text{eff}} \simeq M/(1 + 2\tau_{\text{int},O}) \). Thus, the efficient MCMC method requires the reduction of the variance or the correlation time.

In the Markov chain with DBC, Peskun’s theorem provides us a guiding principle for constructing an efficient MCMC method.7) According to the theorem, the asymptotic variance of any observable is reduced by decreasing the rejection rate of the Markov chain. From this point of view, it turns out that the Metropolis transition probability is more efficient than that used in the heat-bath method. However, this argument relies on DBC and no guiding principle has been established in the case of the MCMC methods without DBC. It is therefore of great concern how MCMC methods are constructed without the use of DBC and how the methods improve the efficiency of performance. For instance, Suwa and Todo have proposed a MCMC method without DBC,3) which brings several times of reduction in the correlation time of the Potts model, in comparison to the corresponding method with DBC. Turitsyn et al.4) and Fernandes and Weigel5) have also proposed other MCMC methods with-

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out DBC and have suggested from numerical simulations that the dynamical critical exponent may be changed in a mean-field Ising model. Although these numerical studies encourage to use the MCMC methods without DBC, it is not well understood theoretically how these methods affect to the dynamics, particularly in statistical-mechanical models.

In this paper, we discuss the dynamics in the Markov chain without DBC in an one-dimensional kinetic Ising model, which is exactly solved in the Glauber dynamics with DBC. By solving time evolution of the order parameter for the model, it is found that some transitions matrices yield the reduction of the relaxation time which significantly depends on the choice of the transition probability.

The paper is organized as follows. In §2, static and dynamic properties of the one-dimensional Ising model are surveyed. In §3, an irreversible Markov chain based on the skew detailed balance condition is constructed for the Ising model and dynamical behavior of the magnetization density is analyzed in the Markov chain. An outline of our MCMC simulation is described and their results are presented in §4. Finally, summary and discussions are given in §5.

2. Reversible Glauber Dynamics

Glauber dynamics is a Markov chain of configuration of an Ising model. In this section, we survey the Glauber dynamics of an one-dimensional Ising model with DBC in order to fix our notation.

2.1 Ising model in one dimension

We study the one-dimensional Ising model with no external magnetic field. A state of the Ising model is denoted by a vector $\sigma = (\sigma_1, \ldots, \sigma_N)$ with $\sigma_j = \pm 1$ being an Ising variable defined on $j$-th site. The Hamiltonian is defined as

$$\mathcal{H}(\sigma) = -J \sum_{j=1}^{N} \sigma_j \sigma_{j+1},$$

(2.1)

where a periodic boundary condition is imposed as $\sigma_{N+1} = \sigma_1$ and $J$ is the exchange interaction constant. For a given inverse temperature $\beta$, in the units where Boltzmann constant is 1, the equilibrium distribution $\pi(\sigma)$ for finding a state $\sigma$ is proportional to the Boltzmann factor $\exp(-\beta \mathcal{H}(\sigma))$.

An expectation of an observable $A = A(\sigma)$ in equilibrium is expressed as

$$\langle A \rangle_{\text{eq}} := \sum_{\sigma} A(\sigma) \pi(\sigma),$$

(2.2)

where $\sum_{\sigma}$ denotes the summation over $2^N$ spin configurations. The order parameter of the Ising model is magnetization density which is given in our notation by the expectation $\langle m \rangle_{\text{eq}}$ of the observable $m(\sigma) = \frac{1}{N} \sum_j \sigma_j$. It is well known that no spontaneous magnetization emerges at any finite temperature and the phase transition does not occur in the one-dimensional Ising model, that is $\langle m \rangle_{\text{eq}} = 0.$

for all $N$ and $\beta > 0$ in this model. The correlation length $\xi(\beta)$ is given by

$$\xi^{-1}(\beta) = -\log(\tanh \beta J),$$

(2.4)

which diverges as the temperature goes to zero.

2.2 Master equation and detailed balance condition

Since the Ising model has no intrinsic dynamics induced by Hamiltonian, a stochastic dynamics introduced by Glauber has been used in the study of dynamics of the Ising models. The stochastic dynamics is a Markov chain of the state $\sigma$, which is described by a master equation.

We define $F_j$ be a spin-flip operator on $j$-th site: $F_j \sigma$ is the state that $j$-th spin is flipped from $\sigma$ with the others fixed. The Markov chain is characterized by a transition probability $w_j(\sigma | \sigma)$ per unit time from $\sigma$ to $F_j \sigma$. Let $p(\sigma, t)$ be a probability distribution for finding the spin state $\sigma$ at time $t$. Then, the master equation is written as follows:

$$\frac{d}{dt} p(\sigma, t) = -\sum_j w_j(\sigma | \sigma)p(\sigma, t) + \sum_j w_j(F_j \sigma)p(F_j \sigma, t),$$

(2.5)

where the first and second terms in the right hand side are outgoing and incoming probability, respectively.

For the master equation in Eq. (2.5), the necessary and sufficient condition that $p(\sigma, t)$ converges to the equilibrium distribution $\pi(\sigma)$ as $t \to \infty$ is that the transition probability $w_j(\sigma | \sigma)$ satisfies a balance condition (BC):

$$\sum_j w_j(\sigma | \sigma) \pi(\sigma) = \sum_j w_j(F_j \sigma)p(F_j \sigma, t).$$

(2.6)

In practice, DBC is widely used for a sufficient condition of BC:

$$w_j(\sigma | \sigma) = w_j(F_j \sigma)p(F_j \sigma, t).$$

(2.7)

This condition is also called reversibility in the field of statistical science. The sequence of states generated by the transition probability with DBC is called reversible Markov chain. While BC means the total balance of the stochastic flow in the state space, DBC requires a local balance of the stochastic flow between each state $\sigma$ and $F_j \sigma$. Imposing DBC, some transition probabilities can be determined explicitly and have been used in MCMC simulations. For instance, Glauber’s transition probability is given for the one-dimensional Ising model as

$$w_j(\sigma | \sigma) = \frac{1}{2^\alpha} \left[ 1 - \frac{1}{2} \gamma \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \right],$$

(2.8)

where $\alpha$ is a time constant and $\gamma = \tanh 2\beta J$. This is equivalent to the heat-bath algorithm in MCMC method.
2.3 Time evolution of magnetization density

An expectation of an observable $A$ at time $t$ is denoted by

$$\langle A(t) \rangle := \sum_{\sigma} A(\sigma)p(\sigma, t). \quad (2.9)$$

From the master equation in Eq. (2.5), time evolution of the magnetization density is reduced to\(^8\)

$$\frac{d}{dt} \langle m(t) \rangle = -(1 - \gamma) \langle m(t) \rangle. \quad (2.10)$$

Then, we have

$$\langle m(t) \rangle = \langle m(0) \rangle \exp[-\alpha(1 - \gamma)t]. \quad (2.11)$$

This indicates that the magnetization density converges exponentially in time to the equilibrium value in Eq. (2.3). The relaxation time of the magnetization density which reflects the rate of convergence is defined as

$$\tau := \int_0^\infty \frac{\langle m(t) \rangle - \langle m\rangle}{\langle m(0) \rangle - \langle m\rangle} dt. \quad (2.12)$$

Using the solution of Eq. (2.11), the relaxation time of this system is obtained as

$$\tau = \frac{1}{\alpha(1 - \gamma)}, \quad (2.13)$$

which means that the convergence rate is slower with decreasing temperature and eventually diverges at zero temperature $\gamma = 1$. This is due to dynamical slowing down induced by the zero-temperature transition. For $\gamma \to 1$, one finds that $\tau \sim \xi^z$ using Eq. (2.4) with the dynamical critical exponent $z = 2$.

2.4 Integrated autocorrelation time

We also discuss an integrated autocorrelation time of the magnetization density. Let $p(\sigma, t + t_\omega, \sigma', t_\omega)$ be a conditional probability for finding a state $\sigma$ at elapsed time $t$ after a state $\sigma'$ at waiting time $t_\omega$. Then, an autocorrelation function of an observable $A$ in equilibrium is defined as

$$C_{eq}(t; A) := \frac{\langle A_{eq}A(t) \rangle - \langle A \rangle^2_{eq}}{\langle A^2 \rangle_{eq} - \langle A \rangle^2_{eq}}, \quad (2.14)$$

where

$$\langle A_{eq}A(t) \rangle := \sum_{\sigma, \sigma'} A(\sigma')\pi(\sigma')A(\sigma)p(\sigma, t + t_\omega|\sigma', t_\omega), \quad (2.15)$$

where $t_\omega$ being a sufficient long time. In the case of the magnetization density, substituting Eq. (2.11) we have

$$\langle m_{eq}(t) \rangle = \langle m^2 \rangle_{eq} \exp[-\alpha(1 - \gamma)t]. \quad (2.16)$$

Combining with Eq. (2.3), we obtain

$$C_{eq}(t; m) = \exp[-\alpha(1 - \gamma)t]. \quad (2.17)$$

Thus, the integrated autocorrelation time of the magnetization density is obtained as

$$\tau_{int, m} := \int_0^\infty dt \ C_{eq}(t; m) = \frac{1}{\alpha(1 - \gamma)}. \quad (2.18)$$

which is identical to the relaxation time of the magnetization density. This indicates that the correlation between states in the Markov chain increases with temperature decreasing and consequently the effective variance of the magnetization density is enlarged.

3. Irreversible Glauber Dynamics

A stochastic process whose transition probability does not satisfy DBC is called irreversible Markov chain. In this section, we construct a Markov chain for the one-dimensional Ising model on a basis of skew detailed balance condition (SDBC)\(^5\) and study time evolution of the magnetization density under SDBC.

3.1 Master equation and skew detailed balance condition

According to the method of Turitsyn et al.,\(^4\) we introduce another Ising spin $\varepsilon = \pm 1$ in addition to the original spin configurations. The enlarged state of the system is denoted by $X := (\sigma, \varepsilon) \in \{-1, +1\}^N \times \{-1, +1\}$. We consider a single spin-flip update for the whole spin including $\varepsilon$ as an elementary Markov process. Let $p(\sigma, \varepsilon, t)$ be a probability distribution which we find a state $(\sigma, \varepsilon)$ at time $t$. The master equation of the system is given as follows:

$$\frac{d}{dt} p(\sigma, \varepsilon, t) = -\sum_j w_j(\sigma, \varepsilon) p(\sigma, \varepsilon, t) + \sum_j w_j(F_j, \varepsilon)p(F_j, \sigma, \varepsilon, t) - \lambda(\sigma, \varepsilon)p(\sigma, \varepsilon, t) + \lambda(\sigma, -\varepsilon)p(\sigma, -\varepsilon, t), \quad (3.1)$$

where $w_j(\sigma, \varepsilon)$ is a transition probability par unit time from a state $(\sigma, \varepsilon)$ to $(F_j, \sigma, \varepsilon)$ and $\lambda(\sigma, \varepsilon)$ is that from a state $(\sigma, \varepsilon)$ to $(\sigma, -\varepsilon)$. We assume that an equilibrium distribution of the master equation is independent of the additional spin $\varepsilon$:

$$\forall (\sigma, \varepsilon), \quad p(\sigma, \varepsilon, t) \to \frac{1}{\pi(\sigma)} \quad \text{as} \quad t \to \infty. \quad (3.2)$$

Therefore, the balance condition (BC) is given by

$$\sum_j \left[ w_j(\sigma, \varepsilon)p(\sigma) - w_j(F_j, \sigma, \varepsilon)p(F_j, \sigma) \right] + \lambda(\sigma, \varepsilon) - \lambda(\sigma, -\varepsilon) \pi(\sigma) = 0. \quad (3.3)$$

In order to determine the transition probabilities $w_j(\sigma, \varepsilon)$ and $\lambda(\sigma, \varepsilon)$ satisfying BC in Eq. (3.3), we impose an alternative condition:

$$w_j(\sigma, \varepsilon)p(\sigma) = w_j(F_j, \sigma, \varepsilon)p(F_j, \sigma). \quad (3.4)$$

This condition is referred as the skew detailed balance condition\(^5\) which requires a local balance of stochastic flows from a state $(\sigma, \varepsilon)$ to $(F_j, \sigma, \varepsilon)$ and that from $(F_j, \sigma, \varepsilon)$ to $(\sigma, -\varepsilon)$. Under SDBC, the condition for $\lambda(\sigma, \varepsilon)$ is obtained from BC in Eq. (3.3) as

$$\lambda(\sigma, \varepsilon) - \lambda(\sigma, -\varepsilon) = \sum_j \left[ w_j(\sigma, -\varepsilon) - w_j(\sigma, \varepsilon) \right]. \quad (3.5)$$
The condition in Eq. (3.5) combined with SDBC ensures that the probability distribution converges to the equilibrium distribution in the Markov chain.

There still remains the degree of freedom for determining the transition probability \( w_j(\sigma, \varepsilon) \) even when SDBC is imposed. In the present work, we choose a Glauber like transition probability

\[
 w_j(\sigma, \varepsilon) = \frac{1}{2} \alpha \left[ 1 - \frac{1}{2} \gamma \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \right] (1 - \delta \varepsilon \sigma_j),
\]

where \( \delta \) is a parameter which characterizes the deviation from DBC. Note that DBC is reduced to the case of \( \delta = 0 \) and the range of the parameter \( \delta \) is restricted to the interval \([-1,1]\) because of the non-negativity of \( w_j(\sigma, \varepsilon) \). The transition probability in Eq. (3.6) is equivalent to the heat-bath transition probability in the one-dimensional Ising model with virtual magnetic field \( \varepsilon H \) with \( \delta = \tanh \beta H \). However, it should be reminded that SDBC leads to the equilibrium distribution of the system without the magnetic field given by Eq. (3.2).

Using the transition probability in Eq. (3.6), the condition in Eq. (3.5) is rewritten as

\[
 \lambda(\sigma, \varepsilon) - \lambda(\sigma, -\varepsilon) = \alpha \delta (1 - \gamma) N \varepsilon m(\sigma).
\]  

(3.7)

There are variations in \( \lambda(\sigma, \varepsilon) \) satisfying the condition of Eq. (3.7). In this work, we discuss the following three types of the transition probabilities:

\[
 \lambda(\sigma, \varepsilon) = \sum_j w_j(\sigma, -\varepsilon)
 = \frac{1}{2} \alpha N \left[ 1 - \gamma u(\sigma) + \delta (1 - \gamma) \varepsilon m(\sigma) \right],
\]

(3.8)

\[
 \lambda(\sigma, \varepsilon) = \frac{1}{2} \alpha \delta (1 - \gamma) N \left( 1 + \varepsilon m(\sigma) \right),
\]

(3.9)

and

\[
 \lambda(\sigma, \varepsilon) = \max \left[ 0, \alpha \delta (1 - \gamma) N \varepsilon m(\sigma) \right],
\]

(3.10)

where \( u(\sigma) = \frac{1}{2} \sum_j \sigma_j \sigma_{j+1} \). We refer the first transition probability of Eq. (3.8) as Sakai-Hukushima 1 (SH\(_1\)) type. Because the condition of Eq. (3.5) means that a difference between \( \lambda(\sigma, \varepsilon) \) and \( \lambda(\sigma, -\varepsilon) \) is equal to that of the summation of \( w_j(\sigma, \varepsilon) \), \( \lambda(\sigma, \varepsilon) \) of the SH\(_1\) type is assigned to one of the summation terms. The second transition probability of Eq. (3.9), referred as Sakai-Hukushima 2 (SH\(_2\)) type, is obtained by imposing that \( \lambda(\sigma, \varepsilon) \) is a linear function of \( \varepsilon \). Then, the non-negativity of \( \lambda(\sigma, \varepsilon) \) further restricts the range of \( \delta \) to \([0,1]\). This transition probability is specific to the Ising model in one dimension. The transition probability of Eq. (3.10) is constructed by allocating all of the right hand side of Eq. (3.5) to either \( \lambda(\sigma, \varepsilon) \) or \( \lambda(\sigma, -\varepsilon) \). Since this transition probability has been proposed originally by Turitsyn et al.,\(^4\) we call it Turitsyn-Chertkov-Vucelja (TCV) type.

### 3.2 Exact solution in the SH\(_1\) type

We discuss time evolution of the magnetization density under the SH\(_1\) type transition probability in this subsection. An expectation of an observable \( A = A(\sigma, \varepsilon) \) of this system at time \( t \) is redefined from Eq. (2.9) to

\[
 \langle A(t) \rangle := \sum_{\sigma = \pm 1} \sum_{\varepsilon} A(\sigma, \varepsilon) p(\sigma, \varepsilon, t).
\]

(3.11)

From the master equation in Eq. (3.1), differential equations for the magnetization density and the expectation of the additive spin \( \varepsilon \) are obtained as

\[
 \frac{1}{\alpha} \frac{d}{dt} \langle m(t) \rangle = -\gamma \langle m(t) \rangle + \delta \gamma \langle \varepsilon u(t) \rangle,
\]

(3.12)

\[
 \frac{1}{\alpha} \frac{d}{dt} \langle \varepsilon(t) \rangle = -\delta (1 - \gamma) N \langle m(t) \rangle - \gamma N \langle \varepsilon u(t) \rangle + \gamma N \langle \varepsilon u(t) \rangle,
\]

(3.13)

respectively. By combining Eqs. (3.12) and (3.13), we have

\[
 \frac{1}{\alpha} \frac{d}{dt} \langle m(t) \rangle = -(1 + \delta^2) (1 - \gamma) \langle m(t) \rangle,
\]

(3.14)

for large \( N \). Thus, we obtain

\[
 \langle m(t) \rangle = \langle m(0) \rangle \exp[-(1 + \delta^2)(1 - \gamma)t],
\]

(3.15)

and the relaxation time is given as

\[
 \tau = \frac{1}{(1 + \delta^2)(1 - \gamma)}.
\]

(3.16)

The autocorrelation function is calculated as well. Let \( p(\sigma, \varepsilon, t + \tau; \sigma', \varepsilon', t_\omega) \) be a conditional probability that we find a state \((\sigma, \varepsilon) \) at elapsed time \( t \) after an equilibrium state \((\sigma', \varepsilon') \) is given at \( t_\omega \). Then, Eq. (2.15) is extended to

\[
 \langle A_{eq} A(t) \rangle = \sum_{\varepsilon, \varepsilon'} \sum_{\sigma, \sigma'} A(\sigma', \varepsilon') \frac{1}{2} \pi(\sigma') A(\sigma, \varepsilon)
 \times p(\sigma, \varepsilon, t + \tau; \sigma', \varepsilon', t_\omega).
\]

(3.17)

Therefore, we have

\[
 C_{eq}(t; \tau) = \exp[-(1 + \delta^2)(1 - \gamma) t],
\]

(3.18)

and the integrated autocorrelation time defined by Eq. (2.18) is obtained

\[
 \tau_{int, \varepsilon} = \frac{1}{(1 + \delta^2)(1 - \gamma)}.
\]

(3.19)

As in the case of DBC discussed in the previous section, the relaxation time and the integrated autocorrelation time of the magnetization density coincide with each other. It is shown analytically that they are reduced by introducing SDBC in the case of the SH\(_1\) type. Interestingly, it is found that the DBC point \((\delta = 0)\) is the worst efficient in this case. The reduction of the relaxation time from DBC is constant and independent of temperature. Therefore, the dynamical exponent does not change from that in DBC by using this type of transition probability satisfying SDBC.

### 3.3 Approximate analyses in the SH\(_2\) type

In this subsection, we discuss another transition probability \( \lambda(\sigma, \varepsilon) \) given by Eq. (3.9). The differential equation for the expectation of the additive spin \( \varepsilon \) is replaced
from Eq. (3.13) to

\[
\frac{1}{\alpha} \frac{d}{dt} \langle \varepsilon(t) \rangle = -\delta(1 - \gamma)N \langle m(t) \rangle - \delta(1 - \gamma)N \langle \varepsilon(t) \rangle,
\]

(3.20)

while that for the magnetization density is identical to Eq. (3.12). It is difficult to solve the differential equation because of the existence of the higher order term \(\langle \varepsilon u(t) \rangle\) in Eq. (3.12), which differs from the case of SH\(_1\) type. It is reasonably assumed

\[
\langle \varepsilon u(t) \rangle \simeq \langle \varepsilon(t) \rangle \langle u \rangle_{eq},
\]

(3.21)

when the system is in the vicinity of the equilibrium state. Under the assumption, Eq. (3.12) is rewritten as

\[
\frac{1}{\alpha} \frac{d}{dt} \langle m(t) \rangle = -(1 - \gamma) \langle m(t) \rangle + \delta \sqrt{1 - \gamma^2} \langle \varepsilon(t) \rangle,
\]

(3.22)

where \(\langle u \rangle_{eq} = \tanh \beta J = (1 - \sqrt{1 - \gamma^2})/\gamma\) for large \(N\). By combining Eqs. (3.20) and (3.22), we obtain

\[
\langle m(t) \rangle = \langle m(0) \rangle \exp[-\alpha(1 - \gamma + \delta \sqrt{1 - \gamma^2})t],
\]

(3.23)

Note that this result could be valid if the initial state is near the equilibrium point. Using Eq. (3.23), we have the autocorrelation function as

\[
C_{eq}(t; m) = \exp[-\alpha(1 - \gamma + \delta \sqrt{1 - \gamma^2})t],
\]

(3.24)

and the integrated autocorrelation time is

\[
\tau_{int, m} = \frac{1}{\alpha(1 - \gamma + \delta \sqrt{1 - \gamma^2})}.
\]

(3.25)

This expression is different from that obtained in the SH\(_1\) type. The relaxation time is not an even function of the parameter \(\delta\). However the parameter takes the value of \([0, 1]\) in this type. Hence, it is also found that the case of DBC with \(\delta = 0\) gives the worst efficiency in the parameter range. Further, the gain from the DBC point significantly depends on temperature and the dynamical critical exponent \(z\) is down to 1 in this type of transition probability of \(\varepsilon\) flip. While some numerical works suggest the reduction of the dynamical critical exponent by using non reversible transition probability,\(^4,5\) the present study shows analytically that the specific type of irreversible transition probability makes the relaxation of the magnetization density accelerated and changes the dynamical critical phenomena.

3.4 Linear analyses of time evolution near equilibrium point

As seen in the previous section, an irreversible transition probability yields the reduction of dynamical critical exponent. Non-local update such as cluster algorithm\(^9,10\) often leads to such acceleration of dynamics. It should be noted that even a local spin update changes the dynamical properties of system by using the irreversible transition probability. However, the irreversible transition probability does not always make the significant changes as seen in §3.2. It turns out that the transition probability for \(\varepsilon\) flip plays an important role for the dynamics of the spin configuration.

In this subsection, we study dynamical trajectory of the magnetization density and the expectation of the additive Ising spin near equilibrium point in the case of the SH\(_1\) type and SH\(_2\) type. Under the assumption in Eq. (3.21), the differential equations of these estimators can be solved for the SH\(_1\) type in a thermodynamical limit

\[
\begin{align*}
\langle m(t) \rangle &= \langle m(0) \rangle \exp[-\alpha(1 + \delta^2)(1 - \gamma)t], \\
\langle \varepsilon(t) \rangle &= -\delta \sqrt{\frac{1 - \gamma}{1 + \gamma}} \langle m(0) \rangle \exp[-\alpha(1 + \delta^2)(1 - \gamma)t],
\end{align*}
\]

(3.26)

and for the SH\(_2\) type

\[
\begin{align*}
\langle m(t) \rangle &= \langle m(0) \rangle \exp[-\alpha(1 - \gamma + \delta \sqrt{1 - \gamma^2})t], \\
\langle \varepsilon(t) \rangle &= -\langle m(0) \rangle \exp[-\alpha(1 - \gamma + \delta \sqrt{1 - \gamma^2})t].
\end{align*}
\]

(3.27)

These solutions are represented as a dynamical trajectory in the parameter space of \(\langle m(t) \rangle\) and \(\langle \varepsilon(t) \rangle\), where the equilibrium point is the origin \((0, 0)\). Using linear analysis at the equilibrium point, it is found that these expectations converge to the equilibrium point \((0, 0)\) along by a straight line, which can be regarded as an eigenvector of the slowest mode of the dynamics. Figure 1 shows a schematic picture of the trajectory. In the case of DBC, \(\langle \varepsilon(t) \rangle\) is an irrelevant parameter and thus the magnetization density \(\langle m(t) \rangle\) converges to zero along by the horizontal axis. A finite slope of the asymptotic line is a consequence of the irreversible transition probability. In fact, the solutions in Eqs. (3.26) and (3.27) provide the estimate of the slope as \(-\delta \sqrt{(1 - \gamma)/(1 + \gamma)}\) for the SH\(_1\) type and \(-1\) for the SH\(_2\) type. The slope for the SH\(_1\) type decreases with temperature decreasing and eventually goes to zero at zero temperature, \(\gamma = 1\). Namely, the dynamics near zero temperature is essentially equivalent to that in DBC. Presumably, this is the reason why the transition probability of the SH\(_1\) type does not change the dynamical critical phenomena. On the other hand, the slope for the SH\(_2\) type is independent of temperature and quite different from that for DBC. This implies that the relaxation dynamics to the equilibrium state with SDBC is accelerated by using the extended state including the additional \(\varepsilon\) spin.
Fig. 2. (Color online) Time evolution of the magnetization density in the one-dimensional Ising model for different values of $\delta$. The chosen values of parameter in the simulations are $N = 2^7$, $\alpha = 10^{-2}$, $\gamma = 0.6$, $N_{\text{ens}} = 10^5$. The transition probability used is the $\text{SH}_1$, $\text{SH}_2$, and TCV types from left to right, respectively.

Fig. 3. (Color online) $\gamma$ dependence of the relaxation time of the magnetization density with the parameter $\delta$ varying. The chosen values of parameter in the simulations are $N = 2^7$, $\alpha = 10^{-2}$, $\gamma = 0.6$, $N_{\text{ens}} = 10^5$ and $M = 2.5 \times 10^5$. The transition probability used is the $\text{SH}_1$, $\text{SH}_2$, and TCV types from left to right, respectively. The solid lines in the left panel for the $\text{SH}_1$ type represent the theoretical results.

4. Monte Carlo simulations

In this section, we explain a procedure of the MCMC method with SDBC for the one-dimensional Ising model described in the previous section. Let $X(n)$ be a state of the system after $n$ steps. Then, the elementary procedure of discrete time evolution in our simulation is as follows:

(a) Set an initial condition $X(0)$ arbitrary.

(b) Suppose that the state $X(n) = (\sigma, \varepsilon)$ at time $n$ and choose a spin $\sigma_j$ from $\sigma$ at random.

(c) Accept the new state as $X(n+1) = (F_j \sigma, \varepsilon)$ with the probability $w_j(\sigma, \varepsilon)$. If it is rejected, accept $X(n+1) = (\sigma, -\varepsilon)$ with the probability

$$
\Lambda(\sigma, \varepsilon) = \frac{\frac{1}{N} \lambda(\sigma, \varepsilon)}{1 - \frac{1}{N} \sum_j w_j(\sigma, \varepsilon)}. \quad (4.1)
$$

If also rejected, set $X(n+1) = X(n)$. Then, return to (b) and repeat the steps (b)–(c).

It is proven that these steps satisfy BC. We consider $N$ steps of (b)–(c) as one Monte Carlo step (MCS). In this work, the initial condition $X(0)$ is fixed as $\sigma_j = +1$ for all $j$ and $\varepsilon = \pm 1$ is chosen at random.

In this method, an expectation of an observable $A = A(\sigma, \varepsilon)$ at time $t$ is estimated as

$$
\langle A(t) \rangle \simeq \frac{1}{N_{\text{ens}}} \sum_{i=1}^{N_{\text{ens}}} A(\sigma^i(t), \varepsilon^i(t)), \quad (4.2)
$$

where $(\sigma^i(t), \varepsilon^i(t))$ is a state of $i$-th trajectory at $t$-th MCS starting from the initial condition and $N_{\text{ens}}$ denotes the number of simulated trajectories. Figure 2 shows the time dependence of the magnetization density estimated by Eq. (4.2) for the transition probabilities discussed in the previous sections. The relaxation time of the magnetization density under the transition probability is estimated as

$$
\tau \simeq \frac{1}{M} \sum_{i=1}^{M} \langle m(t) \rangle, \quad (4.3)
$$

where $M$ is the total number of MCS. Figure 3 shows the $\gamma$ dependence of the relaxation time of the magnetization density with the parameter $\delta$ varying. From Fig. 2, it turns out that the magnetization density decays exponentially in time and it converges to zero rapidly with increasing $\delta$ in the case of all three types. In particular, in the case of $\text{SH}_1$ type, this is completely consistent with the results of Eq. (3.15) for $N$ and $\alpha$ used in the simulations. Moreover, the numerical estimation of relaxation
time, shown in the left panel of Fig. 3, is consistent with the theoretical estimate in Eq. (3.16).

The autocorrelation function and the integrated autocorrelation time are also calculated. Let \( t_\omega \) be a sufficient large integer which ensures equilibrium of the system. Then, the autocorrelation function of the magnetization density is estimated as

\[
\langle m_{eq}(t) \rangle \simeq \frac{1}{N_{ens}} \sum_{i=1}^{N_{ens}} m(\sigma^i(t_\omega))m(\sigma^i(t + t_\omega)),
\]

(4.4)

and the integrated autocorrelation time of the magnetization density is

\[
\tau_{int,m} \simeq \frac{1}{M} \sum_{t=1}^{M} \frac{\langle m_{eq}(t) \rangle - \langle m \rangle_{eq}^2}{\langle m^2 \rangle_{eq} - \langle m \rangle_{eq}^2},
\]

(4.5)

where here \( M \) is the total number of MCS after \( t_\omega \) steps and the equilibrium values of \( \langle m \rangle_{eq} \) and \( \langle m^2 \rangle_{eq} \) are used. Figures 4 and 5 present the numerical results estimated by Eqs. (4.4) and (4.5), respectively. As seen in the magnetization density, the autocorrelation function also decays to zero exponentially in time and the relaxation is accelerated by increasing \( \delta \) for three cases. MC results recover the theoretical solutions of Eqs. (3.18) and (3.19) for the SH1 type. Further, the approximate solution for the SH2 type describes well \( \tau_{int,m} \) obtained by the MC simulation, including that \( \delta \) dependence of \( \tau_{int,m} \) disappears at zero temperature limit with anti-ferromagnetic interaction, \( \gamma = -1 \). This confirms numerically that the transition probability of the SH2 type changes the dynamical critical phenomena. For the TCV type, an oscillating behavior of the autocorrelation function is clearly observed in the right panel of Fig. 4 and consequently the integrated autocorrelation time is reduced more significantly than that for the other types. This implies the existence of complex eigenmode in the relaxation dynamics, discussed later.

As an illustration of the intrinsic dynamics with SDBC, we show the data of trajectory \((\langle m(t) \rangle, \langle \epsilon(t) \rangle)\) in Fig. 6 for the SH1 and SH2 types. In both cases, the slope of the asymptotic line near the equilibrium observed in Fig. 6 coincides with the theoretical prediction discussed in §3.4. A deviation from the straight line is found far from the equilibrium point. This is due to the effect of high-order correlation, approximated to Eq. (3.21) in our analysis, for the SH1 type and due to the finite size effect for the SH2 type, which disappears in the thermodynamical limit.

5. Summary and Discussion

We have studied dynamics of the one-dimensional Ising model in a class of the irreversible Markov chain, where the SDBC, instead of DBC in the reversible Markov
Fig. 6. (Color online) Trajectory of \( \langle m(t) \rangle , \langle \varepsilon(t) \rangle \) from the initial condition (1, 0) to the equilibrium point (0, 0) for the SH\(_1\) type (left) and the SH\(_2\) type (right). The chosen values of parameter in the simulations are \( N = 2^7, \alpha = 10^{-2}, \gamma = 0.6, N_{\text{ens}} = 10^5 \), and \( M = 2.5 \times 10^3 \). Solid lines represent the asymptotic lines near the equilibrium.

Fig. 7. (Color online) Time evolution of the magnetization density for several sizes \( N \) with the TCV transition probability. The chosen values of parameter in the simulations are \( \alpha = 0.05, \gamma = 0.6, \delta = 0.9 \) and \( N_{\text{ens}} = 10^5 \).

Fig. 8. (Color online) Trajectory of \( \langle m(t) \rangle , \langle \varepsilon(t) \rangle \) from the initial condition (1, 0) to the equilibrium point (0, 0) for the TCV type. The chosen values of parameter in the simulations are \( N = 2^7, \alpha = 10^{-2}, \gamma = 0.6, N_{\text{ens}} = 10^5 \), and \( M = 2.5 \times 10^3 \).

The chosen values of parameter in the simulations are \( N = 2^7, \alpha = 10^{-2}, \gamma = 0.6, N_{\text{ens}} = 10^5 \), and \( M = 2.5 \times 10^3 \). Solid lines represent the asymptotic lines near the equilibrium.

chain, ensures the existence of the stationary distribution in a long-time limit. In particular, the relaxation time of the magnetization density and its autocorrelation function have been discussed for three different transition probabilities satisfying SDBC, called the SH\(_1\), SH\(_2\) and TCV types, in which the parameter \( \delta \) controls the deviation from DBC. In the case of SH\(_1\) and SH\(_2\) types, we have obtained theoretical results of the dynamical behavior of the magnetization density and have revealed that the relaxation time and the autocorrelation time are always reduced for non-zero parameter \( \delta \). Furthermore, we have shown that the SH\(_2\) type transition probability changes the dynamical critical exponent while the SH\(_1\) type does not.

Some arguments in the previous sections can be made for more general Ising models in high dimensions. Suppose that the Hamiltonian of the Ising system is given as

\[
\mathcal{H}(\sigma) = - \sum_{j<k} J_{jk} \sigma_j \sigma_k - \sum_j H_j \sigma_j , \tag{5.1}
\]

where \( J_{jk} \) denotes an interaction between \( \sigma_j \) and \( \sigma_k \) and \( H_j \) is a local magnetic field acting on \( \sigma_j \). The transition probability \( w_j(\sigma, \varepsilon) \) for the spin flip discussed here is given as

\[
w_j(\sigma, \varepsilon) = \frac{1}{2} \alpha (1 - \sigma_j \tanh \beta E_j) (1 - \delta \varepsilon \sigma_j), \tag{5.2}
\]

where \( E_j = \sum_k J_{jk} \sigma_k + H_j \) is a local field on \( j \)-th site, including the one-dimensional model as \( J_{jk} = J \delta_{k,j+1} \). This satisfies SDBC and is reduced to the ordinary Glauber transition probability when \( \delta = 0 \), which has been studied. If the transition probability of the SH\(_1\) type is used for the \( \varepsilon \) flip, the magnetization density obeys

\[
\frac{1}{\alpha(1+\delta^2)} \frac{d}{dt} \langle m(t) \rangle = - \langle m(t) \rangle + \frac{1}{N} \sum_j \langle \tanh \beta E_j \rangle , \tag{5.3}
\]

for large \( N \). This indicates that the SH\(_1\) type yields only the change of time constant from \( \alpha \) in DBC to \( \alpha(1+\delta^2) \) in SDBC. Hence, the relaxation time is reduced up to the factor \( 1+\delta^2 \) from DBC, independent of temperature, even when the system exhibits a phase transition at finite temperature in more than two dimensions. Although it is not certain if this argument is valid for other observables, this argument suggests the existence of a class of transition probabilities in the irreversible Markov chain which yields a finite gain, temperature independent, in
the relaxation time compared to that of the corresponding transition probability with DBC.

Finally, let us discuss the eigenvalue in the irreversible Markov chain. Although all eigenvalues of a Markov chain with DBC are real in general, it is considered that whether an eigenvalue is real or complex depends on how to choose transition probabilities if the Markov chain does not satisfy DBC. In the method of SDBC which we consider in this paper, several choices of a transition probability $w_j(\sigma, \varepsilon)$ satisfying SDBC in Eq. (3.4) are possible in general. Even if $w_j(\sigma, \varepsilon)$ is fixed, we can choose some transition probabilities $\lambda(\sigma, \varepsilon)$ satisfying the condition in Eq. (3.5), such as the SH$_1$, SH$_2$, and TCV types. As discussed in §3, it turns out that the eigenvalues which affect to the dynamical behavior of the magnetization density are all real in the case of the SH$_1$ type. However, numerical simulations for the one-dimensional Ising model with other transition probabilities show different dynamical behavior of the magnetization density. For instance, in the case of SH$_2$ type, the magnetization density converges exponentially in time observed in the middle panel of Fig. 2. On the other hand, the existence of complex eigenmode in the relaxation dynamics is strongly implied from numerical simulations in §4 for the TCV type. Figure 7 shows time evolution of the magnetization density for several system sizes $N$, indicating that the complex eigenvalues clearly depend on $N$ and the imaginary part decreases with $N$.

Unfortunately little is known about the dynamics in the TCV type analytically. According to Turitsyn et al.,$^4$ a change in the dynamical critical exponent is induced in the mean-field Ising model with the use of the TCV type In fact, as seen in §4, the transition probability of the TCV type provides the largest reduction of the relaxation time. This may be explained in the dynamical trajectory shown in Fig. 8. The asymptotic slope, which is not derived analytically, is almost vertical, quite far from the horizontal axis in the case with DBC. Therefore, further theoretical studies for the MCMC methods without DBC are of prime importance to clarify the mechanism which induces the change of dynamics.

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