Simulated Tempering and Magnetizing Simulations of the Ising Model

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Abstract

We carried out two-dimensional simulated tempering (ST) simulations of the two-dimensional Ising model with several lattice sizes. We aim to investigate the applicability of the two-dimensional ST to systems with phase transitions, and to study crossover of critical scaling behaviors. In the two-dimensional ST simulations, not only temperature but also external field is treated as a dynamical variable. Thus, this method can be referred to as "Simulated Tempering and Magnetizing (STM)." As has been discussed by previous studies, the ST method is not always compatible with first-order phase transitions. This is also true in the magnetizing process. Processes of flipping the total magnetization hardly occurred during the simulations under T_c in large lattice-size simulations. However, the phase changed through the high temperature region. Therefore, the dimensional extension let us avoid the difficulty of the first-order phase transitions and study a wide area of the phase diagram. We finally study the crossover behavior of the phase transitions with respect to the temperature and external field. The crossover behavior was clearly observed in the simulations in the agreement with the theoretical implications.

Keywords: Monte Carlo simulation, generalized ensemble, Simulated Tempering (ST), Simulated Tempering and Magnetizing (STM), Ising Model, critical phenomenon, crossover
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1. Introduction

Monte Carlo (MC) and molecular dynamics (MD) simulations have been intensively used in statistical physics field. However, the quasi-ergodicity problem, where simulations tend to get trapped in the states of local minima, has often posed a difficulty. To overcome the difficulty, generalized-ensemble algorithms (for reviews see, e.g., Refs. [1, 2]) such as multicanonical algorithm (MUCA) [3, 4], replica-exchange method (REM) [5], and simulated tempering (ST) method [6, 7] have been proposed and applied.

In the ST method, temperature becomes a dynamical variable updated by Metropolis criteria, and consequently a random walk is realized in the temperature space. This random walk, in turn, causes a random walk of the energy, which enables the system to overcome free-energy barriers. However, it is well-known that the ST method is not very efficient when first-order phase transitions are involved (for a review, see e.g., Ref. [8]). Recently, the multi-dimensional generalizations of the generalized-ensemble algorithms, including MUCA, ST, and REM, have been discussed and general formalisms were given [9, 10, 11].

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In this work, we study a two-dimensional version of the generalized ST method. A term $-hM$ is added to the energy term, where h and M are the external field and magnetization, respectively. Not only temperature T but also external field h is updated by the Metropolis criteria. Thus, this simulation can be referred to as the "Simulated Tempering and Magnetizing" (STM). We study the STM's compatibility with phase transitions and investigate the crossover behavior of critical exponents.

This article is organized as follows. In §2 we present the methods. In §3 we present the results. In §4 we conclude this article.

2. Materials and Methods

2.1. System

We study the two-dimensional Ising model. The total energy H is given by $H = E - hM$, where

$$E = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j \,, \tag{1}$$

$$M = \sum_i^N \sigma_i \,. \tag{2}$$

Here, i, N, σ_i, and h are the index of spin, total number of spins, spin at the i-th site, and external field, respectively. The spin σ_i takes on the values ± 1. Here, we set the Boltzmann constant to the unity. The sum in Eq. (1) goes over the nearest neighbor pairs. The spins are arranged on the square $L \times L$ lattice. We employed the periodic boundary conditions. Data were obtained for lattice sizes of 20×20, 80×80, and 160×160.

2.2. Simulation methods

As for spin-updates, we used the single spin update algorithm. We utilized the Mersenne Twister [12] as a random-number generator.

As a simulation method we employed the two-dimensional ST method. Whereas the conventional ST method considers the temperature as a dynamical variable, the two-dimensional ST method considers that not only temperature but also another parameter is a dynamical variable [9, 10, 11]. In this study, the external field h is the second dynamical variable. In other words, we consider the Boltzmann factor $e^{-(E-hM)/T+a(T,h)}$ as a joint probability distribution of the spin configuration, temperature T ($\in \{T_1, T_2, \ldots, T_{N_T}\}$), and external field h ($\in \{h_1, h_2, \ldots, h_{N_h}\}$), where $a(T,h)$ is a parameter.

To find the candidate for $a(T,h)$, we look into the probability of staying in each parameter value (T_i, h_j). It is given by

$$P(T_i, h_j) \propto e^{-f(T_i,h_j)+a(T_i,h_j)} \,,$$

where $e^{-f(T_i,h_j)} = \int dx e^{-(E-h_jM)/T_i}$. The dimensionless free energy $f(T_i, h_j)$ is a good choice for $a(T_i, h_j)$ to acquire the uniform distribution of T and h. Although these values are not generally known *a priori*, they can be estimated with preliminary runs and reweighting methods (the details are provided below).

Any thermal average $\langle A \rangle_{T_i,h_j}$ at given $T_i (\in \{T_1, T_2, \ldots, T_{N_T}\})$ and $h_j (\in \{h_1, h_2, \ldots, h_{N_h}\})$ can be obtained by calculating the conditional expectation: $\langle A \rangle_{T_i,h_j} = \left\langle A | T_i, h_j \right\rangle_{ST}$.

The Metropolis criterion for updating T or h is given by the following transition probability:

$$w(T_i, h_j \rightarrow T_{i'}, h_{j'}) = \min\left(1, \frac{P(T_{i'}, h_{j'})}{P(T_i, h_j)}\right)$$

$$= \min\left(1, \exp\left(-\left(\frac{1}{T_{i'}} - \frac{1}{T_i}\right)E + \left(\frac{h_{j'}}{T_{i'}} - \frac{h_j}{T_i}\right)M + a(T_{i'}, h_{j'}) - a(T_i, h_j)\right)\right). \tag{3}$$

Once an initial state is given, the ST simulations can be performed by repeating the following two steps. 1. We perform a canonical simulation at T_i and h_j for a fixed number of MC sweeps. 2. We update the temperature or external field by Eq. (3) with $a(T, h) = f(T, h)$.

In our implementation, every certain MC sweeps either h or T was updated by Eq. (3) to a neighboring condition chosen at random. Because the external field as well as temperature changes during the simulation, this simulation can be called "Simulated Tempering and Magnetizing" (STM).

2.3. Free energy calculations

We employed two reweighting methods for free energy calculations. One method is the multiple histogram reweighting method (or WHAM) [13, 14] and the other is MBAR [15], which is based on WHAM. Repeating preliminary simulations and free energy calculations, we finally obtained sufficiently accurate free energy values which let the temperature and external field realize random walks during the STM simulations. We then performed the final long STM production run.

The equations of WHAM algorithm that were applied to the system are as follows. For more details, the reader is referred to Refs. [14, 10]. The density of states (DOS) $n(E, M)$ and free energy values $f(T_i, h_j)$ are given by

$$n(E, M) = \frac{\displaystyle\sum_{T_i, h_j} n_{T_i, h_j}(E, M)}{\displaystyle\sum_{T_i, h_j} N_{T_i, h_j} \exp(f(T_i, h_j) - (E - h_j M)/T_i)}, \tag{4}$$

$$f(T_i, h_j) = -\log \sum_{E, M} n(E, M) \exp(-(E - h_j M)/T_i), \tag{5}$$

where $n_{T_i, h_j}(E, M)$ and N_{T_i, h_j} are the histogram of E and M and the number of samples at T_i and h_j, respectively. By solving these two equations self-consistently by iterations, we can obtain $n(E, M)$ and $f(T_i, h_j)$. The obtained $n(E, M)$ allows one to calculate any thermal average at any arbitrary temperature and external field.

The MBAR also enables us to estimate the free energy, but without making histograms or calculating the DOS. For details, the reader is referred to Ref. [15]. Even without DOS, this method also enables one to calculate any thermal average at any arbitrary temperature and external field.

3. Results and Discussion

The STM simulations were carried out properly, because the temperature and external field realized random walk (data not shown). Random walks from the region with $h < 0$ and $T < T_c$ to the region with $h > 0$ and $T < T_c$ were realized through high temperature regions, in which way the simulations went across the first-order phase transition line.

Figure 1 shows the Binder cumulant [16] as a function of temperature, which is defined by

$$U(T, h, L) \equiv \frac{1}{2} \left(3 - \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2} \right). \tag{6}$$

As is well-known, the graphs cross at T_c. The error bars were obtained by the jackknife method [17]. Figure 2 shows the Binder cumulant as a function of temperature under different external fields. The graphs do not cross at one point with finite external field. The amount of error is expected to be on the same level of Figure 1 and the error bars are omitted here for clarity.

We also study the crossover behaviors of the phase transitions. We calculated the magnetization by MBAR around the critical point. We employed the finite-size scaling approach, which is also discussed in Ref. [18]. The scaling form of magnetization per spin m ($\equiv M/L^2$) with respect to the temperature and external field is given by

$$m L^{\beta/\nu} = \Psi(L^{1/\nu} t, L^{(\gamma+\beta)/\nu} h), \tag{7}$$

where $t = |T - T_c|/T_c$ and L is the linear size of lattice. ν and γ are critical exponents. In the two-dimensional Ising model, $\beta = 1/8$, $\delta = 15$, $\nu = 1$, and $\gamma = 7/4$.
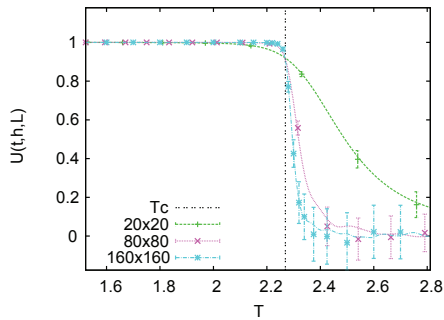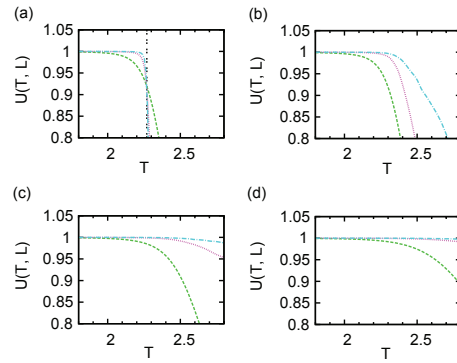
Figure 1: Binder cumulant U versus temperature.

Figure 2: Binder cumulant U versus temperature under different external fields. (a) $h = 0$. (b) $h = 0.01$. (c) $h = 0.05$. (d) $h = 0.1$. The dotted green curve, solid red curve, and dashed blue curve stand for the results for $L = 20$, 80, and 160, respectively.
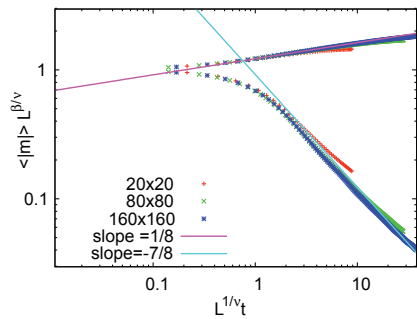

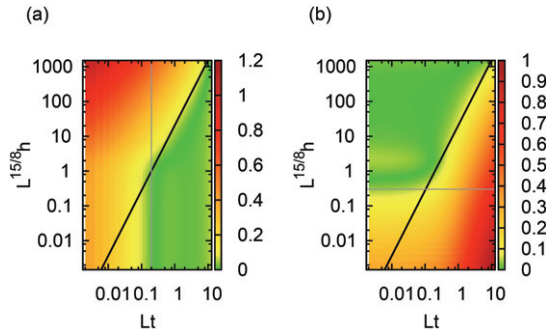Figure 3: Scaled m when $h = 0$. The straight lines are the same as those used in Ref. [18].

Figure 4: Difference between magnetization and expected phenomena about the critical point. The linear lattice size L was 80. (a) $|\langle|m|\rangle - 1.22t^{1/8}|L^{1/8}$ is illustrated. The black line is $t = 0.2h^{8/15}$. The vertical gray line is $Lt = 0.2$. (b) $|\langle|m|\rangle - h^{1/15}|L^{1/8}$ is illustrated The black line is $t = 0.2h^{8/15}$. The horizontal gray line is $L^{15/8}h = 0.3$

Figure 3 shows the magnetization, and we see that it obeys the critical behavior of $m \sim |T - T_c|^\beta$. According to the scaling approach, when Lt is large enough, then the finite effect can be negligible. In this case, Fig. 3 implies that this condition is given by $Lt > 0.2$.

Figures 4(a) and 4(b) show the difference between $\langle|m|\rangle L^{1/8}$ and $1.22(Lt)^{1/8}$ and that between $\langle|m|\rangle L^{1/8}$ and $(L^{15/8}h)^{1/15}$, respectively. These data were obtained by the 80×80 lattice size simulation. According to the crossover scaling formalism [19], if $t^{-15/8}h$ is large enough, then the magnetization critical phenomena obeys $m \sim t^{1/8}$, and if $h^{-8/15}t$ is large enough ($t^{-15/8}h$ is small enough), then it obeys $m \sim h^{1/15}$. Figure 4(a) shows that if the finite-size effects are negligible ($Lt \gg 0.2$) and $t \gg 0.2h^{8/15}$ (i.e., $th^{-8/15}$ is large), then the critical behavior is $m \sim t^{1/8}$. Figure 4(b) shows that when finite-size effects were negligible ($L^{15/8}h \gg 0.3$) and $t \ll 0.2h^{8/15}$ (i.e., $t^{-15/8}h$ is large), then the critical behavior is $m \sim h^{1/15}$. Thus, Fig. 4 clearly shows that the line ($t = 0.2h^{8/15}$) gives the boarder of the two scaling behaviors.

4. Conclusions

In this work, we performed two-dimensional simulated termpring simulations of two-dimensional Ising model. In the simulation, not only temperature but also external field becomes a dynamical variable. Thus, we refer to the method as simulated tempering and magnetizing (STM).

Even though the first-order phase transitions along the external field change did not directly occur, the transitions happened through high temperature regions. Thus, the method realized the two-dimensional random walk in the temperature and external field space and enabled us to study a wide area of phase diagram. These results suggest that the dimensional extension allows one to overcome the first-order phase transitions with the ST methods. The similarity between ST and REM implies that the dimensional extension of REM also gives this kind of behaviors.

We also investigated the crossover behavior of phase transitions. The simulation results showed agreement with the previous theoretical studies. Thus, this supports the validity of STM.

We can calculate the two-dimensional density of state $n(E, M)$. Therefore, we can also perform the two-dimensional multicanonical simulations. This will be our future work. This STM method will be very useful in studying spinglass systems, and work is also in progress. We also remark that the presented methods should be useful not only for spin systems but also for complex systems.

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