Nonequilibrium dynamic-correlation-length scaling method

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The finite-size scaling method in the equilibrium Monte Carlo (MC) simulations and the finite-time scaling method in the nonequilibrium relaxation simulations are compromised. MC time data of various physical quantities are scaled by the MC time data of the dynamic correlation length, which corresponds to changing the system size in the finite-size scaling method. This scaling method is tested in the three-dimensional ferromagnetic Ising spin model and in the three dimensional ±J Ising spin-glass model. The transition temperature and the critical exponents, \( \eta \) and \( \nu \), are obtained by the nonequilibrium relaxation data of the susceptibility and the dynamic correlation length apart from the dynamic exponent. We also comment on the definition of the dynamic correlation length in the nonequilibrium relaxation process. The Ornstein-Zernike formula is not always appropriate.

I. INTRODUCTION

A Monte Carlo (MC) simulation and the finite-size-scaling analysis are very important tools in the study of phase transitions. The applications serve as a strong bridge between the experimental and the theoretical physics. Using this method, we may estimate various physical parameters, predict unknown properties, and propose new experiments on real materials. One of successful applications may be the study on the phase transition. We perform the finite-size-scaling analysis on the numerical data obtained by the MC simulations. Then, the critical temperature and the critical exponents are estimated.

The nonequilibrium relaxation method is an alternate version of the MC simulation that studies the phase transitions. The method directly deals with the MC relaxation functions of physical quantities. In this scheme, time and size are related by the dynamic scaling relation: \( \tau \sim \xi^z \), which connects the correlation time \( \tau \) and the correlation length \( \xi \) via the dynamic exponent \( z \). In the standard equilibrium simulations, we take the infinite-time (equilibrium) limit first. Then, infinite-size limit is taken by the finite-size-scaling analysis. This procedure is reversed in the nonequilibrium relaxation method. We take the infinite-size limit first by preparing a very large system and stopping the simulation before the finite-size effects appear. Then, infinite-time (equilibrium) limit is taken by the finite-time-scaling analysis. The critical temperature and the critical exponents are estimated in the same manner as the standard finite-size-scaling analysis.

An advantage of the nonequilibrium relaxation method is a computational efficiency. We use the nonequilibrium MC data that are usually discarded in the equilibrium simulations. It is very important particularly when the computational resources at hand are limited.

One shortcoming in the nonequilibrium-relaxation method is an ambiguity of the dynamic exponent, \( z \). We obtain the transition temperature and the critical exponent, \( \gamma \), by the finite-time-scaling analysis on the susceptibility. However, the exponent \( \nu \) is not solely obtained but it appears as a form \( z \nu \). We need to estimate \( z \) independently in order to obtain \( \nu \). The dynamic exponent takes a large value in the frustrated and/or random systems. It sometimes depends on the temperature in spin-glass models. The numerical estimate of \( z \) is a tough task in these simulations.

In this paper, we introduce another scaling method based on the nonequilibrium relaxation scheme. The method is free from the estimate of \( z \). We focus on the nonequilibrium relaxation function of the correlation length, which is called the dynamic correlation length. It serves as the system size in the finite-size-scaling analysis. The nonequilibrium relaxation functions of various physical quantities are scaled by the dynamic correlation length. We obtain the transition temperature and the critical exponents by this scaling analysis in the same manner as the finite-size scaling. We just replace the system size \( L \) of the finite-size scaling analysis with the dynamic correlation length \( \xi(t) \), where \( t \) is the MC time step. We also propose a definition of the dynamic correlation length. The Ornstein-Zernike formula is often used to define this value. We show that this definition is not always appropriate particularly in the nonequilibrium relaxation regime.

Section II explains models and a definition of the dynamic correlation length. Section III explains the scaling procedure. Numerical results are presented in Sec. IV. The ferromagnetic Ising model and the ±J Ising spin-glass model are taken as examples. Section V is devoted to the summary and discussions.

II. MODEL AND DEFINITION OF THE DYNAMIC CORRELATION LENGTH

Let us consider the following spin model to demonstrate the present scaling method.

\[
\mathcal{H} = - \sum_{(i,j)} J_{ij} S_i S_j,
\]

where \( \langle i, j \rangle \) denotes the nearest-neighbor pairs in the cubic lattice, \( J_{ij} \) denotes the exchange interaction, and \( S_i \)
denote the Ising spin. We consider the uniform ferromagnetic model \((J_{ij} = 1)\) and the spin-glass model \((J_{ij} = \pm J\) with an equal probability) in this paper.

The correlation length of an ordered domain in spin models is usually defined by the correlation function \(C(r) = \langle S_i S_{i+r} \rangle\) as

\[
C(r) = \langle S_i S_{i+r} \rangle \propto \exp[-r/\xi]
\]

in the equilibrium state near the transition temperature. In the Monte Carlo simulations, it is easier to estimate the correlation length by the Fourier transform of the susceptibility, \(\chi(k)\), as

\[
\xi = \frac{1}{k_{\text{min}}} \sqrt{\frac{\chi(0)}{\chi(k_{\text{min}})}} - 1, \quad k_{\text{min}} = \frac{2\pi}{L} \left( \begin{array}{c} 1 \\ 0 \\ 0 \end{array} \right). \tag{1}
\]

Here, \(k_{\text{min}}\) denotes the smallest wave vector along one direction in a finite-size lattice. The expression is exact in the limit of \(k_{\text{min}} \to 0\).

The \(1/r\)-correction form in the spin correlation function is only guaranteed by the mean-field theory in the equilibrium state.\(^{14}\) It is not trivial that we may use Eq. (1) in the nonequilibrium relaxation process. The system size \(L\) is much larger than the correlation length in the nonequilibrium process. In such a case, the spin correlation function may decay in a simple exponential form without the \(1/r\)-correction. In order to check the \(r\)-dependence, we plot the correlation functions, \(C(r)\) and \(rC(r)\), against \(r\) in the nonequilibrium regime \((t=501)\) and in the equilibrium regime \((t=3981)\). The system is the uniform ferromagnetic model with \(J_{ij} = 1\), the system size \(L = 299\), and the temperature \(T = 4.515\), which is above the transition temperature, \(T_c = 4.511525^{10}\) \(\text{K}\). Figure 1 shows the result. The linearity of \(rC(r)\) is better than that of \(C(r)\) when \(t = 3981\). The \(1/r\)-correction is necessary in estimating the correlation length in the equilibrium state. On the other hand, the linearity is poor and convex upward when \(t = 501\). The linearity of \(C(r)\) seems to be better. If the correlation function exhibits the simple exponential decay as

\[
C(r) = \langle S_i S_{i+r} \rangle \propto \exp[-r/\xi],
\]

the correlation length should be estimated by

\[
\xi = \frac{1}{k_{\text{min}}} \sqrt{\frac{\chi(0)}{\chi(k_{\text{min}})}} - 1. \tag{2}
\]

It is difficult to judge a use of Eq. (1) or Eq. (2) just by the linearity of \(C(r)\) or \(rC(r)\). The difference is small as shown in Fig. 1. Therefore, we compare the time dependences of the dynamic correlation length estimated by both definitions. We judge two definitions by the scaling behavior.

Figures 2 and 3 compare the estimates of \(\xi(t)\) using both definitions, Eqs. (1) and (2). The dynamic correlation length of the size-\(L\) system, \(\xi(t, L)\) divided by the linear scale \(L\) is plotted against \(t^{1/z}/L\). We expect that \(\xi(t, L) \propto t^{1/z}/L\) from the dynamic scaling relation. The correlation length divided by \(L\) becomes scale invariant at the transition temperature. Therefore, the present plot should ride on the single line with its slope unity, if we choose a correct value of \(z\) that satisfies the dynamic scaling relation.

In the uniform ferromagnetic Ising model (Fig. 2), the dynamic correlation length estimated by Eq. (2) yields a good scaling and the slope unity. The dynamic exponent \(z = 2.05\) is taken from the Ref.16.
The finite-size effects appear as the system approaches the equilibrium state. The dynamic correlation length given by Eq. (1) is well-scaled but the slope does not agree with unity. If we choose $z$ so that it yields the slope unity, the relaxation data of different sizes do not ride on the same line. The slope suggests that $\xi(t, L)/L \propto t^{1/2}/L$, but the scaling fails if we take $z = 2.05/1.13 = 1.81$ for $t^{1/2}/L$. Therefore, the dynamic scaling relation contradicts itself even in the ferromagnetic model. It is an evidence that a use of the Ornstein-Zernike expression, Eq. (1), is not appropriate in the nonequilibrium relaxation scheme.

Figure 3 shows the same $\xi(t, L)/L$ scaling in the $\pm J$ Ising spin-glass model in three dimensions. Relaxation data at three temperatures are plotted in the same figure by shifting arbitrary in the vertical direction. The temperatures are above ($T = 1.40$), near ($T = 1.18$), and below ($T = 1.10$) the transition temperature. The dynamic exponent at each temperature is estimated so that the dynamic correlation length are well-scaled at each temperature.

The first two steps below are the standard procedure of the nonequilibrium relaxation method. The relaxation functions of the physical quantity and the correlation length are obtained.

1. We prepare a system with a linear scale $L$, and perform a MC simulation at the temperature $T$. We start the simulation from the paramagnetic state. The data free from the finite-size effects are denoted by $A(T, L, T$). Changing a random number sequence, we perform independent simulations and take an average of $A(T, L, T)$ over these runs.

2. We change the system size and perform simulations. Relaxation functions $A(t, L, T)$ of different sizes are compared to check the finite-size effects. Only data that are free from the finite-size effects are used in the scaling analysis. Examples are Figs. 2 and 7 in Sec. IV. The data free from the size effects are denoted by $A(t, T)$. We obtain a relaxation function of the dynamic correlation length, $\xi(t, T)$, as explained in Sec. II.

We will perform three scaling analyses below. The first scaling analysis determines the dynamic exponent, $z$. Then, the second one determines the anomalous exponent $\eta$, and the last scaling analysis determines the critical temperature, $T_c$, and the exponent $\nu$. It is noted that the first scaling analysis is not necessary and is independent from the other two scaling analyses. It should be done only when we need a value of $z$. This is a clear difference from (and is probably an advantage over) the standard nonequilibrium relaxation method with the finite-time-scaling analysis.

3. The relaxation function of the dynamic correlation length should satisfy the dynamic scaling relation: $\xi(t, T) \sim t^{1/2}$. At the temperature near the critical temperature, We plot $\xi(t, L)/L$ versus $t^{1/2}/L$ so that all the scaled data fall on a single scaling function. This scaling is possible because $\xi/L$ is scale-invariant at the critical temperature. Only a value of $z$ is a control parameter. Examples are Figs. 2 and 3.

Let us take the magnetic susceptibility, $\chi$, as a physical quantity for simplicity.

4. Using the relaxation function of $\chi(t, T)$ and $\xi(t, T)$, we perform the scaling analysis. Since the simulation starts from the paramagnetic state, both $\chi$ and $\xi$
and $\xi$ are expected to increase algebraically in time as $\chi(t, T) \sim \xi(t, T)^{2-\eta}$ when $T$ is near $T_c$. Since $\chi \propto \xi^{2-\eta}$ in the critical region, we expect that the nonequilibrium relaxation functions of $\chi(t, L)$ and $\xi(t, L)$ depend on $L$ as
\[
\frac{\chi(t, L)}{L^{2-\eta}} \propto \left(\frac{\xi(t, L)}{L}\right)^{2-\eta}.
\]
(3)

We plot $\chi(t, L)/L^{2-\eta}$ against $\xi(t, L)/L$ in a log-log scale and determine $\eta$ so that all the relaxation functions falls on the same line with a slope $2-\eta$. Examples are Figs. 5 and 8 in Sec. IV. It is a one-parameter scaling analysis. The determination of $\eta$ is easily done first by this scaling plot. Here, it is not necessary to know the critical temperature precisely. We only need the rough estimate. Since we work with the nonequilibrium relaxation method, the critical relaxation is observed near the critical temperature in the nonequilibrium process. It is sufficient to perform this scaling analysis at one temperature near $T_c$.

5. The critical temperature, $T_c$, and the critical exponent, $\nu$, are determined in the last scaling analysis. The equilibrium value of the correlation length diverges as $\xi \sim |T - T_c|^{-\nu}$. At the same time the susceptibility $\chi(t, T)$ should be scaled by $\xi(t, T)^{2-\eta}$ with $\eta$ estimated above. Therefore, we plot the relaxation functions $\chi(t, T)/\xi(t, T)^{2-\eta}$ versus $\xi(t, T)/(T - T_c)^{-\nu}$ for various temperatures and determine $T_c$ and $\nu$ so that all the data ride on a single scaling function. Examples are Figs. 6 and 9. in Sec. IV.

It is noted that the finite size $L$ in the finite-size-scaling analysis is replaced by the dynamic correlation length $\xi(t, T)$ in the present analysis. We consider that the present scaling analysis is a natural extension from the finite-size-scaling analysis when we work within the nonequilibrium relaxation scheme.

IV. NUMERICAL RESULTS

A. Ferromagnetic model

We present the numerical results in the ferromagnetic Ising model in three dimension. Figure 4 shows the raw relaxation data of the dynamic correlation length, $\xi(t, L)$, and the magnetic susceptibility, $\chi(t, L)$ in the ferromagnetic model. The temperature, $T = 4.512$, is a little above the transition temperature.

FIG. 4: (Color online) Size dependences of raw relaxation data of the dynamic correlation length, $\xi(t, L)$, and the magnetic susceptibility, $\chi(t, L)$ in the ferromagnetic model. The temperature, $T = 4.512$, is a little above the transition temperature.

B. Spin-glass model

In this subsection, we present the numerical results of the $\pm J$ Ising spin-glass model in three dimensions. The spin-glass correlation length is estimated from the Fourier transform of the spin-glass susceptibility, $\chi_{sg}$. It is defined by
\[
\chi_{sg} = \frac{1}{N} \sum_{i,j} \langle S_i S_j \rangle^2,
\]
where the bracket $\langle \cdots \rangle_c$ denotes the configurational average, and the bracket $\langle \cdots \rangle$ denotes the thermal average.
The thermal average is estimated by the average over different real replicas:

$$\langle S_i S_j \rangle = \frac{1}{m} \sum_{A=1}^{m} S_i^{(A)} S_j^{(A)}.$$ 

A replica number is denoted by \(m\), and the superscript \(A\) denotes a replica index. We prepare \(m\) real replicas for each random bond realization with different initial spin configurations. Spin states of each replica are updated using different random number sequences. The thermal average is taken only by this replica average in our nonequilibrium relaxation scheme. A replica number controls an accuracy of the thermal average. It is set to 256 in this paper. The dynamic spin-glass correlation length in this paper is estimated by Eq. (2), where \(\chi\) is replaced by \(\chi_{sg}\). It is usually defined by Eq. (1) \(17,18\).

Figure 6 shows the raw relaxation functions of the spin-glass susceptibility and the dynamic spin-glass correlation length. Figure 5 shows the scaling plot determining a value of \(\eta\). The straight-line scaling is possible near and above the transition temperature. The scaling poor in the low-temperature phase. Using the estimated value of \(2 - \eta\) we plot the dynamic correlation-length scaling results in Fig. 8. The scaling is good when the temperature is above the estimated spin-glass transition temperature, \(T_{sg} = 1.18\). The scaling behavior becomes poor below \(T_{sg}\). The estimated critical exponents may be invalid in the low-temperature phase.

The previous estimates\(18,22\) for \(T_{sg}\) lie between 1.1 and 1.2. They are roughly categorized into two groups. Our\(18,21\) gives \(T_{sg}\) close to 1.1 and \(\nu\) close to 2. The other\(19,20,22\) gives \(T_{sg}\) close to 1.2 and \(\nu\) close to 1.3. The present result is consistent with the latter group. The latter group mostly takes the dynamic approach to the phase transition. Recently, Hukushima and Campbell\(23\) discussed that this discrepancy can be understood by the strong corrections to scaling.

Campbell et al\(24\) proposed the \(\beta\)-scaling analysis,
which uses \((\beta^2 - \beta_s^2)\) as the scaling variable. They estimated the transition temperature and the critical exponents as \(T_c = 1.11, \nu = 2.72, \) and \(2 - \eta = 2.40(4)\). We also try this \(\beta\)-scaling analysis in Fig. 10. Our estimates are \(T_c = 1.11, \nu = 2.62, \) and \(2 - \eta = 2.35, \) which are consistent with their estimates but disagree with our present estimates using \((T - T_c)\). This discrepancy suggests that the present numerical simulation is not sufficient to extract the true critical phenomena both in a size scale and a time scale in the spin-glass model. We checked that the \(\beta\)-scaling is possible using the same transition temperature and critical exponents in the ferromagnetic model. (Figures are not shown.) The present size and time scales are sufficient in the ferromagnetic model.

\section*{V. SUMMARY AND DISCUSSION}

The dynamic correlation-length-scaling method is introduced. The basic idea of this method is that we investigate the phase transition through the correlation length. It is found that the scaling relations among physical quantities hold even in the nonequilibrium relaxation process. We can use finite-time and finite-size data in the scaling analysis. The examples are Figs. 5 and 8. Although the raw relaxation data (Figs. 4 and 7) exhibit the finite-size effects, we can scale them to one scaling line without the size effects. The critical divergence is observed from very early stage of the nonequilibrium relaxation process, if we scale the data by the dynamic correlation length.

The present dynamic-correlation-length-scaling analysis is regarded as an extension of the finite-size-scaling analysis replacing the size \(L\) with the dynamic correlation length \(\xi(t)\). We may consider that the finite-time relaxation data at a time \(t\) corresponds to the equilibrium data of the size \(L\) with \(L = \xi(t)\).

Since the present scaling method is entirely based on the dynamic correlation length, the definition is very important. We found that a use of the definition based on the Ornstein-Zernike formula is not appropriate in our scheme. Since the formula is based on the mean-field approximation, the present nonequilibrium process may be out of the applicable range of the approximation. The relaxation function of the dynamic correlation length estimated by Eq. (1) exhibits an extra increase before reaching an equilibrium value, as shown in Figs 2 and 3. The logarithmic slope, which is \(1/\xi\), is then overestimated. It affects a value of \(\nu\) in the conventional finite-time-scaling analysis of the nonequilibrium relaxation method. The introduced definition, Eq. (2), is based on a simple exponential decay of the correlation function. The relaxation function exhibits a normal behavior. It algebraically increases with \(t^{1/\xi}\), and eventually converges to a finite-size value. We also comment that the definition Eq. (2) may be used even in the equilibrium state where the mean-field approximation is not valid.

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