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Statistical Dependence Time and Its Application to Dynamical Critical Exponent

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A new method for studying dynamical correlation of temporal sequence is proposed. We introduce a new quantity named *statistical dependence time* $\tau_{\rm dep}$ as an estimator for the equilibrium relaxation time. The calculation of $\tau_{\rm dep}$ does not require calculation of any time-displaced correlation function nor numerical fitting in extracting the relaxation time; as a result, the estimation of $\tau_{\rm dep}$ and statistical analysis such as the error estimation are quite straightforward and simple. We apply this method to the critical dynamics of 3D Ising model, and estimate the dynamical critical exponent z as 2.030 ± 0.004, provided $K_c=0.221654$ (if possible error in K_c is taken into account, the error in z becomes 0.01).

§1. Introduction

A number of attempts have been made so far to extract dynamical properties of model systems in equilibrium by dynamical simulations, such as Monte Carlo methods. Time-displaced correlation functions are often used for this purpose; from their asymptotic behaviors one can estimate the equilibrium relaxation time τ, which is the characteristic time scale of the dynamics. Although such an approach is simple and straightforward in concept, it involves some difficulties when applied to actual simulations: First, for precise estimation of τ, acculate knowledge on the correlation functions up to large time displacement is required. Their estimation is often CPU time and memory consuming. Second, statistical analyses becomes complicated and ambiguous, because the data for different time are usually not independent of each other; in fact, if all data of a time-displaced correlation function are simply regarded as independent, the resulting statistical error of τ will be systematically underestimated. Moreover, one has to determine which data are within the asymptotic region and which ones are out of it more or less arbitrarily. These points are in contrast with the case of static properties, where one can easily use mutually independent data set in statistical analyses.

Calculation of the dynamical critical exponent z of spin models is one of the important subjects in dynamical problems. Even for very fundamental systems such as the three-dimensional (3D) Ising model, the value of z still remains controversial, in spite of long history of efforts. In fact, the values of z for this model estimated using time-displaced correlation functions spread within the range $1.99\leq z\leq2.17$.[1-5] Especially, two recent studies based on large-scale Monte Carlo simulations reported mutually incompatible values: 2.04 ± 0.03 by Wansleben and Landau,[4] and 2.10 ± 0.02 by Heuer.[5] Remarkably, the both studies used basically the same procedure: the equilibrium relaxation time τ for the longest relaxation mode was estimated from the time-displaced correlation function of the magnetization, and z was then calculated from τ applying the dynamical finite-size scaling theory.[6] The largest difference between these two studies lies in how the longest relaxation mode was extracted. However, because of complicated statistical analyses used in these studies, it is not easy to find the true origin of this descrepancy.

Another category of methods for estimating z includes ones in which information from the non-equilibrium relaxation is used.[7-10] An advantage of these methods is that calculation of time-displaced correlation functions is unnecessary in them. Dynamical Monte Carlo renormalization-group methods are also within this category.[11,12] Quite recently, one of the authors (N. I.) reported an quite accurate estimate for a combination of critical exponents $\beta/z\nu$ of the 3D Ising model using the non-equilibrium relaxation, where β and ν are the static critical exponents of the magnetization and the correlation length, respectively.[10] An estimate of z in comparable accuracy from equilibrium relaxation is highly expected now.

In the present paper, we propose a new method based on a new quantity named *statistical dependence time* for calculating the equilibrium relaxation time τ and the integrated correlation time $\tau_{\rm int}$ by means of Monte Carlo simulations. This method is quite simple in operation; it no longer requires calculation of time-displaced correlation functions; only the equilibrium (static) averages are used instead. Consequently, it enables us to make statistical analyses in an unambiguous manner, as can be done for static quantities. As the first application of the method, we apply it to the critical dynamics of the 3D Ising model, and thereby estimate z.

The basic idea of the statistical dependence time is the following: When n estimates of a quantity from a dynamical simulation are statistically independent, the variance of the average of these n estimates will be $1/\sqrt{n}$ times the variance of the original quantity. If these n estimates are not completely independent as is often the case with dynamic simulations, the above factor $1/\sqrt{n}$ will be enhanced due to the temporal correlation. Hence, one can expect that the ratio of the two variances, one for the n-averaged quantity and one for the original quantity, is related to the correlation time. In the present paper, we elucidate this possibility and show that the correlation time can be indeed estimated from this ratio.

The paper is organized as follows: In the next section, we describe a new method for calculating the equilibrium relaxation time. A new quantity *statistical dependence time* is introduced there. In §3, we apply the method to an off-critical case, where the relaxation is well described by a single relaxation time. Calculation of z of the 3D Ising model is given in §4. The last section is devoted to the summary and the discussions.

§2. Statistical Dependence Time

Let us consider a situation where N independent simulations of the same system are made under the same external parameters (temperature, external field and so on), with each run consisting of n measurements of a physical quantity m. We assume that the measurements are made at every constant time step; in the following, this interval of successive measurements is used as the unit of time. Let $m_\alpha(k)$ be the value of the quantity m for k-th measurement of α-th run, where $k=1, 2, \cdots, n$ and $\alpha=1, 2, \cdots, N$. We define two kinds of (thermal) averages, namely, (1) average over the measurements in α-th run

$$\langle m\rangle_\alpha \equiv \frac{1}{n}\sum_{k=1}^{n} m_\alpha(k), \tag{2.1}$$

and (2) average of $\langle m\rangle_\alpha$ over all the independent runs

$$\overline{\langle m\rangle} \equiv \frac{1}{N}\sum_{\alpha=1}^{N} \langle m\rangle_\alpha. \tag{2.2}$$

These two averages converge to a common expectation value $\mu\equiv \mathrm{E}\{m\}$ in the limit of $n\to\infty$ or $N\to\infty$, respectively, where $\mathrm{E}\{A\}$ denotes the expectation value of a quantity A.

The expectation value for the variance of $\langle m\rangle$ is

$$\mathrm{E}\{(\langle m\rangle-\mu)^2\} = \frac{1}{n^2}\sum_{k,l=1}^{n} \mathrm{E}\{m(k)m(l)\}-\mu^2. \tag{2.3}$$

Since this expectation value does not depend on α, we omitted the suffix from $\langle m\rangle$. The expectation value $\mathrm{E}\{m(k)m(l)\}$ appearing in the r.h.s. is related to that of the time-displaced correlation function of $(m-\mu)$ as

$$\mathrm{E}\{C(k, l)\} = \mathrm{E}\{m(k)m(l)\}-\mu^2, \tag{2.4}$$

where

$$C(k, l) \equiv \langle (m(k)-\mu)(m(l)-\mu) \rangle \tag{2.5}$$

is the (unnormalized) time-displaced correlation function of the fluctuation in m for "time" k and l.

Let us assume for a moment that the relaxation of this correlation function is described by a single exponential function with the relaxation time τ. Then the correlation function is expressed by

$$\begin{aligned} \mathrm{E}\{C(k, l)\} &= \mathrm{E}\{C(|k-l|)\} \\ &= (\mathrm{E}\{m^2\}-\mu^2)\, \mathrm{e}^{-|k-l|/\tau} \\ &= \sigma^2\, \mathrm{e}^{-|k-l|/\tau}, \end{aligned} \tag{2.6}$$

where σ^2 denotes the variance of m. Thus we get

$$\mathrm{E}\{(\langle m \rangle-\mu)^2\} = \frac{\sigma^2}{n^2} \sum_{k,l=1}^{n} \mathrm{e}^{-|k-l|/\tau}. \tag{2.7}$$

The summation in the last equation can be calculated explicitly:

$$\begin{aligned} \sum_{k,l=1}^{n} \mathrm{e}^{-|k-l|/\tau} &= n + 2\sum_{k>l}^{n} \mathrm{e}^{-(k-l)/\tau} \\ &= n + 2\sum_{k=1}^{n-1} (n-k)\, \mathrm{e}^{-k/\tau} \\ &= n\left[\frac{1+\Lambda}{1-\Lambda} - \frac{2\Lambda(1-\Lambda^n)}{n(1-\Lambda)^2}\right], \end{aligned} \tag{2.8}$$

where $\Lambda \equiv \exp(-1/\tau)$. Now we introduce a new quantity with a dimension of time, named *statistical dependence time* τ_{dep}, defined by

$$\tau_{\mathrm{dep}} \equiv \frac{1}{2}\left[\frac{1+\Lambda}{1-\Lambda} - \frac{2\Lambda(1-\Lambda^n)}{n(1-\Lambda)^2}\right]. \tag{2.9}$$

From eqs. (2.7), (2.8) and (2.9), we get the relationship between the expectation values:

$$\mathrm{E}\{(\langle m \rangle-\mu)^2\} = \frac{2\tau_{\mathrm{dep}}}{n}\sigma^2. \tag{2.10}$$

As can be read intuitively from eq. (2.10), the factor $n/2\tau_{\mathrm{dep}}$ plays a role of the statistical degrees of freedom (DOF); in fact, for statistically independent measurements, $\mathrm{E}\{(\langle m \rangle-\mu)^2\}$ becomes σ^2/n, which agrees with the well-known result with n being the DOF. Equation (2.10), therefore, expresses reduction in the DOF by the factor $1/2\tau_{\mathrm{dep}}$ due to correlations among the successive measurements. In other words, only $n/2\tau_{\mathrm{dep}}$ among n measurements have statistical significance, and $2\tau_{\mathrm{dep}}$ can be interpreted as the mean interval of successive statistically significant measurements. It is worth noting that this reduction factor of DOF depends not only on τ but also on the total number of measurements n. Of course, as it is clear from the derivation of eq. (2.10), the above interpretation of τ_{dep} holds only when τ is larger than, or at least of order of, 1. The factor 2 introduced here in the definition of τ_{dep} is only for convenience.

So far, we have derived the exact relationship between the expectation values, eq. (2.10). Next we will describe how to estimate the corresponding values by actual simulations. The unbiased estimator for l.h.s., $\mathrm{E}\{(\langle m \rangle-\mu)^2\}$, from N independent runs is

$$\begin{aligned} (\delta m)^2 &= \frac{1}{N-1}\sum_{\alpha=1}^{N} (\langle m \rangle_\alpha - \overline{\langle m \rangle})^2 \\ &= \frac{N}{N-1}(\overline{\langle m \rangle^2} - \overline{\langle m \rangle}^2) \end{aligned} \tag{2.11}$$

The quantity $|\delta m|/\sqrt{N}$ is commonly used as the estimator for the statistical error of m. It should be noted that although it has the meaning of the *error*, it is still a well-defined statistical quantity, converging to a definite value for fixed n in the limit $N \to \infty$. On the other hand, the estimator for r.h.s. of eq. (2.10), σ^2, is

$$\chi = \overline{\langle m^2 \rangle} - \overline{\langle m \rangle}^2, \tag{2.12a}$$

or

$$\chi' = \overline{\langle m^2 \rangle - \langle m \rangle^2}. \tag{2.12b}$$

Both expressions are equally valid. Throughout the present paper, we employ χ defined by eq. (2.12a) as the estimator for σ^2. Physically, it has a meaning of the succeptibility associated to m. Combining these equations, we get our final expression for the estimator of τ_{dep}:

$$\tau_{\mathrm{dep}} = \frac{n(\delta m)^2}{2\chi} = \frac{nN}{2(N-1)} \frac{\overline{\langle m \rangle^2} - \overline{\langle m \rangle}^2}{\overline{\langle m^2 \rangle} - \overline{\langle m \rangle}^2} \tag{2.13}$$

The r.h.s. of eq. (2.13) can be calculated by the simulations; once τ_{dep} is thus estimated through eq. (2.13), one can then get τ by solving eq. (2.9).

Taking the large n limit or the continuous-time limit is unnecessary in the above procedure; one can, therefore, estimate τ from arbitrarily short simulations in principle. On the other hand, the value of $\tau_{\rm dep}$ itself can be used as an estimator for τ, if calculated in the large n limit; in fact, expansion of eq. (2.9) in terms of $1/\tau$ gives

$$\lim_{n\to\infty}\tau_{\rm dep}=\frac{1}{2}\left[\frac{1+\Lambda}{1-\Lambda}\right]=\tau\left[1+\frac{1}{12\tau^2}+O\left(\frac{1}{\tau^4}\right)\right]. \tag{2.14}$$

Hence, for large τ, $\tau_{\rm dep}$ coincides with τ in the large n limit.

So far, we have dealed with the single-exponential relaxation, and now we turn to multi-exponential decay. Even for such a complicated situation, we can still show that $\tau_{\rm dep}$ calculated through eq. (2.13) serves as an estimator for, this time, the integrated relaxation time $\tau_{\rm int}$ in the large n limit. The expectation value of the time-displaced correlation function $C(|k-l|)$ is now assumed to be expressed as a sum of many exponential functions:

$$\mathrm{E}\{C(|k-l|)\}=\sigma^2\sum_I a_I\,\mathrm{e}^{-|k-l|/\tau_I}, \tag{2.15}$$

where τ_I denotes the relaxation time of I-th relaxation mode, and a_I is the associated weight, which satisfies the sum rule

$$\sum_I a_I=1. \tag{2.16}$$

For multi-exponential relaxation, it is convenient to treat the integrated relaxation time as a characteristic time scale instead of treating each τ_I separately. The integrated relaxation time is defined as the integral of $C(t)$ from 0 to ∞:

$$\begin{aligned}\tau_{\rm int}&\equiv\frac{1}{\sigma^2}\int_0^\infty \mathrm{E}\{C(t)\}\,\mathrm{d}t\\&=\int_0^\infty\sum_I a_I\,\mathrm{e}^{-t/\tau_I}\\&=\sum_I a_I\tau_I.\end{aligned} \tag{2.17a}$$

Although we have treated the time t as a continuous variable in the above definition, it is actually a discrete one in real simulations. The integral in eq. (2.17a) should then be replaced by an infinite sum, and we get a slightly different definition for the integrated relaxation time:

$$\begin{aligned}\tau'_{\rm int}&\equiv\frac{1}{\sigma^2}\sum_{|k-l|=0}^{\infty}\mathrm{E}\{C(|k-l|)\}\\&=\sum_I\sum_{|k-l|=0}^{\infty}a_I\,\mathrm{e}^{-|k-l|/\tau_I}\\&=\sum_I\frac{a_I}{1-\mathrm{e}^{-1/\tau_I}}.\end{aligned} \tag{2.17b}$$

These two definitions coincide with each other if all the τ_I's, or at least all the principal τ_I's (i.e., τ_I with large weight a_I) are much larger than unity. In other word, the integrated relaxation time has a definite meaning if and only if this condition is satisfied. Now we generalize the statistical dependence time to multi-exponential relaxation. Equations (2.9) and (2.10) now become

$$\mathrm{E}\{(\langle m\rangle-\mu)^2\}=\frac{2\tau_{\rm dep}}{n}\sigma^2$$

and

$$\tau_{\rm dep}\equiv\sum_I\frac{a_I}{2}\left[\frac{1+\lambda_I}{1-\lambda_I}-\frac{2\lambda_I(1-\lambda_I^n)}{n(1-\lambda_I)^2}\right], \tag{2.18}$$

where $\lambda_I=\exp(-1/\tau_I)$. In actual simulations, $\tau_{\rm dep}$ is calculated in the same way as that for the single-exponential relaxation, that is, through eq. (2.13). These three quantities $\tau_{\rm int}$, $\tau'_{\rm int}$, and $\tau_{\rm dep}$ can be used equally as a characteristic time scale in the long-time limit, provided they are much larger than unity; in fact, in this limit we can easily show

$$\lim_{n\to\infty}\tau_{\rm dep}=\tau'_{\rm int}-\frac{1}{2}. \tag{2.19}$$

On the other hand, the relationship between $\tau_{\rm int}$ and $\tau_{\rm dep}$ can be seen most easily under the condition discussed above, i.e., $1/\tau_I\ll 1$: For finite but large n so that $\tau_I/n\ll 1$, λ_I^n vanishes rapidly, and we get

$$\begin{aligned}\tau_{\rm dep}&=\sum_I\frac{a_I}{2}\left[\frac{1+\lambda_I}{1-\lambda_I}-\frac{2\lambda_I}{n(1-\lambda_I)^2}\right]\\&=\tau_{\rm int}\left[1-\frac{\tau_{\rm int}}{n}\sum_I a_I\left(\frac{\tau_I}{\tau_{\rm int}}\right)^2\right.\\&\qquad\left.+\frac{1}{12\tau_{\rm int}}\left(\sum_I\frac{a_I}{\tau_I}+\frac{1}{n}\right)+\cdots\right].\end{aligned} \tag{2.20}$$

Thus, the leading relative differences of $\tau_{\rm int}$,

$\tau'_{\rm int}$, and $\tau_{\rm dep}$ are of $O(1/\tau_{\rm int})$. Consequently, these three time scales are expected to obey the same scaling behavior. In utilizing the above procedure, however, one has to make long enough simulations to ensure the long-time limit. To overcome this difficulty, let us consider to solve eq. (2.9) formally by substituting the above $\tau_{\rm dep}$; the effective relaxation time $\tau_{\rm eff}$ thus obtained is expanded as

$$\tau_{\rm eff}=\tau_{\rm int}\left[1-\left(\frac{\tau_{\rm int}}{n}+2\left(\frac{\tau_{\rm int}}{n}\right)^2\right)\times\sum_I a_I\left(1-\frac{\tau_I}{\tau_{\rm int}}\right)^2+\cdots+\frac{1}{12\tau_{\rm int}^2}\left(\sum_I a_I\left(\frac{\tau_{\rm int}}{\tau_I}-1\right)+\cdots\right)\right]. \quad (2.21)$$

The term $\sum_I a_I(1-\tau_I/\tau_{\rm int})^2$ is the variance of the relaxation spectrum, normalized by $\tau_{\rm int}$. Therefore, if τ_I's contributing mainly to the relaxation process, that is, τ_I's with large weights, spread within much narrower range compared to $\tau_{\rm int}$, then $\tau_{\rm eff}$ can be used as an estimator for $\tau_{\rm int}$ even if $\tau_{\rm int}/n$ is not small.

We make some comments before closing this section. First, the relationship between the susceptibility, the relaxation time, and the statistical error was first discussed by Müller-Krumbhaar and Binder in a different context.[13] However, their expression was derived using the integral approximation of the summation appears in eq. (2.7); as a result, it is valid only in the limit $\tau/n\to 0$ and $1/\tau\to 0$. It is in contrast with eq. (2.8) we have derived above, which is exact for single-exponential relaxations. Berretti and Sokal also discussed the effects of finite correlation time on the statistical errors, again in the large n limit.[14] Second, a systematic error in the susceptibility due to finite number of measurements was discussed by Ferrenberg, Landau, and Binder quite recently.[15] They pointed out that the estimator of the susceptibility commonly used is not an unbiased one; rather, it is biased with a factor $n_{\rm DOF}/(n_{\rm DOF}-1)$, where $n_{\rm DOF}$ stands for the DOF of the measurements. If this bias is taken into account, the r.h.s. of eq. (2.13) should be multiplied by a factor $(n/2\tau_{\rm dep})/(n/2\tau_{\rm dep}-1)$, since the effective DOF is $n/2\tau_{\rm dep}$, as was discussed above. The statistical dependence time thus corrected is:

$$1/\tau_{\rm dep}=\frac{2(N-1)}{Nn}\frac{\overline{\langle m^2\rangle}-\overline{\langle m\rangle}^2}{\overline{\langle m\rangle^2}-\overline{\langle m\rangle}^2}+\frac{2(N-1)}{Nn}. \quad (2.22)$$

The correction term $2(N-1)/Nn$ is smaller than the main term by a factor $2\tau_{\rm dep}/Nn$. In the following sections, we will neglect this correction, since Nn will be taken very large there. But there may be cases where one has to take this term correctly into account. If χ' is used as the estimator of σ^2 instead of χ, this correction term becomes N times larger than that for χ.

§3. A Test of the Method

To test the validity of the method developed in the last section, we performed Monte Carlo simulations for a three-dimensional Ising model at temperature higher than its critical point. We use the simple-cubic lattice consisting of $8\times 8\times 8$ spins, with the periodic boundary conditions imposed on all directions. We employ the Metropolis-type transition probability with two-interpenetrating-sublattice updating, which is commonly used in simulations on vector computers. Figure 1 shows the (unnormalized) time-displaced correlation function of the magnetization at $K\equiv J/T=0.22$. The time t is measured in unit of the Monte Carlo Steps (MCS)/spin. The straight

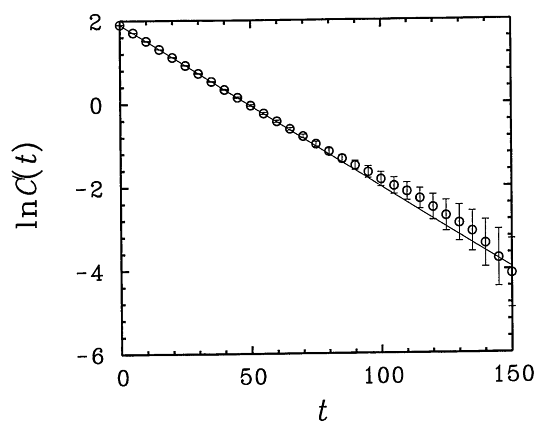

Fig. 1. The unnormalized two-time correlation function of the magnetization for the 3D Ising model on the $8\times 8\times 8$ simple-cubic lattice at $K=0.22$. The straight line represents the single-exponential relaxation of the form $C(t)\sim\exp(-t/\tau)$ with $\tau=25.66$.

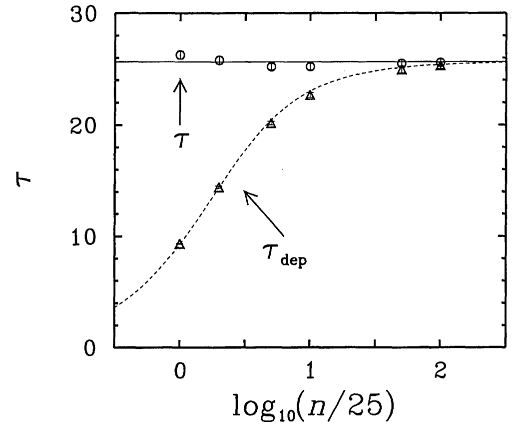

Fig. 2. Dependence of the statistical dependence time $\tau_{\rm dep}$ (○) and the corresponding τ (△) on the length of simulations n for the same system as one treated in Fig. 1. The solid line indicates $\tau=25.66$ and the dotted line expresses the expected n dependence of the corresponding $\tau_{\rm dep}$.

line in the figure represents the single-exponential form of the relaxation, $C(t)\sim\exp(-t/\tau)$, with $\tau=25.66\pm0.07$ obtained by fitting of the data up to $t=100$. We see that the single exponential function describes the relaxation very well. The statistical error of τ is estimated by assuming that all the data points are independent; thus it may be underestimated.

Next we calculated the statistical dependence time $\tau_{\rm dep}$ from the magnetization of the same system. We made 16000 independent runs with 500MCS/spin discarded for each run. Figure 2 shows n-dependence of $\tau_{\rm dep}$ and τ; here we calculated the values for τ by solving eq. (2.9) numerically. The straight line denotes $\tau=25.66$ obtained above and the dotted line expresses the expected behavior of $\tau_{\rm dep}$ from eq. (2.9) for this value of τ. It should be noted that data for wide range of n, from $n\simeq\tau$ to $n\simeq100\tau$, are shown in the figure; we see that both $\tau_{\rm dep}$ and τ agree well with their expected values in this range. The statistical dependence time $\tau_{\rm dep}$ approaches 25.66 slowly as n increases, while τ agrees well with it irrespective of n, as is expected from the discussions in the preceding section. The validity and the effectiveness of the method is thus confirmed.

§4. Dynamical Critical Exponent of 3D Ising Model

We applied the method of statistical dependence time to the critical dynamics of the 3D Ising model to estimate the dynamical critical exponent z. Throughout this section, we use the simple-cubic lattices of the size $L\times L\times(L+1)$, with the skewed boundary conditions imposed on the L-directions, and the periodic boundary condition on the $(L+1)$-direction. Apart from the boundary conditions, we used the same dynamics as one used in the last section. Simulations were performed at the critical point $K_{\rm c}=0.221654$, with 64 independent runs made simultaneously by means of the recycling algorithm.[16,17] For more details of the simulation method in this section, see ref. 10.

First, we show the data taken from long runs. Figure 3 shows the log-log plot of $\tau_{\rm dep}(L)$ against the average linear dimension of the systems, $L_{\rm av}\equiv[L^2(L+1)]^{1/3}$. The quantity we measured for calculating $\tau_{\rm dep}(L)$ is again the magnetization. The length of each simulation was about $100\tau_{\rm dep}(L)$, so that we expect calculated $\tau_{\rm dep}(L)$ is a good estimator for $\tau_{\rm int}(L)$. According to the dynamical finite-size scaling theory,[6] $\tau_{\rm int}(L)$ is expected to be proportional to $L_{\rm av}^z$. The data indeed fit well to

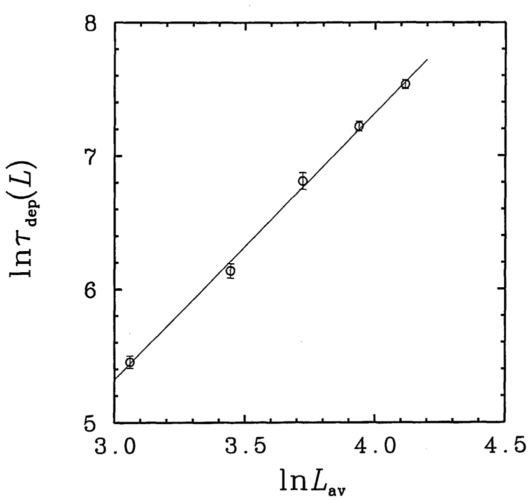

Fig. 3. System-size dependence of $\tau_{\rm dep}$ for the 3D Ising model at $K=K_{\rm c}$. About $100\tau_{\rm dep}$ was taken as n for each size. The horizontal axis is the average linear dimension of the systems, $[L^2(L+1)]^{1/3}$.

a straight line, and from the gradient of the line we get $z=2.00\pm0.05$. Although this value for z is a reasonable one, the error is rather large compared to the other recent studies.

To reduce the statistical errors, it is necessary to increase the number of independent runs. To this end, we next performed shorter runs and calculated the effective relaxation time $\tau_{\rm eff}$ using eq. (2.9). According to the discussions in §2, if the relaxation is approximated well by a single-exponential relaxation, $\tau_{\rm eff}$ serves as a good estimator for $\tau_{\rm int}$. In fact, it was observed that the time-displaced correlation function of the magnetization for the present model is described very well by at most two exponential functions even at the critical point;[4] thus, utilizing $\tau_{\rm eff}$ in the present case is expected to work well.

The results of shorter simulations are listed in Table I as well as detailed information on the simulations such as n and N. Here we took n as of order of $10\tau_{\rm dep}$. It should be noted that in Table I $\tau_{\rm dep}$ and $\tau_{\rm eff}$ are represented in unit of MCS/spin, while we measured the magnetization in every n_0 MCS/spin. Figure 4 shows the log-log plot of $\tau_{\rm eff}(L)$ against $L_{\rm av}$. At first sight, all the data points seem to fit very well to a straight line, $\tau_{\rm eff}(L)\sim L_{\rm av}^z$. We, however, will find by the detailed analyses below that $\tau_{\rm eff}$ for the smallest system $\tau_{\rm eff}(3)$ deviates significantly from the line. To see this deviation, we cutted 19 data points into overlapping sets of 8 successive data points and tried to fit each set to the function $\tau_{\rm eff}(L)\sim L_{\rm av}^z$. The resulting z are shown in Fig. 5 against $L_{\rm mid}\equiv(L_{\rm min}+L_{\rm max})/2$, where $L_{\rm min}$ and $L_{\rm max}$ are the smallest and the largest $L_{\rm av}$ among the 8 data, respectively. The error bars indicate 1σ calculated by the error-propagation law. Only the value of z for the smallest $L_{\rm mid}$ is calculated from the data set includes $\tau_{\rm eff}(3)$, among the values shown in the figure. Evidently, all the values of z except for the smallest $L_{\rm mid}$ fall in the range 2.030 ± 0.005, and coincide with each other within the errors. The goodness of each fit can be deduced from the corresponding chi-square values per the DOF, χ^2/DOF, which is shown in Fig. 6. Again only the value of χ^2/DOF for the smallest $L_{\rm mid}$ shows

Table I. Size dependence of $\tau_{\rm dep}$ and the corresponding $\tau_{\rm eff}$. The errors in the last two digits are given in brackets. In each run, magnetization was measured in every n_0 MCS/spin. The number of measurement is denoted by n. The length of each run is, therefore, $n_0\times n$, after $n_{\rm dis}$ MCS/spin discarded for thermalization. Number of independent runs is denoted by N ($N/64$ is shown). The whole procedure was repeated $N_{\rm rep}$ times, for statistical analyses. It should be noted that $\tau_{\rm dep}$ and $\tau_{\rm eff}$ are shown in unit of MCS/spin (not in unit of the interval of the measurements n_0).

L	$n_{\rm dis}$	n_0	n	$N_{\rm rep}$	$N/64$	$\tau_{\rm dep}$	$\tau_{\rm eff}$
3	90	9	10	8	250	6.044(16)	4.963(25)
5	250	10	25	8	250	13.784(65)	13.936(76)
7	500	10	50	10	150	25.80(14)	26.99(16)
9	800	10	80	10	450	41.517(93)	43.71(10)
11	10000	10	100	10	400	60.85(16)	64.93(18)
13	2000	10	200	10	450	86.05(19)	90.00(20)
15	2300	10	230	8	625	113.99(19)	120.20(22)
17	3000	10	300	8	250	146.51(55)	154.41(61)
19	4000	10	400	10	950	182.84(23)	192.01(26)
21	5000	10	500	7	500	224.16(62)	235.19(68)
23	6000	10	600	10	550	268.87(65)	282.11(71)
25	6500	10	650	8	1400	316.55(66)	333.65(74)
27	8000	10	800	8	625	368.50(77)	387.23(85)
29	9000	10	900	8	300	425.5(14)	447.8(16)
31	10000	10	1000	9	250	484.0(12)	510.0(13)
41	20000	10	2000	8	105	865.7(57)	906.9(62)
51	30000	10	3000	7	28	1345(14)	1412(15)
61	50000	10	5000	10	30	1934(13)	2017(15)
91	50000	50	1000	10	23	4068(60)	4471(73)

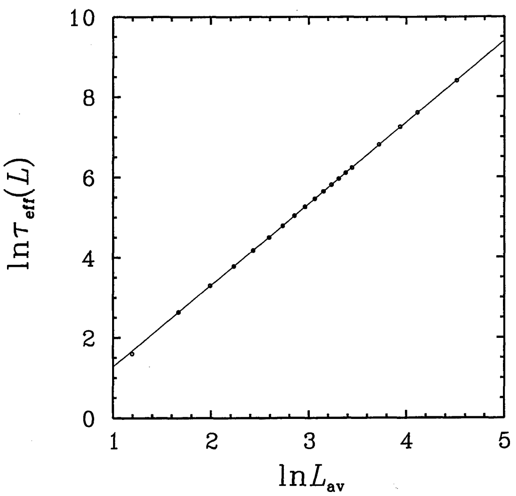

Fig. 4. System-size dependence of $\tau_{\rm eff}$ for the 3D Ising model at $K=K_{\rm c}$. About $10\tau_{\rm dep}$ was taken as n for each size. The horizontal axis is the average linear dimension of the systems, $[L^2(L+1)]^{1/3}$. Error bars are not shown, since the errors are much smaller than the symbol size.

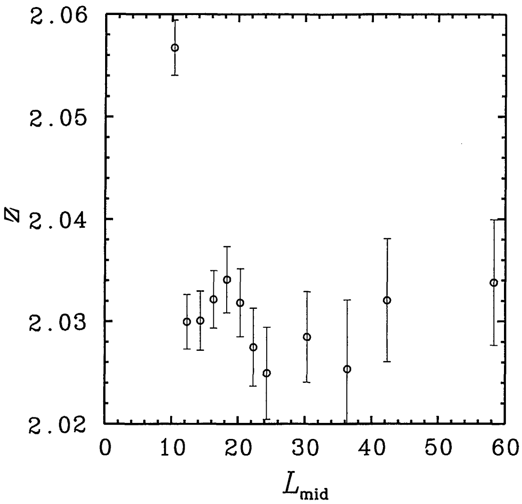

Fig. 5. Estimated z for sets of $\tau(L)$, with each set consisting of 8 successive data points. The horizontal axis L_{mid} denotes the average value of the smallest and the largest L_{av} among 8 data.

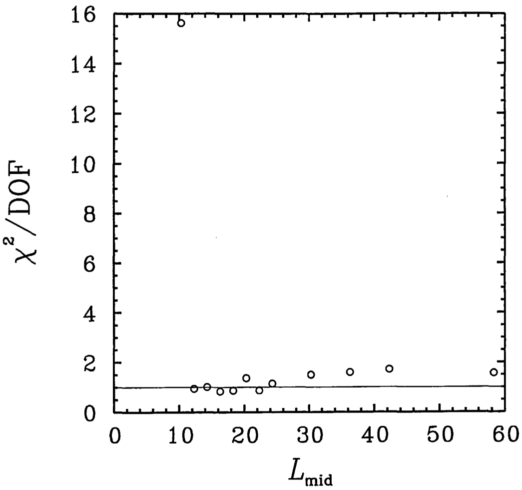

Fig. 6. Chi-square value per DOF corresponding to the fit in Fig. 5. The horizontal line indicates $\chi^2/\mathrm{DOF}=1$.

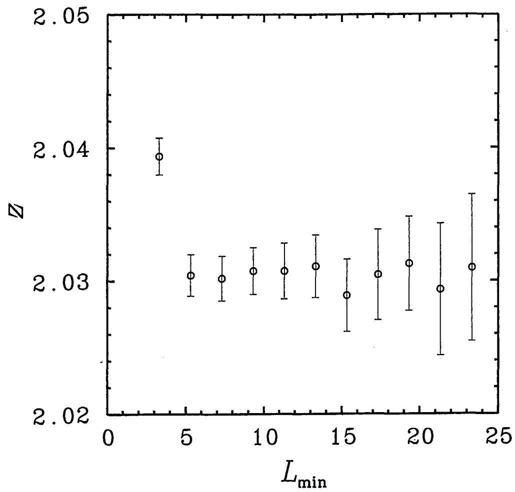

Fig. 7. Estimated z for sets of $\tau(L)$, with each set consinting of data data from L_{min} to $L=91$.

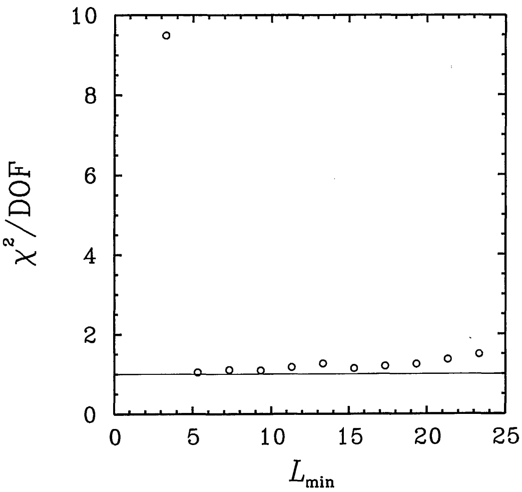

Fig. 8. Chi-square value per DOF corresponding to the fit in Fig. 7. The horizontal line indicates $\chi^2/\mathrm{DOF}=1$.

anormalous behavior; this time it is found to be extraordinarily large, so that this fitting is not statistically acceptable. On the other hand, chi-square values for other sets have reasonable values.

As an alternative analysis, we tried to fit the data from $L_{\mathrm{av}}=L_{\mathrm{min}}$ through $L=91$ to the same function as above. The number of data points fitted now decreases with increasing L_{min}. The z thus obtained and the corresponding χ^2/DOF are plotted in Figs. 7 and 8, respectively, against L_{min}. We again see that only z for $L_{\mathrm{min}}=3$ deviates significantly from the others, and the corresponding χ^2/DOF is extraordinarily large at the same time. The reason of this large χ^2/DOF can be understood by the examination of the residuals of the fit. In Fig. 9, we plot the residuals against L_{av} for fitting of whole 19 points and for 18 points other than $L=3$. The residuals of 19-point fitting, which includes $\tau_{\mathrm{eff}}(3)$, shows evident

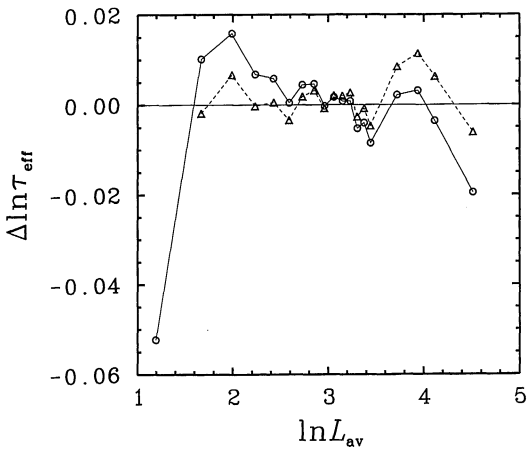

Fig. 9. Residuals against L_{av} for fitting of whole 19 data (○) and for 18 data other than $L=3$ (△).

downward tendency with increasing L_{av}, after jumping up between $L=3$ and 5. Clearly, this tendency is the origin of the large value for χ^2/DOF. On the other hand, no special tendency can be seen in the residuals of 18-point fitting.

According to these two analyses, it is natural to conclude that all the 18 values for $\tau_{\mathrm{eff}}(L)$ other than $\tau_{\mathrm{eff}}(3)$ fit well to the straight line, and thus to the finite-size scaling. Our final estimate of z using the linear-least-square fitting of these 18 data is 2.030 ± 0.004 with corresponding $\chi^2/\mathrm{DOF}=1.05$; here we took 2σ region as the range of the error instead of 1σ for the sake of safety. The present estimate of z agrees well with that of Wansleben and Landau, but the error is of one order of magnitude smaller. As is seen in Fig. 4 and the value of χ^2/DOF, the fitting of the data to the straight line is extremely good, in spite of the fact that several parameters, such as n, were taken rather arbitrarily for each L_{av}. We believe that such a goodness of fit itself justifies the use of τ_{eff} as a characteristic time scale in the present study.

§5. Summary and Discussions

We have proposed a new method for estimating the equilibrium relaxation time τ from dynamical simulations. Calculation of the time-displaced correlation function or any other dynamical correlation is unnecessary in this method; only static averages are used instead. As a result, it is quite simple in operation. The greatest advantage of the method is that it allows unambiguous statistical analyses, in contrast to the traditional methods which use time-displaced correlation functions. It is thus suitable to precise analyses of dynamics. Effectiveness of the method has been shown for off-critical relaxation of the 3D Ising model. The present method is quite general so that it is applicable not only to Monte Carlo simulations but also to other dynamical simulations such as molecular dynamics simulations, or even to some sort of real experiments.

As the first application of the present method, we have applied it to the critical dynamics of the 3D Ising model. Although the relaxation of the magnetization at $K=K_c$ is expected to be of multi-exponential type, we found that the present method works very well, and we successfully estimated z. The value $z=2.030\pm0.004$ we obtained agrees very well with the recent estimation by Wansleben and Landau, 2.04 ± 0.03;[4] we, however, improved the accuracy in z by about one order of magnitude. Most importantly, possibility of $z=2$ is clearly excluded by the present result. On the other hand, the present result is not compatible with the estimate by Heuer, $z=2.10\pm0.02$.[5] We believe that the present investigation thus resolved the controversy in the value of z. One possible source of systematic errors in z which has not been taken into account in the present study is the error due to an uncertainty in K_c; in fact, it was found from the non-equilibrium relaxation of the magnetization, that the shift in z caused by the different choices of K_c between 0.22165 and 0.22166 is about 0.01.[18] Since the error of K_c used here is expected to be at most 0.000005, we expect the resulting error of z is less than 0.005; as a result, the above conclusions are supposedly not affected by this correction, only the error bar becomes to be about 0.01.

As was stated briefly in §1, one of the authors (N. I.) estimated $\beta/z\nu$ of the same model from the non-equilibrium relaxation process quite recently.[10] The value obtained is 0.250 ± 0.002. Combining it with the present result, we get $\beta/\nu=0.5075\pm0.0050$. On the other hand, two recent Monte Carlo renormalization group studies estimated the value of exponent η as 0.027 ± 0.005[19] and 0.026 ± 0.003,[20] which imply $\beta/\nu=0.513\pm0.002$ and 0.514 ± 0.003, respectively; a finite-size scaling study for $L=8$ to 96 gave $\beta/\nu=0.518\pm0.007$.[21] Thus, the value we obtained seems slightly smaller than these recent estimates using large-scale Monte Carlo simulations, although the error regions are overlapping. In order to conclude definitely about this discrepancy, more accuracy is required, not only in dynamic exponents we obtained but also in static exponents calculated in refs. 19–21; in fact, a value 0.505 was also reported for the same exponent in ref. 21, which is very close to the present one, when only the data for $L\geq 24$ are used in the finite-size scaling fit. It should be noted that we obtained the ratio of the static critical exponents β/ν using informations both from equilibrium and non-equilibrium dynamics. The present method is thus useful in estimating both the dynamical and static critical exponents.

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