Dynamic finite-size effect in the three-dimensional classical *XY* model

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Explicit dynamic finite-size scaling in the time-dependent correlation functions for the three-dimensional classical *XY* model is explored. The dynamic scaling method, proposed by us previously, is utilized for finding the time-scaling variables of the model. Time-dependent correlation functions of the model for different numbers of spins could be collapsed into universal curves. Compared to infinite-range spin models, the width of the scaling region is found to be much narrower. [S0163-1829(97)01045-X]

I. INTRODUCTION

In our previous work,[1] we developed a method which could take into account the dynamic finite-size scaling property appearing *explicitly* in the time-dependent correlation function. We applied the method to study the finite-size effect in the time-dependent correlation functions of the classical spin van der Waals model[2–4] (CSVW) with infinite-range ferromagnetic interaction and an infinite-range antiferromagnetic classical spin model[5] (IRCAS). With the time-scaling variable determined by applying this method, the time-dependent correlation functions for systems with different numbers of spins collapsed into universal curves. We could also interpret the meaning of the system size-dependent *maximum time interval*, where the calculation of Dekeyser and Lee[2] is valid. In fact, the maximum time interval is found to be related to the interval, i.e., the size of the characteristic time, where the dynamic scaling is maintained. In both models, the dynamic finite-size scaling phenomena persist even far away from criticality. This is in contrast with most static finite-size scaling phenomena which usually appear only close to criticality.

In this note, we further apply our dynamic scaling method to a short-range spin model to elucidate the effect of the interaction range on the dynamic finite-size scaling behavior. One possible choice for a short-range spin model is the well-known Heisenberg model. Since the total spin components are constants of motion, their time-dependent behavior is trivial. Hence, we investigate the dynamic finite-size behavior of the three-dimensional classical *XY* model (3DC*XY*), in which the total spin components have nontrivial time evolutions. Since neither the statics nor the dynamics of this model is exactly solvable, we shall appeal to the spin dynamics simulation[6] (SDS) approach.

Recently, Chen and Landau[7] developed a dynamic finite-size scaling theory in the frequency–wave-number domain, which inherits the features of the dynamic scaling theory of Halperin and Hohenberg[8] for bulk systems. However, their dynamic finite-size scaling explores the size dependence of a characteristic frequency ω_m, which can only be *indirectly* attained by integrating the dynamic structure factor $S(k,\omega)$ with respect to angular frequency ω. Hence, they did not intend to explore the existence of *direct* dynamic finite-size scaling in the time-dependent correlation function (or equivalently in the dynamic structure factor) like the present work.

II. DESCRIPTION OF THE DYNAMIC SCALING METHOD

In our previous work,[1] we developed a finite-size dynamic scaling method in which the time-dependent correlation functions are *directly* scaled in the time domain. The time-scaling variable can be found by comparing the orders of magnitude of both sides of the equations of motion, $\dot{\mathbf{s}}_i = -\mathbf{s}_i \times \delta H/\delta \mathbf{s}_i$ for the single spin vector $\mathbf{s}_i$ at site i, and $\dot{\mathbf{S}} = -\Sigma_{i=1}\mathbf{s}_i \times \delta H/\delta \mathbf{s}_i$ for the total spin vector $\mathbf{S}=\Sigma_{i=1}\mathbf{s}_i$. Usual quantities considered in simulations are the ensemble averages of the absolute value of spins. The order of magnitude of these quantities in each side can be determined from the results of statics, which in most cases are obtained through Monte Carlo (MC) simulations.[9] In general, the size dependence of the spin variable is changed by taking the derivative with respect to time. We introduced a characteristic time $\mathcal{T}$, which represented this change. The change may depend on the system size N and the N dependence of $\mathcal{T}$ is expressed in the form $\mathcal{T} \sim O(N^e)$, where e is to be determined. We asserted that the equations of motion for a system in the thermodynamic limit are well defined only within this characteristic time $\mathcal{T}$. Thereby we chose $t/\mathcal{T}$ or equivalently tN^{-e} as the finite-size time-scaling variable τ. This assertion and the above proposition were fully justified for the CSVW and IRCAS models.[1]

Following the above analysis, we arrived at the finite-size scaling form for the time-dependent correlation functions, namely

$$\frac{\langle s_i^{\alpha}(t) s_i^{\alpha}(0)\rangle}{\langle (s_i^{\alpha})^2\rangle} = F_{\alpha}(\tau) \tag{1}$$

for the single spin components ($\alpha = x,y,z$), and

$$\frac{\langle S_{\alpha}(t) S_{\alpha}(0)\rangle}{\langle S_{\alpha}^2\rangle} = G_{\alpha}(\tau), \tag{2}$$

for the total spin components. Here, $F_{\alpha}(\tau)$ and $G_{\alpha}(\tau)$ are universal dynamic scaling functions.

The exponent e can be determined with the help of the identity $\langle \dot{B}(t)A(0)\rangle = -\langle B(t)\dot{A}(0)\rangle$, i.e.,

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$$\frac{\langle(\dot{s}_i^\alpha)^2\rangle}{\langle(s_i^\alpha)^2\rangle}=-\frac{\langle\ddot{s}_i^\alpha s_i^\alpha\rangle}{\langle(s_i^\alpha)^2\rangle}=N^{-2e}\ddot{F}_\alpha(0), \tag{3}$$

for the single spin components, and

$$\frac{\langle(\dot{S}_\alpha)^2\rangle}{\langle S_\alpha^2\rangle}=-\frac{\langle\ddot{S}_\alpha S_\alpha\rangle}{\langle S_\alpha^2\rangle}=N^{-2e'}\ddot{G}_\alpha(0), \tag{4}$$

for the total spin components at time $t=0$. The first expressions in these equations are usually accessible from static simulations and the equations of motion. Then log-log plots of Eqs. (3) and (4) yield the exponents e and e'. This implies that the time-scaling variables tN^{-e} or $tN^{-e'}$ can be found from static simulations such as MC. It should be noted that once we take the dynamic finite-size scaling ansatz, Eqs. (1) and (2), for granted, our dynamic scaling method, Eqs. (3) and (4), is *exact* at least in the short-time region.

III. SIMULATION OF 3DC*XY*

Now we apply the *direct* dynamic scaling method described above to the 3DC*XY* model. The model is defined by the Hamiltonian

$$H=-J\sum_{\langle i,j\rangle}(s_i^x s_j^x+s_i^y s_j^y), \tag{5}$$

where s_i^α denotes the α component of a classical Heisenberg spin at site i; J is the positive coupling constant. Note that the sum runs over nearest-neighbor pairs i,j of the system. For simplicity we choose the simple cubic lattice, which should not affect the result according to the universality argument.

We now proceed to find out the time-scaling exponents e and e', and hence the time-scaling variables of the model τ by utilizing the dynamic scaling method described in the previous section. Since the relevant static correlation functions are not known analytically, we make use of MC simulations. In our MC simulations, we have studied $5\times5\times5$, $7\times7\times7$, and $10\times10\times10$ lattices. Ensemble averages are obtained through the heatbath algorithm.[10] In the simulations, we have discarded the first 4 000 Monte Carlo steps per spin (MCS) for the equilibration of the system. Ensemble averaging is carried out by collecting three sets of 10 000 to 30 000 configurations, where successive configurations are separated by 10 to 20 MCS to assure the statistical independence between the configurations. The error in our MC calculation is estimated to be less than 2%.

We obtained the dimensionless inverse critical temperature from the MC data via the Binder cumulant plot;[9] $\beta_c J=0.64(1)$, where $\beta_c=1/k_BT_c$. The number inside the parenthesis denotes the standard error in the last digit.

For the 3DC*XY* model, the equations of motion for a single spin vector are given by

$$\dot{s}_i^x=-Js_i^z\sum_{j\in \mathrm{NN}}s_j^y, \tag{6}$$

$$\dot{s}_i^y=Js_i^z\sum_{j\in \mathrm{NN}}s_j^x, \tag{7}$$

TABLE I. Time-scaling exponents e and e' of the time-scaling variable $\tau=tN^{-e(e')}$ for the time-dependent spin-correlation functions of the 3DC*XY* model. Numbers in parentheses are the errors in the last digits.

	Time-scaling exponent e		
	$T\gg T_c$	$T\approx T_c$	$T\ll T_c$
Single spin	0.00(1)	0.03(1)	0.00(1)
Total spin	0.00(1)	0.34(1)	0.49(1)

$$\dot{s}_i^z=-Js_i^y\sum_{j\in \mathrm{NN}}s_j^x+Js_i^x\sum_{j\in \mathrm{NN}}s_j^y, \tag{8}$$

where $\Sigma_{j\in \mathrm{NN}}$ denotes the sum over nearest neighbors j of site i. Among the equations of motion for the total spin components, S_z is a constant of motion which is not of our interest, and we get

$$\dot{S}_x=-J\sum_i s_i^z\sum_{j\in \mathrm{NN}}s_j^y, \tag{9}$$

$$\dot{S}_y=J\sum_i s_i^z\sum_{j\in \mathrm{NN}}s_j^x. \tag{10}$$

In order to obtain the scaling exponent, we have calculated $\langle(\dot{s}_i^\alpha)^2\rangle/\langle(s_i^\alpha)^2\rangle$ and $\langle(\dot{S}_x)^2\rangle/\langle S_x^2\rangle$. Then Eqs. (3) and (4) enable us to find the time scaling exponents, e and e'. The results are summarized in Table I. Unlike the CSVW or IRCAS models, there is no size dependence away from criticality except for the remarkably strong one at $T\ll T_c$ for the total spin correlations. In the critical region, $T\approx T_c$, the time-scaling exponents show extremely weak size dependence within the error bound for the single spin correlations, while the dependence is strong for the total spin correlations. The reason why the behavior of the 3DC*XY* model is so different from that of the CSVW model will be discussed below.

Having obtained the time-scaling variables, we now proceed to find the range of the variable, within which the time-dependent spin-correlation functions for the systems with different number of spins collapse into a universal curve. To do so, we calculated the time-dependent spin-correlation function for the model through the SDS.

In the SDS, ensemble averages of the time-dependent correlations are obtained through MC simulation as described above. From each configuration, the equations of motion are integrated using the fourth-order Runge-Kutta algorithm. The time interval between each step in the present work is 0.01 in units of J.

In Fig. 1, we depict the time-dependent single spin-correlation functions $F_x(\tau)=\langle s_1^x(t)s_1^x(0)\rangle/\langle[s_1^x(0)]^2\rangle$ vs time-scaling variables, which are given in Table I, at different temperature regimes. Although our result is given only for site 1, it is also valid for any site. $F_y(\tau)$ shows an identical behavior due to the symmetry of the model. We witness almost perfect collapse of curves at least up to $J\tau\lesssim0.3$ for

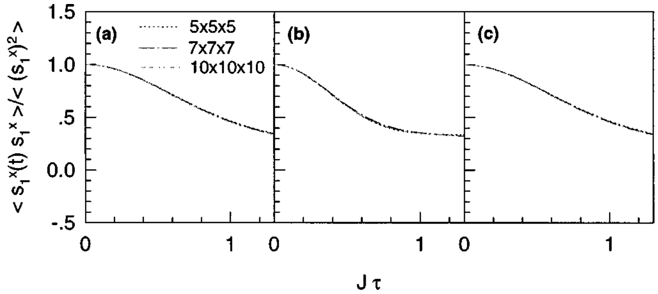

FIG. 1. $F_x(\tau)$ vs $J\tau$ at (a) $\beta J=0.30$, (b) $\beta J=0.64$, and (c) $\beta J=0.90$, respectively.

all temperature regimes. The data collapsing range is reduced substantially at the critical temperature from that of the CSVW and IRCAS models.[1]

Figure 2 shows the time-dependent total spin-correlation functions $G_x(\tau)=\langle S_x(t)S_x(0)\rangle/\langle S_x^2(0)\rangle$ vs time-scaling variables, which are given in Table I, at different temperature regimes. $G_y(\tau)$ also shows an identical behavior due to the symmetry of the model. From the figure, almost perfect collapse of the curves at least up to $J\tau\lesssim0.2$ can be seen for all temperature regimes. Note here that the data collapsing range is reduced dramatically at the critical temperature from that of the CSVW and IRCAS models.[1]

In both cases, we observe that the data collapsing regions (or equivalently the dynamic scaling regions) are much narrower than those of the infinite-range CSVW and IRCAS models. At the same time, the finite-size dependence of the time-scaling variables becomes much weaker for the single spin correlations at all temperature regimes. These differences can be understood by examining Eq. (5). We immediately note that each spin is coupled only to nearest neighbors in the 3DCXY model. Therefore, practically no collective effect of spin-spin interactions would arise at high temperatures, thus the size dependence would be minimal. This causes the zero in the first column in Table I. Near T_c, due to diverging correlation length effectively all the spins become correlated with each other. Hence, each spin will have effective dynamical coupling to all other spins, and there will be some collective effect which in turn causes appreciable size dependence. At low temperatures, the dynamic finite-size scaling of the total spin is strong although the correlation length becomes short. We suppose this is caused by the long-range order related to the variable S_x, which we have chosen to investigate. Onset of long-range order in the XY limit almost sets the motion of the x component of the total spin in a single phase, and hence effectively all the spins behave as if they are dynamically coupled.

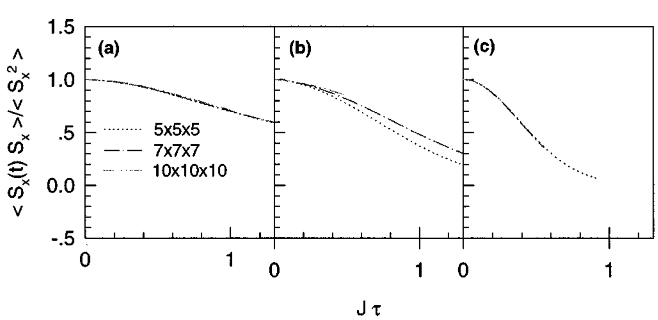

FIG. 2. $G_x(\tau)$ vs $J\tau$ at (a) $\beta J=0.30$, (b) $\beta J=0.64$, and (c) $\beta J=0.90$, respectively.

As time increases, however, this correlation vanishes quickly, so that corrections to scaling make the collapsing less apparent. As a consequence, the dynamic scaling region in the 3DCXY model becomes narrow. This narrow scaling region and weak size dependence should be contrasted to the CSVW model, where the coupling is inherently of infinite range. It is indeed the infinite-range coupling of spins which gives rise to the collective effect, and thus the finite-size scaling for the correlation function is strong at all temperature regimes for infinite-range models. This intrinsic collectiveness of the model makes dynamic coupling of all spins diminish only gradually in time, so that corrections to scaling appear at a much later stage. However, the small scaling region is rather normal in many critical phenomena and it should be interpreted that the CSVW model has an extraordinarily long scaling region.

We briefly mention an interesting but anomalous behavior of the total spin-correlation function at $T\approx T_c$. Our dynamic scaling method predicts $e'=0.34(1)$ and the time-dependent correlation function fits well within the characteristic time interval (at small $J\tau$). On the contrary, we found afterwards that the correlation function fits the scaling function with $e'=0.50$ within a fairly broader range even beyond $J\tau=1.0$. Since our dynamic finite-size scaling is exact at short times as mentioned in Sec. II, we suspect this might be a manifestation of the so-called intermediate asymptotics.[11] However, to inquire into this matter further would require more study.

IV. CONCLUSION

We have studied the *explicit* dynamic finite-size scaling in the time-dependent correlation function of the 3DCXY model. Applying the dynamic scaling method proposed by us previously, we have found the appropriate time-scaling variables in various temperature regimes using static MC simulations. Time-dependent correlation functions have been calculated using dynamic SDS simulations. With the scaling variables, collapsing of the dynamic correlation functions into universal curves is successfully carried out.

The results confirm our proposition of using $\tau=t/\mathcal{T}$ as the time-scaling variable for *direct* dynamic finite-size scaling of the time-dependent correlation functions. It also supports our assertion of interpreting the *maximum time interval* of Dekeyser and Lee[2] as the region $\mathcal{T}$ within which our dynamic finite-size scaling holds. Therefore, our direct finite-size scaling method correctly describes the behavior of a short-range model, as it did for infinite-range models, such as CSVW and IRCAS. In the 3DCXY model, however, the data collapsing regions are found to be much narrower than those of infinite-range models. Also, the size dependence is much weaker. These changes are attributed to the short-range nature of the coupling in the model.

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