PHYSICAL REVIEW E **69**, 045103(R) (2004)

Critical exponents of isotropic-hexatic phase transition in the hard-disk system

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(Received 6 September 2003; published 26 April 2004)

The hard-disk system is studied by observing the nonequilibrium relaxation behavior of a bond-orientational order parameter. The density dependence of characteristic relaxation time τ is estimated from the finite-time scaling analysis. The critical point between the fluid and the hexatic phase is refined to be 0.899(1) by assuming the divergence behavior of the Kosterlitz-Thouless transition. The value of the critical exponent η is also studied by analyzing the fluctuation of the order parameter at the criticality and estimated as $\eta=0.25(2)$. These results are consistent with the prediction by the Kosterlitz-Thouless-Halperin-Nelson-Young theory.

DOI: 10.1103/PhysRevE.69.045103 PACS number(s): 64.60.−i, 64.70.Dv, 02.70.Ns

Although the hard-disk system is the simplest model which involves the melting transition [1,2], there are still unanswered questions [3]. Recently, the nonequilibrium relaxation behavior of a bond-orientational order parameter has been studied, and two Kosterlitz-Thouless (KT) transitions have been observed [4]. This behavior is consistent with the prediction proposed by Halperin and Nelson [5] and Young [6]. They discussed unbinding processes of disclinations and dislocations based on the KT transition [7], and introduced a new phase named the hexatic phase. This melting scenario is now referred to as the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory.

Besides the KTHNY theory, there are other scenarios for predicting the first-order transition. Chui [8] studied the spontaneous generation of grain boundaries, and concluded that two-dimensional melting occurs through a single first-order transition. Ryzhov and Tareyeva [9] estimated the stability limits of the solid and hexatic phases based on the density-functional approach and concluded that the two-electron electron system can have two separate transitions, but the hard-disk system does not have the hexatic phase.

Many numerical studies have been carried out to clarify the two-dimensional melting phenomena. Two densities characterizing two-dimensional melting are denoted by ρ_i and ρ_m; which correspond to the starting and ending points of an intermediate phase, respectively. The intermediate phase is understood to be the coexisting phase in terms of the first-order transition, and the hexatic phase is that of the KTHNY theory. This range of density becomes smaller when the system becomes larger. Alder and Wainwright [2] studied the system with number of particles $N=870$, using a molecular dynamics simulation. They concluded that the transition is of the first order on the basis of a van der Waals looplike behavior of pressure. They obtained $\rho_i=0.880$ and $\rho_m=0.912$. (Hereafter, we use the definition of density which is reduced by the hard-disk diameter as $\rho=4N\sigma^2/A$ with the area A of the system, the total number of particles N, and the radius σ of particles.) Fernandez *et al.* [10] studied the system of $N=15\,876$ by a constant-pressure Monte Carlo (MC) simulation and obtained $\rho_i=\rho_m=0.916(5)$. They concluded that the intermediate phase does not exist or its range is small. Zollweg *et al.* [11] examined the size dependence in the hard-disk system of $N=16\,384-65\,535$ by the MC method and found a strong finite-size effect (physical quantities drift over long MC runs) near the criticality. They pointed out that the density range of the intermediate phase becomes smaller with increasing system size. Hence it is unclear whether the intermediate phase survives or vanishes in the thermodynamic limit. Jaster [12] studied the divergence of the bond-orientational correlation length and the susceptibility by the MC method. He treated systems with $N=1024-65\,535$ and showed that the behavior of the bond-orientational correlation and the susceptibility as well as the value of the critical exponent η are consistent with the KTHNY theory. He obtained $\rho_i=0.899(1)$ and $\rho_m>0.91$. Weber *et al.* [13] studied the bond-orientational susceptibility as a function of density with the $N=16\,384$ system, and obtained $\rho_i>0.880$ and $\rho_m<0.905$. They fitted a plot based on the KTHNY theory, and obtained an unphysical value of the critical point $\rho_i'\sim0.913(1)$ which is larger than the value of ρ_m. They concluded that the result was not compatible with the prediction of the KTHNY theory.

Most of the numerical works introduced above used the equilibrium Monte Carlo (EMC) simulations. The EMC method is popular and has been widely used in statistical physics. However, the EMC method encounters some trouble for systems with slow relaxation. In particular, it makes the analysis of large systems involving the KT transition difficult, since the correlation length diverges exponentially near the criticality.

Instead of the EMC method, a method is proposed by which the nonequilibrium behavior of order parameters is studied to obtain properties in the thermodynamic limit [14]. This analysis is called the nonequilibrium relaxation (NER) method. This method has been used to study phase diagrams and to determine accurate values of critical points and critical exponents for transitions of various systems: spin-glass transition [15], chiral-glass transition [16], and the KT transition [17,18].

The NER method has some advantages over the EMC method. It is less influenced by finite-size effects. For a fixed time t, the time-dependent correlation length $\xi(t)$ remains finite when t is smaller than the correlation time τ. Thus, up to the correlation time, the finite-size effect of the system is

negligible. Furthermore, the NER method makes use of only the relaxation processes, so the attainment of equilibration, which is the most time-consuming process in the EMC simulations, is unnecessary.

In our previous work [4], we studied hard-disk melting of the system with $N=23\,288$ by observing the nonequilibrium behavior of the bond-orientational order. From scaling analyses based on the dynamic scaling hypothesis, we obtained $\rho_i=0.901(1)$ and $\rho_m=0.910(1)$. Ozeki *et al.* [18] proposed a more efficient method of determining the critical point of the KT transition. In their method, relative values of the relaxation times τ are estimated by scaling. Then the critical point can be determined from the divergence behavior of the obtained values of τ. In this paper, we study the transition between the fluid and the hexatic phase by analyzing the NER behavior of the bond-orientational order. We obtain an accurate value of ρ_i using dynamic KT scaling. With the obtained critical point, we determine the value of the critical exponent η by observing a nonequilibrium fluctuation of the order parameter.

We introduce the bond-orientational order parameter to characterize the two-dimensional melting. The parameter is denoted by ϕ_6 and is defined as

$$\phi_6 = \left| \frac{1}{N} \sum_k^N \sum_l^{n_k} \frac{\exp(6i\theta_{kl})}{n_k} \right|^2, \tag{1}$$

where n_k denotes the number of neighbors of particle k, and θ_{kl} denotes the angle between a fixed axis and the bond connecting particles k and l.

The neighbors in an off-lattice model are strictly defined with the Voronoi construction [12], but this is a very time-consuming method. In this paper, two particles separated by a distance less than 2.6 times their radius are defined as neighbors. We confirmed that the value of ϕ_6 is approximately the same value as the obtained value with the Voronoi construction.

The scaling behavior of the NER process is constructed, assuming a time-dependent form of free energy, as

$$F(\epsilon,h,L,t) = L^{-d}\overline{F}(\epsilon L^{y_T}, hL^{y_H}, tL^{-z}), \tag{2}$$

where L, h, and ϵ denote the linear system size, the external field, and the reduced density $(\rho-\rho_c)/\rho_c$, respectively. The exponents y_T and y_H are $1/\nu$ and $d-\beta/\nu$, respectively, with the exponent of correlation length ν, magnetization β, and system dimensionality d. The dynamical exponent is denoted by z. On the basis of the dynamical scaling hypothesis (2), the correlation length ξ and characteristic relaxation time τ have the relationship

$$\tau \sim \xi^z. \tag{3}$$

This means that finite-scaling analyses are easily applicable to finite-time scaling by replacing L with $t^{1/z}$.

In the KT transition, the correlation length diverges exponentially as $\xi \sim \exp(a'/\sqrt{\varepsilon})$ [7]. From Eq. (3), the divergence behavior of the relaxation time τ is expected to be

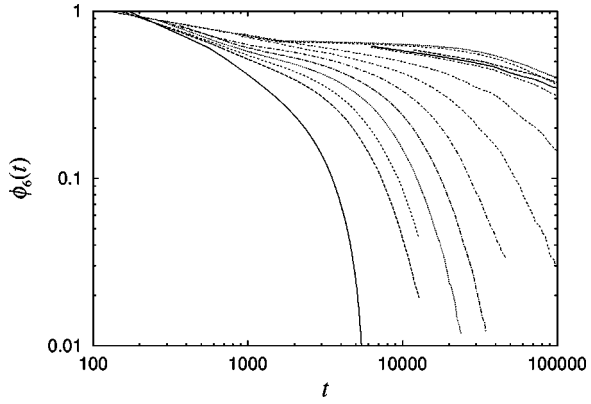

FIG. 1. Relaxation of the bond-orientational order $\phi_6(t)$ for various densities from $\rho=0.800$ to 0.890 in log-log plot. Natural logarithms are used for all figures.

$$\tau(\epsilon) = b\ \exp(a/\sqrt{\varepsilon}). \tag{4}$$

Using this scaling function, one can obtain the critical point. It is difficult to determine absolute values of relaxation time for each density. Instead, one can estimate relative values of $\tau(\epsilon)$ from finite-time scaling [18]. A natural scaling form of the bond-orientational order parameter can be expressed as

$$\phi_6(t,\epsilon) = \tau(\epsilon)^{-\lambda}\overline{\phi}_6[t/\tau(\epsilon)], \tag{5}$$

where λ is the dynamic exponent which is independent of density. Based on Eq. (5), we plot $\tau^\lambda\phi_6$ as a function of t/τ. With appropriately chosen λ and $\tau(\epsilon)$, the relaxation curves $\tau^\lambda\phi_6$ would collapse to a single curve. After that, we can estimate the critical point by fitting divergence behavior (4) to $\tau(\epsilon)$ obtained above.

At the critical point, one can estimate the values of the critical exponents from the nonequilibrium behavior of fluctuations. From Eq. (2), the asymptotic behavior of $\phi_6(t)$ at the critical point is expected as

$$\phi_6(t) \sim t^{-\eta/2z}, \tag{6}$$

with the exponents η and z [14]. Similarly, the fluctuation of ϕ_6 is expected asymptotically $(t\to\infty)$ to be

$$f_{mm}(t) = N\left[\frac{\langle\phi_6(t)^2\rangle}{\langle\phi_6(t)\rangle^2} - 1\right] \sim t^{d/z}. \tag{7}$$

With Eqs. (6) and (7), we can estimate the values of the critical exponents η and z from the asymptotic behavior of the relaxation of ϕ_6 and its fluctuation.

We monitor the relaxation behavior of the bond-orientational order parameter of the hard-disk system. The starting configuration is set to be the perfect hexagonal-packed configuration, that is, $\phi_6(0)=1$. The particle number N is fixed at 23 288 throughout our simulations. We performed simulations of several system sizes and confirmed that this system size is large enough to regard the behavior of the longest simulation as the behavior of the infinite system with adequate accuracy. Periodic boundary conditions are taken for both directions of the simulation box. Up to 512 independent samples are averaged and about 10^9 collisions

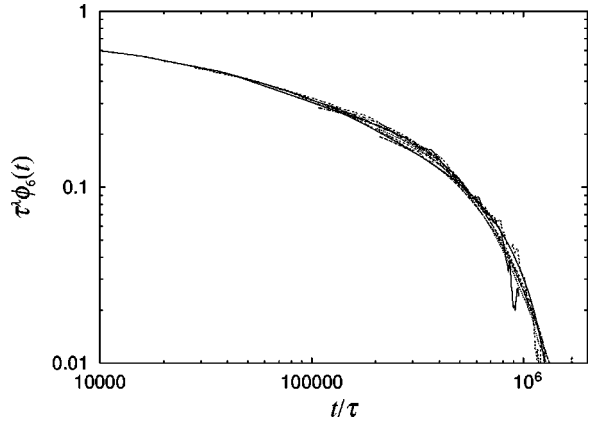

FIG. 2. Scaling plot of bond-orientational order for all densities with appropriately chosen $\tau(\epsilon)$ and λ in log-log plot.

are performed for each density. We study the range of densities from $\rho=0.800$ to 0.880 with the resolution of 0.01 and from $\rho=0.880$ to 0.890 with a fine resolution of 0.002.

Time evolution of the system is performed by event-driven molecular dynamics (EDMD) simulation. The EDMD method was first seen in 1959 [19]. The computational process advances by proceeding collision events of hard particles. In this method, the amount of the computation time required to proceed a single collision is $O(N^2)$. Using a neighbor-search algorithm with an exclusive grid mesh [20], it reduces to $O(N)$. With additional optimization techniques, such as the complete binary tree search and the dynamical upper time cutoff [21], it is finally reduced to $O(\ln N)$. The efficiency of the EDMD and the time-step molecular dynamics (TSMD) simulation depends on the detailed properties of systems. For the case of the hard-disk system, Rapaport [22] reported that EDMD exhibits better performance than TSMD up to $N\sim 10^5$.

The relaxation curves of $\phi_6(t)$ for each density are shown in Fig. 1. We made a scaling plot using Eq. (5) and the result with $\lambda=0.15(1)$ is shown in Fig. 2. Natural logarithms are used for all figures. The estimated $\tau(\rho)$ is plotted in Fig. 3, and we obtain the critical density $\rho_i=0.899(1)$, which is the

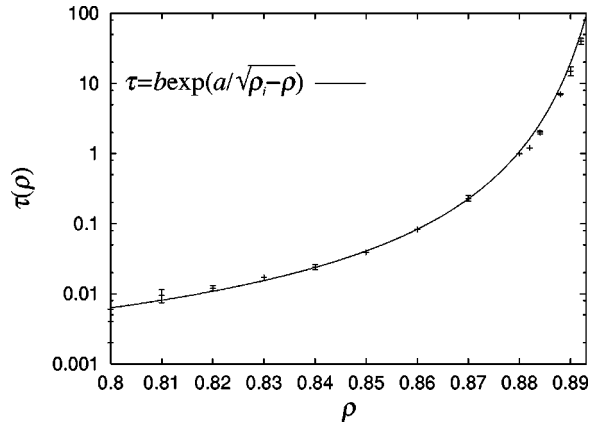

FIG. 3. Relaxation times $\tau(\epsilon)$ in units of τ at $\rho=0.888$ in semi-log plot. The solid curve is the line fitted using scaling form (4) with $\rho_i=0.899(1)$, $a=0.876(2)$, and $b=1.63(1)\times 10^{-3}$.

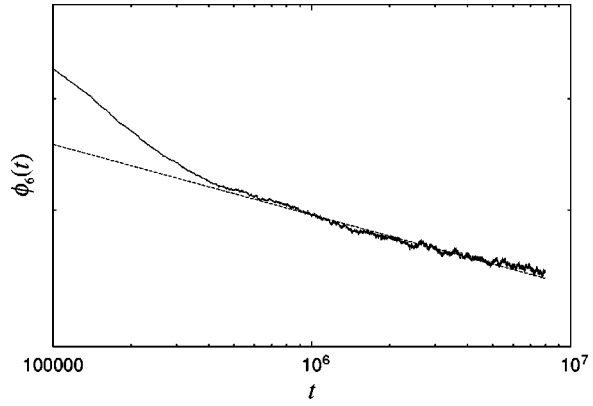

FIG. 4. Time evolution of the bond-orientational order parameter $\phi_6(t)$. After initial relaxation, $\phi_6(t)$ shows power-law decay. From the asymptotic behavior $\phi_6\sim t^{-\eta/2z}$, the value of $\eta/2z$ is determined to be 0.05(1).

transition point between the liquid and the hexatic phase.

With the critical point $\rho_i=0.899$ obtained above, we estimate the critical exponents η and z from the NER fluctuation analysis. The time evolution of $\phi_6(t)$ and its fluctuation at the criticality are shown in Figs. 4 and 5, respectively. From the asymptotic behavior of $\phi_6(t)$, we determine the value of $\eta/2z$ to be

$$\eta/2z = 0.05(1). \tag{8}$$

Similarly, from Eq. (7), we obtain the value of d/z to be

$$d/z = 0.8(1), \tag{9}$$

with the dimensionality $d=2$. From Eqs. (8) and (9), we obtain the values of the critical exponents $\eta=0.25(2)$ and $z=2.5(2)$.

In this paper, we observe the NER behavior of the bond-orientational order parameter ϕ_6 of the hard-disk system. We obtain (i) a critical point ρ_i of 0.899(1) with the dynamical KT scaling, and (ii) the critical exponent η of 0.25(2) by observing the fluctuation of ϕ_6.

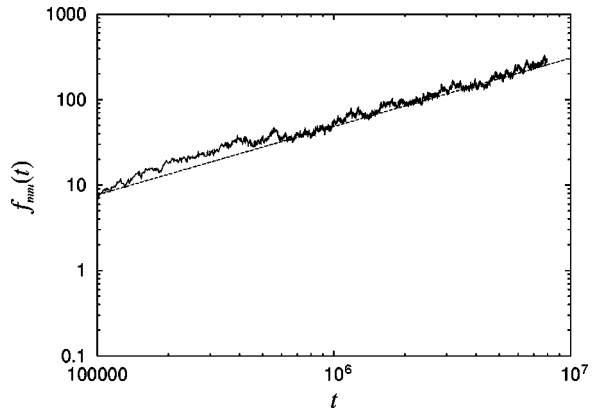

FIG. 5. The behavior of the fluctuation of the bond-orientational order parameter. After an initial relaxation, it shows good power-law behavior. From the asymptotic behavior (7), the value of d/z is determined to be 0.8(1). With $d=2$, one can obtain $z=2.5(2)$.

The critical density ρ_i obtained here is different from ρ_i' $\sim 0.913(1)$ which was obtained by a similar fitting performed by Weber *et al.* [13]. However in their study, the resolution of density near the criticality was insufficient. Therefore it is difficult to obtain an accurate value of the critical point by fitting.

We do not observe the saturation of the correlation time (i.e., that of the correlation length) near the critical point up to a system size of $N=23\,288$. This indicates that the transition would not be first order since the correlations would be finite in the first-order transition. However in a larger system, the correlation length may be finite; we thus cannot avoid the possibility of the first-order transition. To clarify this problem, we need more computational power or alternative analytical approaches.

The value of ρ_i obtained here is close to the crossing point of the fourth-order cumulant (the Binder parameter) ρ_{cross} $\sim 0.8985(5)$ estimated by Weber *et al.* While the Binder parameter should collapse over a finite range of density with KT transitions, they did not observe this and they concluded that this is one of the discrepancies with the KTHNY theory. It is difficult to thermalize the system in the KT phase because of the divergence of the correlation time. Thus the collapse behavior of the Binder parameter can be improved with a longer simulation time.

To summarize, the NER behavior of the bond-orientational parameter indicates that the transition between the isotropic and the hexatic phase is a KT transition. The results are consistent with the prediction of the KTHNY theory for the transition point and the critical exponents. The value of $\eta \sim 1/4$ is strong evidence that the transition is of the KT type. We do not study the transition between the hexatic and the solid phase in this paper. In our previous study [4], the transition point was estimated to be $\rho_m = 0.910(2)$, but we did not obtain the critical exponent at the transition. This issue is a problem for future consideration.

This work was carried out on SGI 2800 at the Supercomputer Center, Institute for Solid State Physics, University of Tokyo and CP-PACS at the Center for Computational Physics, University of Tsukuba. We thank S. Miyashita for valuable discussions. This work was partly supported by the Nestlé Science Promotion Committee, Grant-in-Aid for Scientific Research (C) No. 15607003 from the Japan Society for the Promotion of Science, and Grant-in-Aid for Young Scientists (B) No. 14740229 of the Ministry of Education, Science, Sports and Culture of Japan.

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