Dynamical scaling in two-dimensional quenched uniaxial nematic liquid crystals

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(Received 15 October 2004; published 23 February 2005)

The phase-ordering kinetics of the two-dimensional uniaxial nematic has been studied using a cell dynamic scheme. The system after quench from $T=\infty$ was found to scale dynamically with an asymptotic growth law similar to that of the two-dimensional O(2) model (quenched from above the Kosterlitz-Thouless transition temperature), i.e., $L(t)\sim[t/\ln(t/t_0)]^{1/2}$ (with nonuniversal time scale t_0). We obtained the true asymptotic limit of the growth law by performing our simulation for a sufficiently long time. The presence of topologically stable 1/2-disclination points is reflected in the observed large-momentum dependence k^{-4} of the structure factor. The correlation function was also found to tally with the theoretical prediction of the correlation function for the two-dimensional O(2) system.

DOI: 10.1103/PhysRevE.71.026119 PACS number(s): 61.30.Jf, 05.70.Ln, 64.60.Cn

The phase ordering of various systems with scalar, vector, and tensor order parameters has gained considerable interest over the last few years [1]. The system quenched from a high-temperature homogeneous disordered phase into an ordered phase does not get ordered instantaneously, instead the various degenerate ground states compete to be selected [1,2]. In the process, the system develops length scales that grow with time and topological defects, if present, are eliminated. An infinite system will never achieve complete ordering and the length scale will increase without any bound. If a single growing length scale characterizes the evolving system then it is said to scale dynamically. Rutenberg and Bray [3] proposed a very general technique, known as the energy scaling approach, to estimate growth laws in purely dissipating systems that scale dynamically. However, their scheme could also be applied to find out the relation between various length scales for a system in which dynamical scaling does not hold. If the growth law observed is different from their estimation then we can say that the system violates dynamical scaling. There are a large number of systems where the failure of dynamical scaling is observed, e.g., the one-dimensional *XY* model [4], the nonconserved two-dimensional O(3) model [5], and the conserved spherical model [6], etc.

The model we have studied is described by the Hamiltonian

$$H=-\sum_{\langle i,j\rangle}(\phi_i,\phi_j)^2,$$

where ϕ is the usual O(n) vector spin. Due to the spin inversion symmetry, the model represents a uniaxial nematic. The phase ordering of the same model was studied by Blundell and Bray [7] using a cell dynamic scheme for $d=2$, $n=2$, and $d=3$, $n=3$. In the present paper we have studied it for $d=2$ and $n=3$. It differs from the usual two-dimensional O(3) model due to its local inversion symmetry. While in the two-dimensional O(3) model, there is no stable topological singular defect, in the present model, due to presence of local inversion symmetry. The order parameter space, instead of being a simple three-dimensional sphere [as in the case of the usual O(3) models], is a three–dimensional sphere with antipodal points identified. This gives rise to topologically stable singular point defects of strength $\pm1/2$ (where the director rotates around the defect core by 180°). The mapping of other 1/2 integrals' defects are homotopically equivalent to the mapping of 1/2 defects. A $-1/2$-defect configuration is continuously deformable to a 1/2 defect configuration. Integral defects are topologically unstable due to the so-called "escape to the third dimension." Hence the first or the fundamental homotopy group of the system is just the two element group Z_2 ({0,1}) [8].

In general, the O(n) model with $d=n-1$ supports nonsingular topologically stable extended spin configurations carrying an integral topological charge, known as topological textures (or antitextures, for negative topological charges) [9]. In the two-dimensional O(3) model the textures are known as Skyrmions, instantons, or baby Skyrmions. The various length scales associated with these weakly interacting textures evolve with different growth laws in the one-dimensional *XY* model and in the two-dimensional O(3) model, which give rise to scaling violations in these systems [4,5]. In the two-dimensional O(3) model, the minimum energy configuration for an isolated texture is obtained by stereographically projecting the order parameter sphere on the physical space [3]. The configuration covers the order parameter space exactly once and hence the texture is associated with a topological charge 1. In the present model one would expect the presence of the two-dimensional O(3)-like textures, but our effort to find them using the algorithm prescribed by Berg and Luscher [10] resulted in the detection of no textures at all. This may be explained purely on the basis of homology of the order parameter space. Hindmarsh [11], on the basis of topology or more specifically homology of the order parameter space (which is the projective plane RP^2 in the nematics), has shown that in three-dimensional quenched nematics the probability of occurrence of monopoles is very low. Unlike in the Heisenberg model, in real

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nematics, in order to get a monopole, the order parameter space has to be covered twice and a special arrangement over many uncorrelated domains is required. This is responsible for a very low probability ($\sim 10^{-8}$) of occurrence of the monopoles. In case of the two-dimensional RP^2 model (an example of which is the present model) a similar argument should also be valid for the textures and this, perhaps, explains why we could not find the textures in this model. In case of the two-dimensional O(3) model, the different growth rates associated with the internal and external length scales of the extended textures are responsible for the failure of single length scaling [5,3]. Since in the present model textures (or antitextures) are highly suppressed due to topological reasons, the scaling violation is less likely. In the present paper we have established that the system scales dynamically.

We have used the cell dynamic scheme [7,13] for studying the coarsening dynamics of the soft-spin version of the concerned model. The discrete time updating relation is

$$\phi_{n+1}(i) = D\left[\frac{1}{4}\sum_{j}\left(\hat{\phi}_n(i),\hat{\phi}_n(j)\right)\phi_n(j) - \phi_n(i)\right] + E\hat{\phi}_n(i)\tanh(|\phi_n(i)|).$$

The sum is over nearest neighbors of i. The parameter D is called the diffusion constant, which determines the strength of the coupling between various cells evolving with time. The value of the parameter E should always be greater than unity and it determines the depth of quench [13]. In the above discrete time updating relation, the unit vectors (represented by hats) are used for stability of the iteration process. However one must avoid using both $\phi(j)$ as unit vectors as this leads to a freezing of the configuration in some metastable region [7].

The phase-ordering kinetics of the two-dimensional uniaxial nematic have been studied in details by Zapotocky *et al.* [12]. Using a cell dynamic scheme, they have shown that dynamical scaling is violated in two-dimensional uniaxial nematics films. They observed different values of the growth exponents, in the familiar algebraic growth law $L(t) \sim t^{\phi}$ (ϕ is known as a growth exponent), corresponding to different length scales. In determining the effective growth exponents they used the time range between 200 and 2000. However, as indicated by Rojas and Rutenberg [16], in the context of the issue of dynamical scaling in two-dimensional *XY* model quenched from above T_{KT} (the Kosterlitz-Thouless transition temperature), that in order to decide whether a system violates dynamical scaling or not, one must find the effective growth exponent in the true asymptotic limit after it is constant with time and before the finite size effect starts playing its role. They observed no violation in the dynamical scaling in the two-dimensional *XY* model. Like integral singular point defects (known as vortices) present in the two-dimensional XY model, the present two-dimensional model also supports topologically stable $\pm 1/2$ disclination points. This is the main finding of this paper. In Fig. 1, we have shown the Schlieren patterns in a 180×180 uniaxial nematic placed between crossed polarizers at different times as indicated in the figure. The patterns were obtained in the same way as discussed in Refs. [12,14,15]. So it is expected that the growth laws should be similar. By performing the simulation for a sufficiently long run to get the true asymptotic limit, we have shown that the two-dimensional uniaxial nematic scales dynamically by establishing that the same asymptotic growth law is valid for various length scales. Instead of the usual t^{ϕ} growth law, the system was found to scale asymptotically in a manner similar to the two-dimensional *XY* model quenched from above T_{KT} with the growth law, $L(t) \sim [t/\ln(t/t_0)]^{1/2}$ (t_0 nonuniversal time scale) [16,17]. We have performed our simulation with two lattice sizes 256×256 and 512×512. By comparing the results of the two lattice sizes, we did not find any significant finite size effect up to the time limit we have investigated.

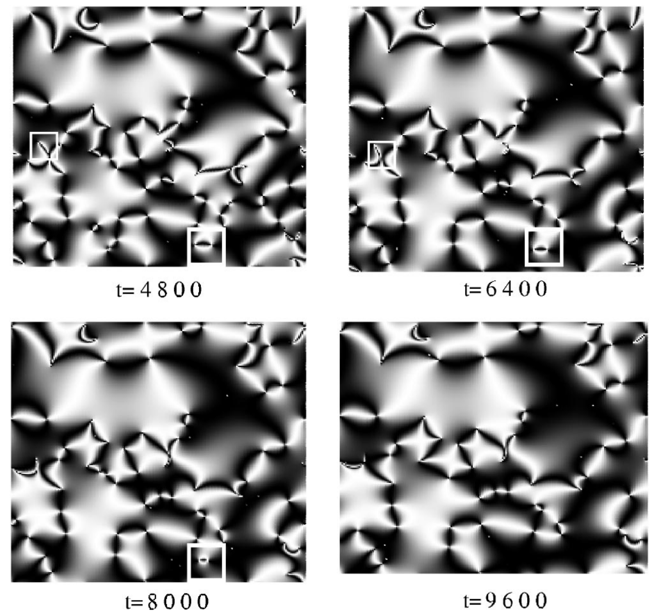

FIG. 1. The Schlieren patterns of the 180×180 uniaxial nematic placed between a crossed polarizer at different times as indicated in the figure. The polarizing microscope textures were obtained using the Muller matrices approach [12,14,15]. The 1/2-disclination point defects are identified by the intersection of two dark brushes and two white brushes. Two annihilating pairs of point defects are indicated by marked portions within the figure.

The normalized correlation function in the present model is given by

$$C(r,t) = 3/2\langle(\hat{\phi}(0),\hat{\phi}(r))^2\rangle - 1/2,$$

where $\langle\ \rangle$ represents the average over various random initial states (random length and direction). The scaling form of correlation function is given by

$$C(r,t) = f(r/L_{cor}(t)),$$

where the $L_{cor}(t)$ is the length scale required to collapse the correlation functions for different time. In Fig. 2 we have shown the scaling plot of $C(r,t)$ averaged over 20 initial states for a 256×256 lattice.

The structure factor scales with respect to $L_k = 1/\langle k\rangle$ [16], where $\langle k\rangle = \Sigma S(k,t)K/\Sigma S(k,t)$, is the first moment of struc-

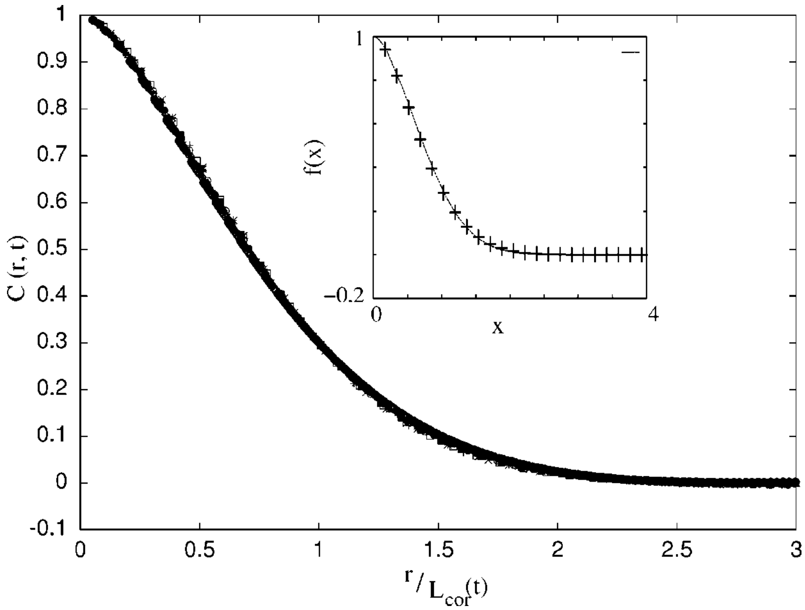

FIG. 2. Scaling plot of the correlation function $C(r,t)$ against $r/L_{cor}(t)$ for a 256×256 lattice ($D=0.1$, $E=1.1$) obtained after collapsing the correlation function at different time steps (as indicated in Fig. 4). The correlation length is obtained by using $C[L_{cor}(t),t]=0.3$. The agreement of the Bray-Puri prediction [19] for the O(2) ($\cdots$) model with the scaled correlation function($+$) ($t=400$) is shown in the inset. The BP function $f_{\mathrm{BP}}(x)=(1/\pi)\exp(-x^2/2)\ [B(1/2,3/2)]^2\ F[1/2,1/2,2;\exp(-x^2)]$. The maximum value of the L_{cor} obtained is 19.35, which is much smaller than the linear size of the lattice, i.e., 256.

ture factor. The scaling form of the structure factor is given by

$$S(k,t)=L_k^2 g[kL_k(t)].$$

In Fig. 3 we have shown the plot of $\ln[L_k^{-2}S(k,t)]$ against (kL_k). From the generalized Porod's law, the large-momentum structure factor for a two-dimensional system with point defects should be proportional to $\rho_{def}k^{-4}$ [1,12,18,19]. In the present system the density of the point defects (ρ_{def}) scales as L_{def}^{-2}, where L_{def} is the typical defect separation length. In the large-momentum limit we obtained the slope of $\ln[L_k^{-2}S(k,t)]$ versus kL_k plot equal to -4 as shown in Fig. 3, which verifies Porod's law. The good collapse of the tail verifies that L_k and L_{def} have asymptotically the same growth law. In Fig. 4, where we have tried the collapse of the correlation function with respect to the defect separation, poor collapse at the initial stage of dynamics does not, however, indicate the violation of dynamical scaling. At late stages the collapse shown in Fig. 4 is quite acceptable. In Fig. 5 we have verified that the growth law for all concerned lengths is asymptotically the same as that for the two-dimensional *XY* model, because of the linear dependence of $t/L^2(t)$ on $\ln(t)$. Figure 5 also verifies that the present system does not violate dynamical scaling. The correlation function that we obtained in our simulation also tallies with the Bray-Puri prediction [19] of the equal time correlation function for O(2) model, i.e.,

$$C(r,t)=(\gamma/\pi)[B(1/2,3/2)]^2F(1/2,1/2,2;\gamma^2),$$

where

$$\gamma(r,t)=\exp(-r^2/8t),$$

$B(x,y)$ is the beta function, and $F(a,b,c;z)$ is the hypergeometric function.

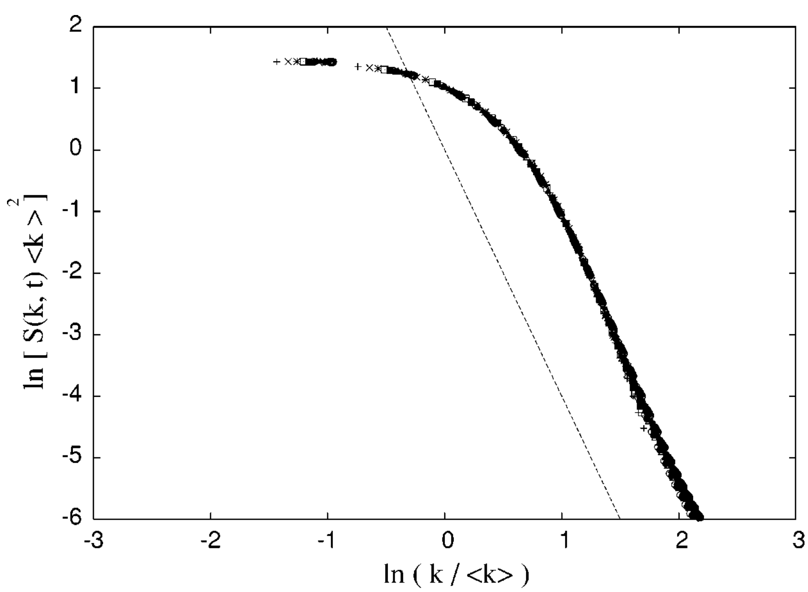

FIG. 3. Log-log plot of the structure factor scaling function of a 256×256 lattice ($D=0.1$, $E=1.1$). The first moment $\langle k\rangle$ is used for rescaling of momenta. The straight line (dotted) has a slope of -4, which indicates the validity of the generalized Porod's law.

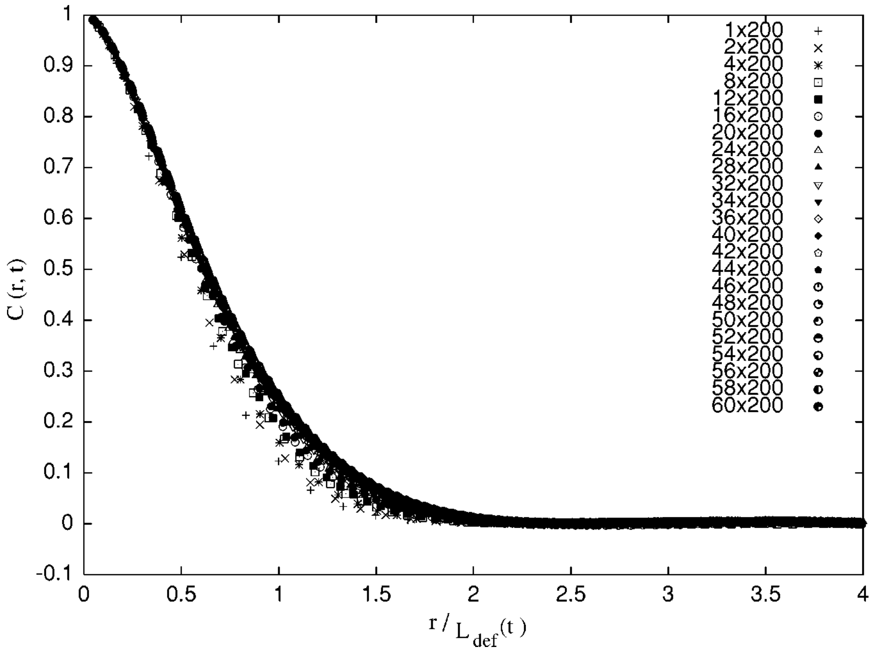

FIG. 4. The attempted collapse of the correlation function for a 256×256 lattice ($D=0.1$ and $E=1.1$) with respect to the defect separation length $L_{def}=1/\rho_{def}^{1/2}$. The failure of collapse at the initial stages of phase ordering does not indicate the violation of dynamical scaling. In the asymptotic limit the correlation function scales well with respect to the defect separation, indicating the proportionality of $L_{cor}(t)$ and $L_{def}(t)$.

Thus in the scaling form we have $C(r,t)=f_{\mathrm{BP}}(x)$ (BP stands for Bray and Puri), where $x=r/L(t)$ and $L(t)=(4t)^{1/2}$. The logarithmic factor is not correctly reflected in that function. However, for comparison we have plotted the $f_{\mathrm{BP}}(x)$ and the scaled correlation function (for $t=400$) in the inset of Fig. 2. We performed our simulation with higher values of D (0.5) and got similar asymptotic results. Higher values of D are useful in achieving the asymptotic regime faster. However, the finite size effect is also more prominent in case of large D. We have not considered noise in the time evolution equation; hence we are effectively working at $T=0$. However, it is known that quenching to $T=0$ may lead to metastable freezing [20]. In order to check that our results are not influenced by such freezing, we performed a number of simulations (almost 100 steps) with noise, by adding a constant amplitude (of the order of 0.1) random configuration to the order parameter. The noise amplitude used was enough to generate a large number of pairs of disclination point defects. We could not find any discrepancy with the results obtained without noise.

To summarize we would like to focus on the main findings of our paper. We have confirmed that dynamical scaling is not violated in a two-dimensional nematic with order parameter dimensionality three, and asymptotically the growth laws are the same as that of the two-dimensional *XY* model quenched from above T_{KT} (i.e., the initial state with free vortices). Consideration of topological defects in the issue of dynamics is very necessary, because the structure of the defects determines the large-momentum dependence of the structure factor, which has an important role in the determi-

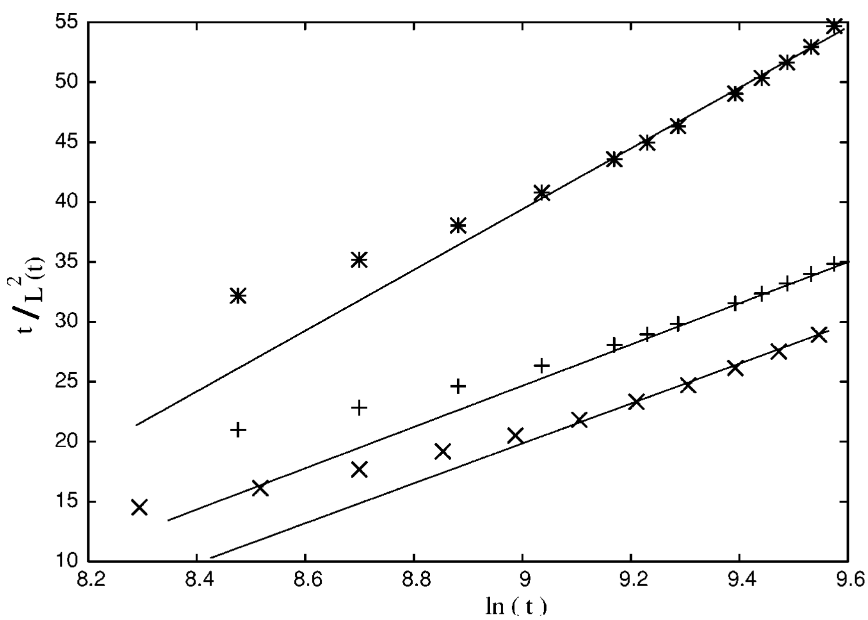

FIG. 5. The plot of $t/L^2(t)$ vs $\ln(t)$ for three lengths $L_{cor}(\times)$, $L_{def}(+)$, and $L_k(*)$ for a 512×512 lattice ($D=0.1$ and $E=1.1$). The observed linear dependence at late times (over a wide range from $t=5500$ to $t=14\,400$) indicates that the dynamical scaling growth law $L(t) \sim [t/\ln(t/t_0)]^{1/2}$ holds. However, the time scale t_0 is found to be nonuniversal.

nation of the growth laws [3]. In the O(n) model with $n \leqslant 2$, the topological defects dominate the dynamics. Since both the present two-dimensional model and the two-dimensional *XY* model support singular point defects, it is expected that the dynamics should be similar and this is established in this paper. We were able to establish the expected result and achieved the true asymptotic limit of the dynamical scaling by performing longer simulation with the help of increased computational power now available.

The authors are thankful to Dr. A.D. Rutenberg for useful discussions. One of us (S.D.) acknowledges the financial assistance from the Council of Scientific and Industrial Research (CSIR), India.

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