Cell dynamics simulation for the phase ordering of nematic liquid crystals

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A discrete model is presented to describe the dynamics of nematic liquid crystals for the case where topological defects dominate the spatial pattern. A numerical study is given of the annihilation kinetics of the defects in the two-dimensional nematic system with P^2 symmetry. The structure factor is found to obey a scaling law $S(k,t)=\langle k\rangle_t^2 g(k/\langle k\rangle_t)$ where the first moment $\langle k\rangle_t$ varies as $\langle k\rangle_t \sim t^{-0.42}$. The asymptotic power-law tail $g(x)\sim x^{-4.5}$ is found.

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The phase-ordering dynamics of quenched disordered systems has been an area of very active research for some time [1]. A typical example is spinodal decomposition of binary alloys and fluids. Recently, effort has been devoted to the study of systems with more complicated order parameters, such as n-component vectors and nematic liquid crystals, [2–8]. These systems exhibit scaling laws characterized by a few parameters such as the internal symmetry and the dimensionality of space. This universality is due to the fact that the spatial patterns exhibited by these systems are governed by topological defects. Thus the study of the kinetics of defects is crucial in understanding the phase-ordering dynamics.

Liquid crystals are ideally suited for experimental study of defect dynamics. Indeed, recent experiments [9–11] have provided much insight on defect kinetics. However, analytical understanding is limited to the vector order-parameter systems with O(N) symmetry. Although the nematic liquid crystal differs from vector systems only in whether the order parameter has a distinction between head and tail, this makes topological singularities of nematic liquid crystals somewhat complicated. The order-parameter space is a projective plane P^2, whose topological defects are characterized by the homotopy groups [12] $\pi_1(P^2)=Z_2$, $\pi_2(P^2)=Z$, and $\pi_3(P^2)=Z$; i.e., in two-dimensional (2D) nematic liquid crystals there can be singly charged point defects and extended defects (textures) with integer charge, and there are one species of line defects, point defects with integer charge, and textures in three dimensions. In this paper, we consider the 2D system with P^2 symmetry.

The Frank free energy has been used to describe the macroscopic characters of nematic liquid crystals. This is, however, not suitable for systems including topological defects, since the one-parameter approximation of the Frank energy is identical to that of the classical spin system with S^2 symmetry. This means that the stationary solution of the Frank energy can involve topological defects found in the spin system whose homotopy groups are $\pi_1(S^2)=0$ and $\pi_2(S^2)=Z$, which is different from that of the P^2 system.

In this paper, we construct a discrete model to describe the growth kinetics of the P^2 system. As the order parameter is nonconserved, the evolution equation is simply given by

$$\partial_t \psi = -\frac{\delta F}{\delta \psi} , \tag{1}$$

where ψ is a 3D vector field. The key point is the construction of the energy F. When ψ lies on the minima of a local potential $V(|\psi|)$, the energy should be invariant under the global SO(3) rotation of ψ and under the local inversion, i.e., $\psi(\mathbf{r})\rightarrow -\psi(\mathbf{r})$. A simple model satisfying these condition was given by Khveshchenko, Kogan, and Nechaev [13] as

$$F_{\mathrm{KKN}} = -\sum_{i,j} v_{ij}\mathbf{n}_i\cdot\mathbf{n}_j , \quad \mathbf{n}_i\in S^2 , \quad v_{ij}\in\pm 1 . \tag{2}$$

They considered the phase transition in two space, employing the mean-field-approximation method in lattice-gauge theory. They treated $\{\mathbf{n}_i\}$ and $\{v_{ij}\}$ as independent variables in their calculation of the partition function. However, the gauge v_{ij} is an auxiliary field depending intrinsically on ψ because the energy should be determined solely by the configuration of the director. For this Z_2 gauge, for example, we could take

$$v_{ij}=\mathrm{sgn}(\mathbf{n}_i\cdot\mathbf{n}_j) . \tag{3}$$

Note, however, that since the gauge is required only to preserve the symmetry of the system, it is not restricted to be Z_2 symmetric. The only constraint on v_{ij} is simply that it be an increasing odd function of $\mathbf{n}_i\cdot\mathbf{n}_j$. We avoid Eq. (3) because of unphysical pinned structures, appearing as follows.

Let us consider the P^1 system for simplicity, where the director is planar. A typical pinned structure for the model (3) is shown in Fig. 1. The change of the nearest-neighbor (NN) interaction associated with the rotation of the central director $\mathbf{n}_i$ is given by

$$-\sum_{j\in NN \text{ of } i} v_{ij}\mathbf{n}_i\cdot\mathbf{n}_j = -\sqrt{2}\sin\left[\theta\pm\frac{\pi}{4}\right] ,$$

where the plus and minus signs are taken for $0\le\theta<\pi/2$ and $\pi/2<\theta<\pi$, respectively. Thus, the energy has double minima: one at $\theta=\pi/4$ corresponds to a two-defect state, and the other at $3\pi/4$ is a no-defect state. When

the system starts from a random configuration, there appear some pinned structures such as the former. In contrast, for a similar structure for the XY model, the energy is unchanged by the rotation of the central spin. Since the model with a P^1 director should be dynamically identical to the XY model, we choose v_{ij}, which keeps the energy unchanged by rotation. A simple energy satisfying this condition is the linear relation $v_{ij}=\mathbf{n}_i\cdot\mathbf{n}_j$. In this way, we avoid the unphysical, pinned configurations. Consequently, the free energy is written as

$$F=\tfrac{1}{2}\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\{-[\boldsymbol{\psi}(\mathbf{r})\cdot\boldsymbol{\psi}(\mathbf{r}')]^2+\tfrac{1}{4}(|\boldsymbol{\psi}(\mathbf{r})|^2+|\boldsymbol{\psi}(\mathbf{r}')|^2)^2\}+\sum_r f(|\boldsymbol{\psi}(\mathbf{r})|)$$
$$=\tfrac{1}{4}\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}[(|\boldsymbol{\psi}(\mathbf{r})|^2+|\boldsymbol{\psi}(\mathbf{r}')|^2)|\boldsymbol{\psi}(\mathbf{r})-\boldsymbol{\psi}(\mathbf{r}')|^2-\tfrac{1}{2}|\boldsymbol{\psi}(\mathbf{r})-\boldsymbol{\psi}(\mathbf{r}')|^4]+\sum_r V(|\boldsymbol{\psi}(\mathbf{r})|)\ ,\quad \boldsymbol{\psi}\in\mathbb{R}^3\ , \tag{4}$$

where the quadratic terms in the first summation are added so that, under the condition $|\boldsymbol{\psi}(\mathbf{r})|=\text{const}$, the energy should take the minimum value when directors align uniformly. In the planar rotator case (P^1), this is equivalent to the XY spin model under a transformation that doubles the angle between nearest-neighbor pairs of spins; i.e., if $[\boldsymbol{\psi}(\mathbf{r})\cdot\boldsymbol{\psi}(\mathbf{r}')]^2=(\mathbf{s}_\mathbf{r}\cdot\mathbf{s}_{\mathbf{r}'}+1)/2$ under $|\boldsymbol{\psi}(\mathbf{r})|=|\mathbf{s}_\mathbf{r}|=1$, we have $F=-\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\mathbf{s}_\mathbf{r}\cdot\mathbf{s}_{\mathbf{r}'}$.

Thus we obtain a cell dynamical model:

$$\boldsymbol{\psi}(\mathbf{r},t+1)=\tau c\sum_{\mathbf{r}'}z_{\mathbf{r}\mathbf{r}'}\{[\boldsymbol{\psi}(\mathbf{r},t)\cdot\boldsymbol{\psi}(\mathbf{r}',t)]\boldsymbol{\psi}(\mathbf{r}',t)-\tfrac{1}{2}(|\boldsymbol{\psi}(\mathbf{r},t)|^2+|\boldsymbol{\psi}(\mathbf{r}',t)|^2)\boldsymbol{\psi}(\mathbf{r},t)\}+(1+\tau)\boldsymbol{\psi}(\mathbf{r},t)-\tau|\boldsymbol{\psi}(\mathbf{r},t)|^2\boldsymbol{\psi}(\mathbf{r},t) \tag{5}$$

where the sum is taken over the nearest-neighbor (NN) and the next-neighbor (NNN) cells. The conventional local energy $V(x)=-x^2/2+x^4/4$ was chosen. In the present simulation, $z_{\mathbf{r}\mathbf{r}'}$ is unity for NN and $\frac{1}{2}$ for NNN cells. The value of the parameters $c=0.2$ and $\tau=0.1$ are chosen so that the core size of defects ($\sim c^{1/2}$) is less than unity. Experience has shown that even such a parameter does not cause pinning, though it is problematic in the conserved order-parameter cases. Shown in Fig. 2 are three snapshots of directors and defects. The positions of the defects were found as follows. Consider a map $\mathbf{r}\rightarrow\boldsymbol{\psi}(\mathbf{r})$ for a closed loop of real space. The paths on the order-parameter space, which is half of a sphere, are classified into two homotopy classes. One runs from a point to its opposite one, identical to the starting point, and the other returns to the starting point. If the loop in rel space is mapped to a former path, a defect is inside the loop. In our discrete model, we check this for each unit square of cells. Let $\{\hat{\boldsymbol{\psi}}^{(j)}|1\le j\le 4\}$ be the normalized projection of $\boldsymbol{\psi}$'s at the corners of a square to a plane in the order-parameter space whose normal unit vector is denoted by $\hat{\mathbf{z}}$. We then compute the angles θ_j between $\hat{\boldsymbol{\psi}}^{(j)}$ and $\hat{\boldsymbol{\psi}}^{(j+1)}$ defined on $[-\pi/2,\pi/2]$ through $\theta_i=\text{sgn}(a_jb_j)\arccos(|b_j|)$, where $a_j=\hat{\mathbf{z}}\cdot(\hat{\boldsymbol{\psi}}^{(j)}\times\hat{\boldsymbol{\psi}}^{(j+1)})$, $b_j=\hat{\boldsymbol{\psi}}^{(j)}\cdot\hat{\boldsymbol{\psi}}^{(j+1)}$, and $\hat{\boldsymbol{\psi}}^{(5)}=\hat{\boldsymbol{\psi}}^{(1)}$. By definition, $\zeta=\sum_{j=1}^4\theta_j$ must be zero or $\pm\pi$ within numerical error. If $|\zeta|=\pi$, we

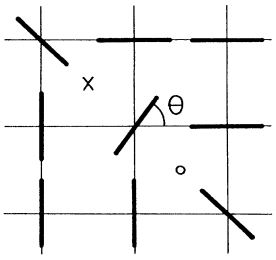

FIG. 1. A pinned configuration of a nematic model with Z_2 gauge.

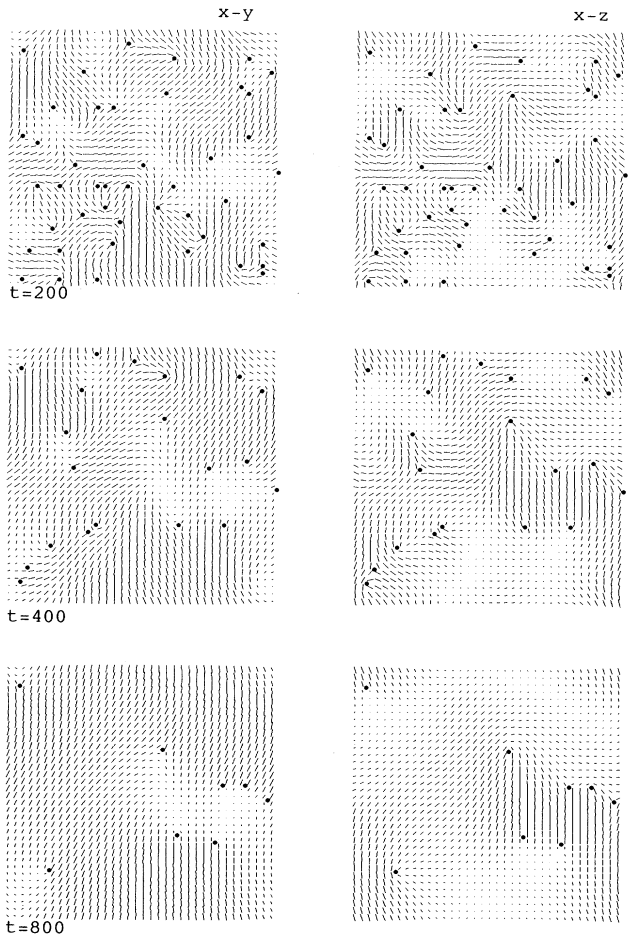

FIG. 2. A time sequence showing the growth of directional order and the annihilation of defects. The left and right columns show the x-y and x-z components of directors, respectively, and the dots represent defects.

regard the center of the square as a defect position. Since the sign of ζ depends on the choice of the projection plane, the sign makes no sense topologically. Thus the defect charge is classified into two values 0 and 1, and the collision of any two defects results in the annihilation, i.e., $1+1=0$. One can see the pair-annihilation process of defects in Fig. 2. As shown in Fig. 3, the number of defects decreases in a power law $N \propto t^{-0.84}$ in the late stage $800 \lesssim t \lesssim 7000$, where the mean separation of defects changes from 10 to approximately 30. The data for N as well as the following structure factor were taken on 256^2 lattices and averaged over ten initial conditions.

The structure factor is written as

$$S_{ij}(k)=\langle \Xi_{ij}(\mathbf{k})\Xi_{ij}(-\mathbf{k})\rangle \ , \tag{6}$$

$$\Xi_{ij}(\mathbf{k})=L^{-1}\sum_{\mathbf{r}} e^{2\pi i \mathbf{k}\cdot\mathbf{r}/L}\Phi_{ij}(\mathbf{r}) \ , \tag{7}$$

where Φ_{ij} is the tensor order parameter defined in terms of the components of $\boldsymbol{\psi}$, $\{\psi_i\}$ as

$$\Phi_{ij}(\mathbf{r})=\psi_i(\mathbf{r})\psi_j(\mathbf{r})-\tfrac{1}{3}\delta_{ij} \ , \tag{8}$$

and $L=256$. Considering the isotropy of the system, we calculate two averaged structure factors

$$S_d(k,t)=\tfrac{1}{3}\sum_i S_{ii}(k,t) \quad \text{(diagonal part)} \ , \tag{9}$$

$$S_o(k,t)=\tfrac{1}{6}\sum_{\substack{i,j \\ i\neq j}} S_{ij}(k,t) \quad \text{(off-diagonal part)} \ . \tag{10}$$

Figure 4 shows the two structure factors which have been scaled by the first moment of $\langle k\rangle = \sum_k kS(k,t)/\sum_k S(k,t)$ as $S(k,t)=\langle k\rangle^2 g(k/\langle k\rangle)$. Figure 5 shows that the characteristic length increases in a power law $\langle k\rangle \propto t^{\phi}$, $\phi=0.42$, consistent with the behavior of the number of defects. This exponent is somewhat less than the value $\phi=\frac{1}{2}$ expected by the dimensional analysis. Such a lower exponent was also observed in simulations of the vector order-parameter systems [5,14]. This fact has been determined to mean that the system

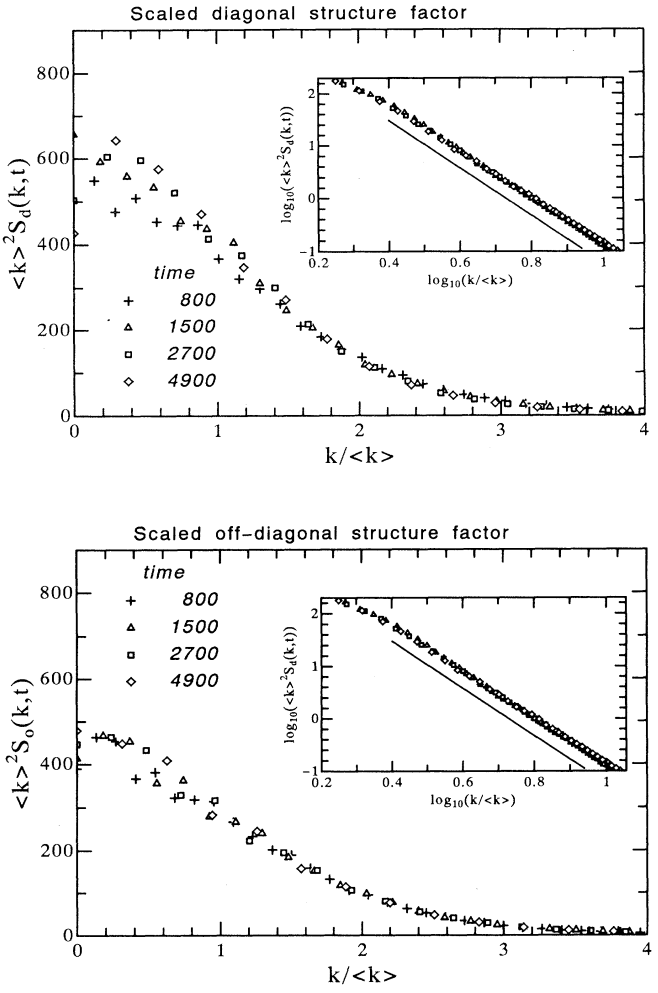

FIG. 4. The scaled structure factor: (a) diagonal part, (b) off-diagonal part. The inset is a log-log plot of the large-k regime which shows the power-law tail. The solid lines indicate the slope (-4.5).

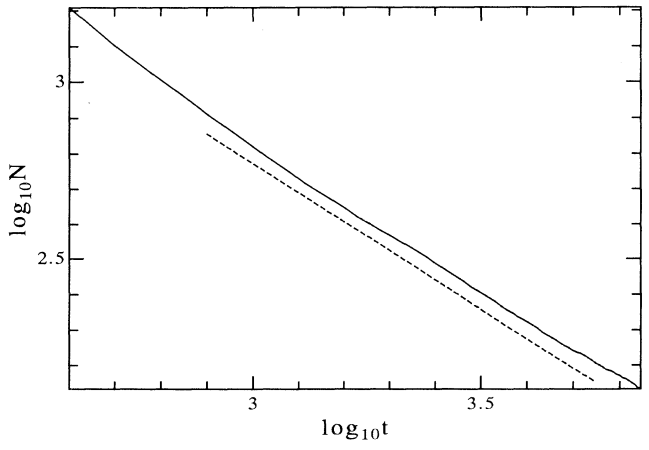

FIG. 3. The number of defects vs time (solid line). The dashed line indicates the slope (-0.84). The data were taken on 256^2 lattices and averaged over ten initial conditions.

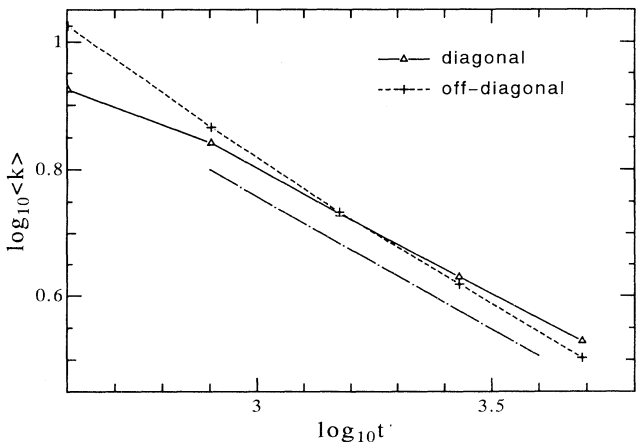

FIG. 5. The first moment of structure vs time. The dotted-dashed line indicates the slope (-0.42).

has not reached the asymptotic regime. It is, however, still possible that the lower exponent is a property of systems with defects.

Another significant behavior is the power-law tail $g(x) \sim x^{-\chi}$, $\chi = 4.5$. The exponent 4.5 is an intermediate exponent between XY and Heisenberg systems [15]. This fact is naively expected from the local configuration around a defect; i.e., the dimensionality of the director is like that of Heisenberg system and the pointlike defect is like that of the XY system.

In summary, we have presented a discrete model for the phase ordering of the nematic liquid crystals. By numerical simulations, we found the scaling behavior of the structure factor, which has a power-law tail with the noninteger exponent 4.5 distinguishing the P^2 nematic liquid crystals from the O(N) vector systems. The 2D nematic liquid crystals with P^2 symmetry are, however, hard to observe experimentally because the director is trapped in the plane or in the vertical direction due to the boundary effect. To compare the simulation with experiment, therefore, we had to study 3D systems. Our model can be used for this purpose, and this is now in progress. After this paper was submitted for publication, the author received a preprint from Blundell and Bray [16], who have performed a 3D simulation result for P^2 symmetry and a 2D simulation for P^1 symmetry using a similar model. The 3D simulation shows a growth exponent $\phi = 0.42$ and a noninteger power-law tail ($\chi = 5.3 \pm 0.1$) consistent with the present one.

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