Motion of Interacting Point Defects in Nematics

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The motion of interacting point defects in a uniaxial nematic is considered in the one-constant approximation. It is shown that the dynamics depends in a decisive way on the reduction in nematic order near the defect core. The computed velocities of interacting defects are inversely proportional to their separation when defects approach each other from afar.

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Motion of topological defects plays a decisive role in the dynamics of ordered media. Rheology of nematics is dominated by the formation and motion of defects, mostly in the form of "thin" and "thick" lines [1]. The statics of defects is understood rather well. At the same time, very little is known so far on dynamics of defects in nematics either theoretically or experimentally. A recent state-of-the-art survey [2] contained theoretical results almost exclusively on the defect statics. There seems to be no experimental studies of the motion of defects under controlled conditions that would yield "clean" data of the kind that became available recently for motion of defects in convective patterns [3].

The topological theory [1, 4] predicts for a uniaxial nematic topologically stable point defects with integer charges and line defects with the charge $\frac{1}{2}$. The latter are identified with thin lines, but the abundance of thick lines with the integer charge that should be topologically unstable, apparently, cannot be explained in the framework of the static theory. The singularity of the free energy in the vicinity of a defect can be removed by relaxing the presumption of perfect local alignment. Nonsingular symmetric static solutions for isolated point defects with an isotropic core were obtained by Schopohl and Sluckin [5]. Another possibility is the splitting of a point defect into a ring singularity due to biaxiality effects [6], which is forced by the absence of topologically stable point defects in a biaxial nematic [4]. In the following, we shall not consider this alternative, presuming the nematic to be strictly uniaxial.

The standard Leslie-Ericksen nematodynamics [7] that presumes perfect local nematic alignment becomes clearly inadequate when defects are present. An attempt to incorporate the imperfections of local alignment into the hydrodynamic theory in a consistent way has been undertaken recently [8]. Olmsted and Goldbart [9] took into account reduction in nematic order explicitly to predict the influence of shear on the isotropic-nematic phase transition; their results were restricted, however, to computations of a nonequilibrium phase diagram in a static system with a homogeneous orientation of the director.

In this Letter we consider the problem of interaction of two point defects in a nematic liquid crystal assuming the simplest model of friction-dominated dynamics in the "one-constant" approximation. We shall show that the motion depends in a decisive way on the reduction in nematic order near the defect core, so that the dynamics is frozen when the local molecular alignment is presumed perfect.

Our starting point is the Landau–de Gennes Lagrangian that expresses the free energy of the nematic as a functional of the order parameter field [1, 10]. We shall consider a uniaxial nematic with the order parameter expressed by a symmetric traceless tensor $Q^{ab} = u^a u^b - \frac{1}{3}\delta^{ab}|\mathbf{u}|^2$. The length $\rho = |\mathbf{u}|$ of the vector $\mathbf{u}$ measures the local coherence of molecular alignment. The unit vector $\mathbf{n} = \mathbf{u}/|\mathbf{u}|$ is called the *director*. The tensor form of the order parameter Q implies the invariance to the inversion of the director.

The vector $\mathbf{u}$ can be expressed using any coordinate system in the order parameter space with a metric tensor g_{ab} that does not need to coincide with the coordinate system in the real space. The state of a perfect local nematic alignment $\rho = 1$ corresponds to the minimum of the Landau–de Gennes potential $V(\rho) = \epsilon^{-2}(\rho^2 - \frac{1}{2}\rho^4)$, where ϵ is the healing length. We shall write the elastic energy connected with the rotation of the director in the one-constant approximation neglecting the distinction between the energies of splay, bend, and twist deformations. Thus, we assume

$$G(u) = \frac{1}{2} \int \left[g_{ab} \nabla u^a \cdot \nabla u^b + V(|u|) \right] d^3x \,. \qquad (1)$$

Formulation of elastohydrodynamic equations describing the motion of nematics under weakly nonequilibrium conditions with the account of local reduction of nematic order remains a major open problem that we do not aspire to solve in the framework of this Letter. The dynamical ansatz we shall assume here is the friction-dominated dynamics with a single friction coefficient that can be incorporated into the time scale. The mathematical expression of this ansatz is the *gradient dynamics*

$$\partial_t u^a = -g^{ab}\, \delta G / \delta u^b \,. \qquad (2)$$

This model assumes relaxation to a stationary state via rotation of the director field and change in local degree of molecular alignment, and neglects convective "backflow" effects. It also neglects anisotropy of friction coefficients, as well as the anisotropy of elastic constants. While we do not expect the model to be quantitative, it allows us to demonstrate most clearly the crucial role of the loss of nematic order in the defect dynamics. The dynamic equations (2) can be written in a general form [11] using Cristoffel symbols Γ^a_{bc} corresponding to the chosen metric of the order parameter space:

$$\partial_t u^a = \nabla^2 u^a + \Gamma^a_{bc} \nabla u^b \cdot \nabla u^c - g^{ab}\, \partial V/\partial u^b. \qquad (3)$$

The static problem at $\rho = 1$ [i.e., restricted to the minimal stratum of the potential $V(\rho)$] is equivalent to the nonlinear σ model [12]. It possesses a variety of exact analytic solutions that are obtained using the correspondence between the complex analytic structure of the sphere $\rho = 1$ in the order parameter space, on one side, and a suitable 2D manifold of the real space, on the other side. In the context of this work, two families of analytic solutions are useful [11]. One of them is the family of topologically unstable vortex solutions with circular symmetry:

$$\alpha = 2\arctan(r/l)^N, \quad \beta = \pm N\phi, \qquad (4)$$

where α and β are, respectively, the polar and azimuthal angles defining the orientation of the director, and l is an arbitrary parameter measuring the spatial extent of the vortex. In 3D, this family of solutions corresponds to straight line vortices with the circulation $\pm 2N\pi$. Line defects with $N = \pm 1$ are quite common in sheared nematics, and can be identified with thick lines, as opposed to topologically stable thin lines with the circulation $\pm\pi$.

Another family of solutions corresponding to point defects with the charge N can be constructed using polar coordinates (r, θ, ϕ) in the real space and presuming the orientation of the director to be independent of r. This leads to the "combed hedgehog" solution family

$$\alpha = 2\arctan\left(k \tan\frac{\theta}{2}\right)^N, \quad \beta = \pm N\phi. \qquad (5)$$

Both families of solutions are degenerate, so that the energy per a cylindrical shell of the vortex solution (4) is independent of l and the energy per a spherical shell of the hedgehog solution (5) is independent of k. The hedgehog solution (5) with $N > 0$ is "combed" towards the north pole at $k > 1$ and towards the south pole at $k < 1$; the slant is opposite at $N < 0$. At large k, the director rotates within a narrow polar region only. The limiting form at $k \to \infty, N > 0$ is the singular line along the ray $\theta = 0$, which coincides with the limiting form of the line solution (4) at $l \to 0$. The limiting forms of solutions for two defects with charges of equal absolute value and opposite signs will be thus matched precisely when the director is parallel to the line connecting the defects in the entire space and turns infinitely fast by π on the connecting line itself. This implies that the pair of defects will be stationary, provided the perfect alignment is not destroyed even when the director rotates arbitrarily fast.

This (rather unphysical) conclusion is in accordance with the mathematical result of Brezis, Coron, and Lieb [13] who found that the above singular solution minimizes the energy of a stationary pair of point defects. The same result can be obtained with the help of Peach-Köhler type arguments. Suppose that the elastic energy is mainly concentrated in the vicinity of the connecting line and that the energy per unit length F is constant. Then the rate of change of the total energy due to the motion of the pair of defects with the velocity v towards their common center of gravity is $2Fv$, so that F plays the role of the Peach-Köhler force. On the other hand, the same change of energy can be expressed by considering the quasistationary motion of each defect in the comoving frame as $2v^2I$, where the dissipative integral I is computed using the combed hedgehog solution (5) with $N = 1$ as

$$I = \int_0^\pi \alpha_z^2 \sin\theta\, d\theta = \int_0^\pi \sin\alpha/\sin^2\theta\, d\alpha. \qquad (6)$$

As $k \to \infty$, F remains finite while I diverges, and, as a consequence, the velocity $v = F/I$ vanishes.

Returning to the full Lagrangian (1) accounting for imperfect local alignment, we interpret the above result as the indication that local reduction of nematic order in the regions of rapid rotation of the director is essential for the defect interaction. The stationary solution with perfect constant alignment everywhere except the singular connecting line appears in the limit $\epsilon \to 0$ only, and the propagation velocity must be finite at $\epsilon \neq 0$.

The mechanism setting the defects into motion is seen qualitatively in the following way. "Combing" the interacting hedgehogs one towards another is necessary to smoothly connect their director fields. Tight combing leads to increased local rotation, and reduction in nematic order helps to reduce energetic costs. In the immediate vicinity of point defects, only spherically symmetric hedgehog solutions are admissible, but the presence of other defects or containing walls break the spherical symmetry globally. By analogy with two-dimensional dissipative dynamics with a complex order parameter for which the analytical asymptotic theory is available [14], we infer that the defect core is set into motion by deviations from spherical symmetry in its vicinity caused by the presence of another defect. The interaction is mediated by the director field changing on a scale large compared to the core size in the "outer" region where the nematic order is nearly perfect. Unlike the two-dimensional case, the field equations are, however, nonlinear even in the outer region, and the analytic solution is unavailable.

For numerical solution of the dynamic problem (3), we consider a single defect in a large box with the reflecting boundary at $z = 0$. By symmetry, this arrangement is equivalent to a pair of interacting defects. We set $\beta = \phi$ and reduce the remaining systems to a single equation for the complex variable $u = \rho e^{i\alpha}$ that we write in cylindrical coordinates as

$$\partial_t u = u_{zz} + r^{-1}(ru_r)_r + \epsilon^{-2}(1-|u|^2)u + r^{-2}(\overline{u}-u). \tag{7}$$

Further on, we set $\epsilon = 1$; thus, the defect separation is measured in units of the healing length. The interaction with the reflecting wall at $z = 0$ is equivalent to the interaction with the mirror image (the defect of the opposite charge). The other boundaries must be dynamically neutral, which is best approximated by imposing the orientation of the director parallel to the z axis on the side wall and presuming the alignment to be perfect in the far field. Thus, we assume the "far" boundary condition $\alpha = \pi$, $\rho = 1$, or $u = -1$.

At the start, the defect velocity is determined by the initial conditions which define the director field in the vicinity of the defect core. In the first run, we placed the defect at some point $z = -L$ on the axis $r = 0$, and took as the initial condition the orientation field $\alpha(r, z)$ corresponding to the hedgehog solution (5) with some suitable k. The degree of local alignment is approximated by some field $\rho(r, z)$ vanising at the defect location and increasing to unity with the distance from the defect. Setting $k > 1$ directs the motion towards the plane $z = 0$, and, at sufficiently large k, makes the solution rather insensitive to the location of the back wall. The motion is initially fast but slows down as the director field adjusts before accelerating again at close approach to the reflecting wall.

In order to eliminate the dependence on arbitrary initial data, we adopted the following iterative procedure. At the moment when the velocity is minimal, the computation is stopped, and the field is rescaled $u(r, z) \to u(2r, 2z)$. As a result of the rescaling, the value of α at the side wall deviates from π by some angle $\delta\alpha(z)$. The required alignment at the side wall $r = R$ is then restored by turning the director by the angle $\delta\alpha\, r/R$. This procedure allows the order parameter field in the vicinity of the defect to relax to a quasistationary distribution that well approximates the order parameter field around the defect that had traveled to the specified location from infinity. Three such iterations were sufficient to eliminate the initial deceleration. Apart from the effect of the side wall, the order parameter field obtained in this manner (Fig. 1) is universal, and simply rescales as the separation decreases. Accordingly, the defect velocity changes inversely proportional to the separation. In dimensional units, $v = a\epsilon/L$ with the numerical constant $a = 6.5$ (Fig. 2).

The radial distribution of the director at $0 > z > -L$ (Fig. 3) was found to follow, except near the side wall and the z axis, rather closely Eq. (4) with slowly changing $l(z) \approx 2$. The local molecular alignment is imperfect near the line connecting the defects [Fig. 1(c)]. This region can be identified therefore with a nontopological "thick line." Note that the distances in all figures are measured in the units of healing length, and the aspect ratio must

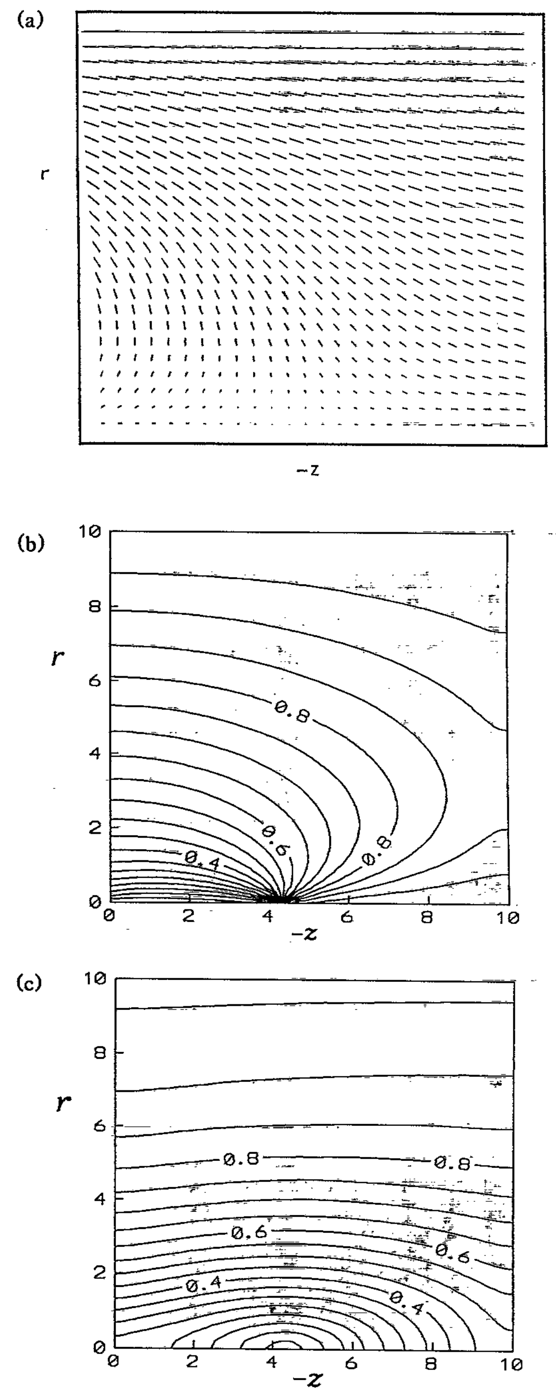

FIG. 1. The quasistationary order parameter field for a moving defect: (a) graphic representation of the director field with the length of lines proportional to ρ; (b) levels of $\alpha(r, z)$; (c) levels of $\rho(r, z)$.

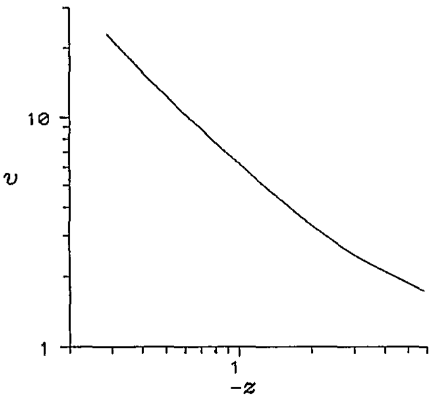

FIG. 2. The dependence of the velocity on distance from the reflecting wall for a defect moving in a quasistationary director field.

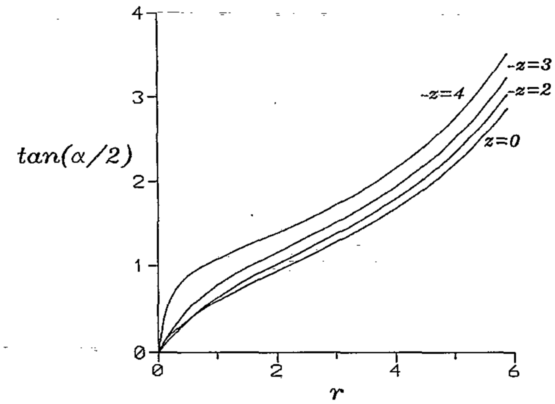

FIG. 3. The quasistationary director field of a moving defect as a function of radius at different values of z.

be large in realistic macroscopic systems. The modest aspect ratios shown here are due to obvious limitations of numerical computations but the extension to larger L must be straightforward. At macroscopic distances far exceeding the healing length, the interaction between the defects is very weak, and can be counterbalanced by advection due to a weak extensional flow that would keep the point defects apart and prevent the connecting line from shrinking. This can account for the abundance of thick line defects in flowing nematics.

The effect of concentration of the changes in the director orientation in an ellipsoidal region around the axis connecting the interacting defects can be seen as the resolution of a singular line in Ref. [13] in a more realistic physical model allowing for partial reduction in nematic order. The quantitative results should be, of course, modified when the model is made more elaborate by accounting for the anisotropy of elastic constants and friction coefficients and imposing realistic boundary conditions on containing walls. All these, however, should not change the principal qualitative mechanism which sets the hedgehog core with an imperfect nematic order into motion when its spherical symmetry is disrupted due to the presence of other defects or side walls.

An interesting unsolved problem is the dynamic effects of a strong deformation of the defect core, that may eventually lead to the splitting of a point defect into a ring singularity when biaxiality is significant. One can expect that interacting rings aligned perpendicular to their common axis will be set into motion due to disruption of symmetry with respect to the plane of the ring. Dynamical effects sensitive to the scale and symmetry of the core could well provide a mechanism for discriminating between different models of core structure.

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