Defect Core Structure in Nematic Liquid Crystals

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The core structure of half-integer wedge disclinations in nematic liquid crystals has been investigated within the Landau–de Gennes theory, by solution of the appropriate Euler-Lagrange equations. Close to the nematic-isotropic transition the energy density exhibits a domain-wall-like structure around the core which disappears at low temperatures. The inner core does not consist of isotropic fluid, and the core is heavily biaxial at all temperatures.

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Nematic liquid crystals owe their name to the Greek word for thread.[1] The threads in question, however, are not, as might be thought, the molecules themselves, but rather defect lines along which the nematic director $\hat{\mathbf{n}}$ is not well defined; they present the most dramatic optical signature of nematic behavior. Defects in liquid crystals have been the subject of much interest, partly because of their striking appearance, and partly because their complexity has been an ideal topic for study by homotopy theorists.[2] Topological studies, however, cast no light on the nature of the core region of the defect, which depends in addition on details of material properties of particular nematics and which hitherto has remained comparatively unexplored.[3] In this Letter we make the first steps towards a theory of defect core structure.

Nematic liquid crystals are usually described by a traceless symmetric tensor order parameter Q_{ij}. In uniform systems, however,

$$Q_{ij}=Q(3\hat{n}_i\hat{n}_j-\delta_{ij}). \tag{1}$$

The Frank-Oseen picture of nonuniform nematics constrains Q_{ij} to be of this form. This hydrodynamic description of nematic deformation describes the asymptotic behavior far from a defect, but fails close to the singularity in the $\hat{\mathbf{n}}$ field which occurs at a disclination core. To describe this regime, it is necessary to work with the full order parameter Q_{ij} in the context of the Landau–de Gennes theory.[4] In the limit of a weakly nonuniform system, this description reduces to the hydrodynamic picture.[5]

The quantity Q_{ij} exhibits no anomalous behavior at the singularity of the $\hat{\mathbf{n}}$ field and the resulting Euler-Lagrange equations remain quasilinear. In contrast, the Frank-Oseen picture and extensions thereof give rise to cumbersome Euler-Lagrange equations, which are nonlinear in the gradients.[6]

The system is described by the Landau–de Gennes free energies F_{bulk} and F_{kin}, where

$$F_{\text{bulk}}=A\,\text{tr}\mathbf{Q}^2+\tfrac{2}{3}B\,\text{Tr}\mathbf{Q}^3+\tfrac{1}{2}C\,\text{Tr}\mathbf{Q}^4, \tag{2a}$$

$$F_{\text{kin}}=L_1\frac{\partial Q_{ij}}{\partial x_k}\frac{\partial Q_{ij}}{\partial x_k}+L_2\frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k}+L_3\frac{\partial Q_{ij}}{\partial x_k}\frac{\partial Q_{ik}}{\partial x_j}, \tag{2b}$$

and the summation convention is assumed. The constraints $Q_{ij}=Q_{ji}$ and $\text{tr}\mathbf{Q}=0$ are taken into account by the introduction of the Lagrange parameter tensor:

$$\Lambda_{ij}=\lambda_0\delta_{ij}-\epsilon_{ijk}\lambda_k. \tag{3}$$

The full free-energy functional

$$F(\mathbf{Q},\mathbf{\Lambda})=F_{\text{bulk}}+2\,\text{tr}(\mathbf{\Lambda}\mathbf{Q})+F_{\text{kin}} \tag{4}$$

is then minimized with respect to $\mathbf{Q}$ and $\mathbf{\Lambda}$, yielding the nine coupled Euler-Lagrange equations

$$[L_1\Delta\cdot\mathbf{1}+(L_2+L_3)\boldsymbol{\partial}\times\boldsymbol{\partial}^{\text{T}}]\mathbf{Q}-[(A+\text{tr}\mathbf{Q}^2)\mathbf{1}+B\mathbf{Q}]\mathbf{Q}=\mathbf{\Lambda}. \tag{5}$$

Equation (5) can be put into tractable form by elimination of the constraint forces λ_0 and λ_k, leaving five coupled equations for five independent unknowns, which we take to be Q_{xx}, Q_{xy}, Q_{xz}, Q_{yz}, and Q_{zz}.

For calculational purposes, it is convenient to introduce a scaling in which free energy is measured in units of $B^4/(9C)^3$, $\bar{A}=9AC/B^2$ defines the temperature scale, and length is measured in units of $\xi=(9CL_1/B^2)^{1/2}$, the characteristic scale for order-parameter changes. In these units, the bulk nematic-isotropic transition T_{NI} occurs at $\bar{A}=\frac{1}{3}$, to a nematic state in which $Q=1$.[7] Below T^*, $\bar{A}=0$, the isotropic state ceases even to be metastable. In our calculations, $L_2+L_3=3L_1$, which is roughly speaking in the experimental range.[7]

In this Letter we discuss wedge disclination lines. The line is in the z direction, and we seek solutions to Eq. (5) independent of z. Far from the disclination core their director $\hat{\mathbf{n}}$ lies in the x-y plane. Traveling along a closed path around the line rotates the director through an angle $2m\pi$, where m, which is integral or half integral, is the disclination index. We study here the cases $m \pm \frac{1}{2}$. We now generate the asymptotic values $Q_{ij}(r \rightarrow \infty, \theta)$ (with use of cylindrical polar coordinates), from $\hat{\mathbf{n}} = (\cos m\theta, \sin m\theta, 0)$ and Eq. (1).[8] We solve Eq. (5) by standard relaxation techniques.[9]

All the solutions we discuss have the form

$$Q = \begin{pmatrix} Q_{xx} & Q_{xy} & 0 \\ Q_{xy} & Q_{yy} & 0 \\ 0 & 0 & Q_{zz} \end{pmatrix} \tag{6}$$

with three free parameters. The symmetry of Eq. (5), subject to the wedge disclination boundary conditions, guarantees the existence of such a three-parameter ("unbroken symmetry") type for $m = \pm \frac{1}{2}$. There also exist five-parameter ("broken symmetry") solutions. These solutions can be classified into two types, depending on their symmetries with respect to reflections and combinations thereof in the x-y and x-z planes.[10]

The solutions to Eq. (5) have a number of striking features. In Fig. 1 we plot the three eigenvalues of the matrix $\mathbf{Q}$ along the $y=0$ axis for the $m=-\frac{1}{2}$ defect at temperature $\bar{A}=0.25$. These features are roughly azimuthally symmetric and are preserved for the $m=\frac{1}{2}$ defect. Outside about 10ξ from the defect line, the tensor order parameter essentially takes the form (1), although the magnitude of the scalar $Q(r)$ is reduced from its asymptotic value. Inside this region the order parameter becomes increasingly *biaxial*, in that the degeneracy between two of the eigenvalues is broken. On a ring around the core, of diameter $\simeq 2\xi$, the liquid crystal is *maximally* biaxial; one of the eigenvalues is now zero. However, over the whole defect, Q_{zz} shows the least change from its bulk value. For this case, $Q_{zz}(\text{core}) \simeq 0.4 Q_{zz}(\text{bulk})$. In the very central core region, the order parameter once again approximately takes the form (1). However, now the symmetry axis is the defect axis itself, and as compared with the bulk, the order parameter has changed its sign.

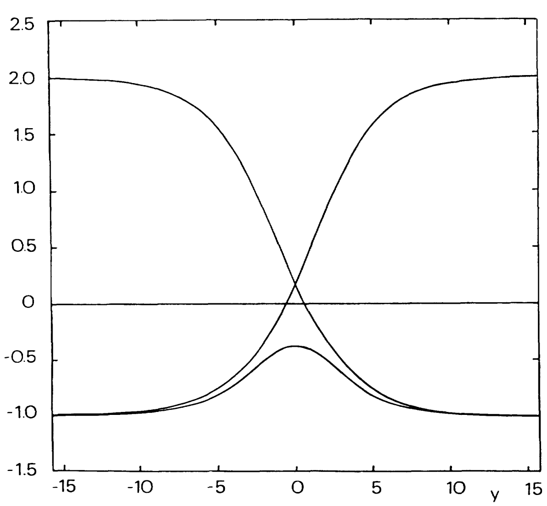

FIG. 1. Eigenvalues of $\mathbf{Q}$ along the slice $x=0$, for $m=-\frac{1}{2}$, $\bar{A}=0.25$, and length scale measured in units of ξ.

These features remain qualitatively similar if the temperature changes, and for $m=\frac{1}{2}$ defects. Very close to T_{NI}, $\bar{A}=\frac{1}{3}$, the reduction in Q_{zz} becomes larger. In contrast, at lower temperatures the core becomes smaller, and Q_{zz} remains relatively impervious to the presence of the defect, e.g., at $\bar{A}=-1$, $Q_{zz}(\text{core}) \simeq 0.8 Q_{zz}(\text{bulk})$.

Another quantity of interest is the free-energy density $\epsilon(x,y)$, which can be derived, with use of a viriallike formula, from Eqs. (4) and (5):

$$\epsilon(x,y) = -\{\tfrac{1}{3} B \operatorname{tr}(\mathbf{Q}^3) + \tfrac{1}{2} C[\operatorname{tr}(\mathbf{Q}^2)]^2\}. \tag{7}$$

This quantity shows how the system distributes the strain imposed on it by topological constraints. We show in Fig. 2 the free-energy surface $\epsilon(x,y)$ for $\bar{A}=0.25$, $m=-\frac{1}{2}$. The picture shows an outer core region, in which the triangular symmetry of this defect is just discernible, and an inner core of diameter $\simeq 10\xi$ which is essentially circular. What is dramatic here, however, is the crater structure of the surface, with a minimum at the center, and a rim separating the inner and outer cores. The quantitative details of this picture are represented in Fig. 3, which shows $\epsilon(0,y)$, a typical slice through the crater.

For the $m=\frac{1}{2}$ defect, the inner core structure is almost identical, although the outer core structure now reflects the different symmetry of this defect. As the

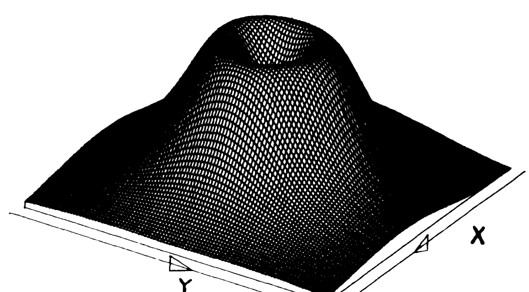

FIG. 2. Energy surface $\xi(x,y)$ in the region $-12 < x,y < 12$ for the same defect as in Fig. 1, showing the crater structure.

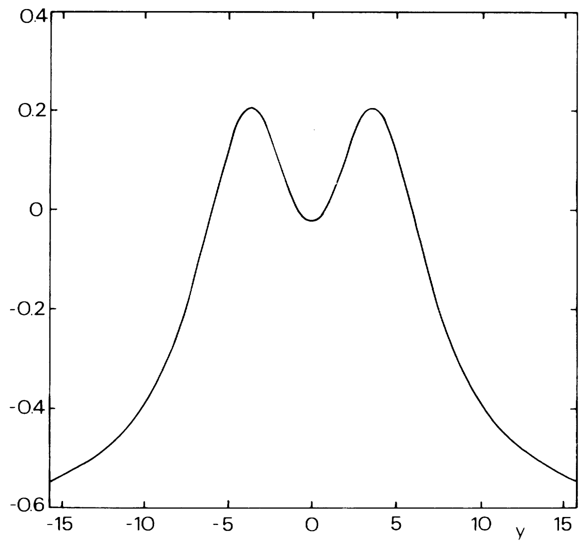

FIG. 3. Energy density along the slice $x=0$ for the same defect. At this temperature $\epsilon_{\text{bulk}} = -0.60$ in these units.

temperature is increased, the rim height and extent both increase; nevertheless, the defect remains finite at T_{NI}. The minimum in the free-energy intensity is always close to zero, which in our units is the (metastable) bulk isotropic free energy. At lower temperatures, however, the rim height decreases until finally, around $\bar{A}=-1$, this structure is replaced by a single peak structure in $\epsilon(x,y)$.

We now comment on these results. The crater structure in $\epsilon(x,y)$ found for $\bar{A}>0$ is presumably related to the double-well structure of $F_{\text{bulk}}(\mathbf{Q})$, as described by Eq. (2a) in the same regime. In some weak sense the core of the disclination is attempting to find the isotropic minimum, and the rim of $\epsilon(x,y)$ corresponds to a nematic-isotropic interface. This picture of the disclination core was proposed some time ago on phenomenological grounds.[2] However, below $\bar{A}=0$, the minimum at $F_{\text{bulk}}(\mathbf{Q}=0)$ disappears, and the disappearance of the crater structure at low $\bar{A}$ is clearly related to this. We note nevertheless that the relation cannot be too close, because the crater structure still persists below $\bar{A}=0$. A simple picture of a disclination core consisting of isotropic fluid was put forward some time ago by Fan.[11] This model exploits the analogy between disclination cores and vortex cores in superfluid ^{4}He which are known to contain normal fluid. The crater structure of $\epsilon(x,y)$ gives it partial support.

However, examination of the eigenvalues of $\mathbf{Q}$ inside the core shows that the core is *never* isotropic, even when the structure of $\epsilon(x,y)$ suggests that it might be. Rather, the topology has a minor effect on Q_{zz} (which always remains an eigenvalue in our calculations), decreasing dramatically the two eigenvalues in the x-y plane. The net effect is that inside the core the nematic acts as though it were constrained not to lie in the direction of the disclination line. In the outer core, on the other hand, the order parameter has the same structural form as it has in the bulk, with the degree of order asymptotically approaching that in the bulk. In between there is a matching region where the liquid crystal is biaxial. There is a ring around which the biaxiality is maximal. This is all that the topology demands. Only if the ring shrinks to a point does the condition $\text{tr}\mathbf{Q}\equiv 0$ insist that $\mathbf{Q}\equiv 0$ at that point. Only then would the disclination core be isotropic.

The picture presented in this Letter has experimental consequences. In particular, core size should be affected by magnetic and electric fields directed along the core. It may also be possible to investigate the core structure more directly, perhaps with liquid crystals consisting of macromolecules such as viruses.

In conclusion we have used the Landau–de Gennes formalism to make an exact calculation of the structure of a wedge disclination in a nematic liquid crystal. The core is always biaxial, sometimes contains structures which resemble an isotropic-nematic interface, but never contains a core of isotropic fluid.

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[7]The Euler-Lagrange equation (5) depends only on the combined quantity $L_{23}=L_2+L_3$. The only independent quantities are therefore the scaled temperature $\bar{A}$ and the ratio L_{23}/L_1. The quantity L_2-L_3 only affects (hydrodynamic) surface integrals, as discussed in Ref. 4 above.

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[9]See, for example, S. L. Adler and T. Piran, Rev. Mod. Phys. **56**, 1 (1984). The equations are solved in a square box of length $n\xi$, for $30\le n\le 50$, with use of a grid of size $\lambda\xi$, where $0.1<\lambda<0.5$. The results in the core region are essentially independent of n and λ.

[10]The symmetry group leaving the asymptotic order parameter invariant contains a little group generated by the reflections S_y and S_z sending $(x,y,z)\Rightarrow(x,-y,z)$ and $(x,y,-z)$, respectively. Three-component solutions are invariant under the little group $\{1,S_y,S_z,S_yS_z\}$, while five-component solutions are not. We find five-component solutions invariant under S_y and a different set invariant under S_yS_z.

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