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Fine structure of point defects and soliton decay in nematic liquid crystals

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Résumé. — Nous démontrons, sur la base d'une théorie de Landau-de Gennes, que les défauts ponctuels des phases nématiques peuvent avoir un corps biaxial non singulier. A partir de ce résultat nous calculons le diamètre critique de solitons topologiques linéaires. Les solitons de petits diamètres peuvent se relaxer *via* une phase biaxiale en un état nématique uniforme, sans avoir à franchir une barrière de potentiel.

Abstract. — On the basis of Landau-de Gennes-theory it is demonstrated that point defects in nematic liquid crystals may have a biaxial nonsingular core. From this result a critical diameter is derived for linear topological solitons in nematics. Solitons of smaller diameter can relax to the uniform nematic state without energy barrier *via* an intermediate biaxial phase.

1. Introduction.

Point singularities in nematic liquid crystals have found much attention recently due to their topological properties [1] and their similarity with magnetic monopoles in non-Abelian gauge theories [2]. There are arguments, that in bulk samples of nematic liquid crystals point singularities do not exist, because immediately after growth they connect by linear topological solitons with their antidefects or, close to free surfaces, with their mirror image. The solitons then retract to thin strings and decay [3]. Homeotropic (orthogonal) boundary conditions, however, either at the walls of capillaries [4] or on the surface of nematic droplets, enforce the existence of point defects. Nematic droplets, immersed in a polymer matrix, are promising candidates for window material of tunable light transmission [5].

The standard point singularity is the spherically symmetric hedgehog (Fig. 1), where the director field lines stream away radially from the center in a scale-invariant, selfsimilar fashion. A simple calculation yields a diverging Frank-Oseen elastic energy,

$$F = 8 \pi K R \quad (1)$$

for a spherical volume of radius R , where K denotes the splay constant.

In the framework of Landau-de Gennes theory Schopohl and Sluckin [6] have studied the core structure of the hedgehog by the following *ansatz* for the tensor order parameter \mathbf{Q} :

$$\mathbf{Q}(\mathbf{x}) = \sqrt{\frac{3}{2}} Q_0(r) \left(\hat{\mathbf{e}}_r \otimes \hat{\mathbf{e}}_r - \frac{1}{3} I \right) \quad (2)$$

where $\hat{\mathbf{e}}_r$ is a unit vector in radial direction. The *ansatz* describes a uniaxial nematic hedgehog similar to that presumed in (1). The difference is that now the degree of order $Q_0(r) = \sqrt{\text{Tr } \mathbf{Q}^2}$ is not constant, but varies, leading to an isotropic core as solution of the Euler-Lagrange equation for $Q_0(r)$.

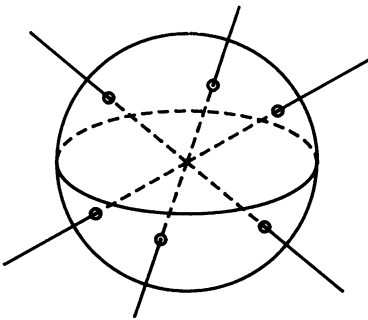


Fig. 1.

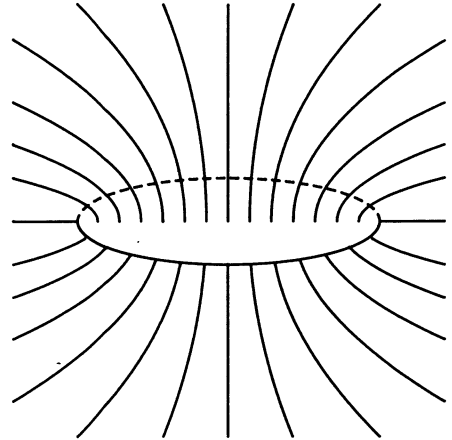


Fig. 2.

Fig. 1. — The hedgehog singularity of a uniaxial nematic phase.

Fig. 2. — The core of the hedgehog singularity can be broadened to a 180°-disclination ring.

However, it is well known [1, 7], that a point defect may broaden out to a line singularity. The spherical symmetry of the hedgehog is broken to cylindric symmetry by transformation of the point defect into a 180°-disclination ring (Fig. 2). For this geometry Mori and Nakanishi [8] have calculated the Frank-Oseen elastic energy in the director representation. A ring has been observed by Lavrentovich and Terentev [9], but this structure arises when the center of a hedgehog is changed from radial to hyperbolic, and it is of much larger diameter than the broadened core (see discussion in Sect. 10).

Lyuksyutov [10] and later Meiboom *et al.* [11] have proposed, that the core of 180°-disclination lines in uniaxial nematic liquid crystals is not an isotropic, but a biaxial phase. The model has been confirmed quantitatively by Schopohl and Sluckin [12]. In the present article we let the ring singularity of the nematic hedgehog escape to biaxiality and thus arrive at a cylindrically symmetric droplet configuration with biaxial interior which nowhere is isotropic. By a simple variational procedure it is proved that its energy is lower than that of equation (1).

From the biaxial droplet configuration we derive a decay channel for linear topological solitons. These are nonsingular director fields, which far away from a line are constant [1]. Under this boundary condition they cannot be deformed continuously to the uniform ground state unless singularities are introduced or the order parameter space is left in between. In reference [3] it was shown that the soliton is unstable with respect to a break-up into a chain of

point defects. These alternate in sign and annihilate in pairs. Here we prove that linear topological solitons vanish away if intermediately their cores become biaxial. For the proof we take advantage of the fact, that the director field on a cross-section of the soliton is identical to that on a sphere enclosing the center of the hedgehog. By peeling off one shell after the other of the biaxial hedgehog configuration and by flattening it out, we construct a continuous sequence of order parameter fields which leads from the topological soliton to a constant director field. Comparison of the field energies yields that below a critical diameter no energy barrier obstructs the decay. Ostlund [13] has demonstrated in the director representation that a linear topological soliton, which is spanned between two point singularities, contracts to infinitesimal diameter. According to our results it then must decay. Thus the hypothesis, that point defects in nematic liquid crystals of open boundary conditions are not existent, is hardened by yet another argument.

Details of the present article are documented in reference [14].

2. The Landau-deGennes free energy density.

The basis of our discussion is the Landau-de Gennes-expansion of the free energy F in powers of the tensor order parameter \mathbf{Q} and its gradient $\text{grad } \mathbf{Q}$. It consists of bulk terms f_v and elastic terms f_{el} [15] :

$$F = \int (f_v + f_{el}) dV \tag{3}$$

$$f_v = \frac{a}{2} \text{Tr } \mathbf{Q}^2 - \frac{b}{3} \text{Tr } \mathbf{Q}^3 + \frac{c}{4} (\text{Tr } \mathbf{Q}^2)^2 \tag{4}$$

$$f_{el} = \frac{L_1}{2} (\text{grad } \mathbf{Q})^2 + \frac{L_2}{2} (\text{div } \mathbf{Q})^2 \tag{5}$$

$$(\text{grad } \mathbf{Q})^2 = \sum_{i,\ell,m} (\partial_i Q_{\ell m})(\partial_i Q_{\ell m}) \tag{6}$$

$$(\text{div } \mathbf{Q})^2 = \sum_{i,\ell,m} (\partial_i Q_{i\ell})(\partial_m Q_{m\ell}) . \tag{7}$$

Since in the following we compare order parameter fields which are identical at infinity, we can omit the surface term of the Landau-de Gennes-theory.

The order parameter \mathbf{Q} is a traceless, symmetric, real, second rank tensor of five components. The tensor can be represented in the form :

$$\mathbf{Q} = \sqrt{2} Q_0 \left[\sin \left(\phi + \frac{1}{3} \pi \right) \left\{ \hat{\mathbf{n}} \otimes \hat{\mathbf{n}} - \frac{1}{3} I \right\} + \sin (\phi) \left\{ \hat{\mathbf{m}} \otimes \hat{\mathbf{m}} - \frac{1}{3} I \right\} \right] \tag{8}$$

where Q_0 is the modulus of the order parameter, $\text{Tr } \mathbf{Q}^2 = Q_0^2$, and $\hat{\mathbf{n}}$ and $\hat{\mathbf{m}}$ are mutually perpendicular unit vectors. The angle ϕ describes the degree of biaxiality of the tensor \mathbf{Q} . When $\phi = 0$, \mathbf{Q} is uniaxial, and $\hat{\mathbf{n}}$ is denoted director.

In the free energy density one can establish a hierarchy of terms. In case of weak variations of the order parameter field the elastic energy density f_{el} is much smaller than the bulk energy f_v .

In f_v the quadratic term $\frac{a}{2} \text{Tr } \mathbf{Q}^2$ and the quartic term $\frac{c}{4} (\text{Tr } \mathbf{Q}^2)^2$ dominate in most cases over the cubic term $-\frac{b}{3} \text{Tr } \mathbf{Q}^3$. The last term is responsible for the transition isotropic-nematic to be first order. But according to experiment the latent heat [15] is small and the transition is only weakly first order.

Therefore we allow ourselves first to minimize the dominant part of the free energy density :

$$f_t = \frac{a}{2} \text{Tr } \mathbf{Q}^2 + \frac{c}{4} (\text{Tr } \mathbf{Q}^2)^2 . \quad (9)$$

We substitute $\text{Tr } \mathbf{Q}^2 = u$ and minimize (9) with respect to u :

$$\partial_u f_t = \frac{a}{2} + \frac{c}{2} u = 0 \quad (10)$$

$$u_{\min} = \frac{-a}{c} =: Q_0^2 . \quad (11)$$

Within the set of order parameters satisfying $\text{Tr } \mathbf{Q}^2 = Q_0^2 = \text{const}$ (these form a sphere in the five-dimensional order parameter space) we now minimize the remaining terms of the bulk free energy density. With equations (8) and (11) we obtain for an unstrained nematic liquid crystal :

$$f_v = \frac{a}{2} Q_0^2 - \frac{b}{3} \cos(3\phi) Q_0^3 + \frac{c}{4} Q_0^4 . \quad (12)$$

Further minimizing (12) with respect to ϕ yields $\phi = 0$, provided $b \geq 0$. Thus for $b \geq 0$, only the uniaxial prolate state is stable. The cubic term enforces the uniaxiality of the system. If we represent the order parameter by an ellipsoid of three axes, then the eigenvalues of the tensor field represent the length of these axes (more exactly : the deviation from the mean axis length). In the uniaxial case two eigenvalues of the tensor field are degenerate ; in case of weak distortions the eigenvalues of the tensor field are constant in space, only the orientation of the ellipsoid changes. Therefore a possible field representation is :

$$\mathbf{Q}(\mathbf{x}) = \sqrt{\frac{3}{2}} Q_0 \left(\hat{\mathbf{n}}(\mathbf{x}) \otimes \hat{\mathbf{n}}(\mathbf{x}) - \frac{1}{3} I \right) . \quad (13)$$

Close to defects the distortion strongly increases, and it can happen that the elastic energy overcomes the cubic term in the bulk energy, so that the system converts to biaxiality. The length scale of the distortion, where the escape to biaxiality occurs, depends on the ratio of elastic energy to cubic volume term and is expressed by a biaxial coherence length :

$$\xi_b = \sqrt{\frac{L_1 + L_2}{2bQ_0}} . \quad (14)$$

For MBBA ξ_b is about 200 Å.

By further increasing the distortion the elastic energy even may overcome the terms of second and fourth order in the volume energy. The characteristic length scale :

$$\xi_0 = \sqrt{\frac{L_1 + L_2}{2|a|}} \quad (15)$$

is the well-known coherence length, which for MBBA is about 20 Å.

3. Cores of singularities.

Frequently, it is assumed that the core of singularities contains the isotropic phase (vanishing order parameter). In references [10-12] it is proposed that the isotropic state is replaced at the

expense of a biaxial phase. Following this view we study the core of a 180°-disclination by the following *ansatz*, which admits eigenvalues to vary in space :

$$\mathbf{Q}(\mathbf{x}) = \sqrt{\frac{3}{2}} Q_0 \left[\left(A(\mathbf{x}) \left\{ \hat{\mathbf{n}}(\mathbf{x}) \otimes \hat{\mathbf{n}}(\mathbf{x}) - \frac{1}{3} I \right\} + B(\mathbf{x}) \left\{ \hat{\mathbf{m}}(\mathbf{x}) \otimes \hat{\mathbf{m}}(\mathbf{x}) - \frac{1}{3} I \right\} \right) \right]. \quad (16)$$

By appropriate choice of the scalar functions A and B we can keep $\text{Tr } \mathbf{Q}^2 = \text{const} = u_{\text{min}}$ (11).

Let the singular line be perpendicular to the paper plane and located at the origin. The directors $\hat{\mathbf{n}}$ and $\hat{\mathbf{m}}$ are laying in the paper plane. Now consider a continuous change of the scalar functions A and B along the x -axis. Far away from the singularity the tensor field is uniaxial and for example represented by $\hat{\mathbf{n}}$ for $x \rightarrow -\infty$ and by $\hat{\mathbf{m}}$ for $x \rightarrow \infty$. By diminishing A and increasing B along the x -axis it is possible to change the direction of uniaxial ordering from $\hat{\mathbf{n}}$ to $\hat{\mathbf{m}}$ in a continuous way *via* a biaxial intermediate state. Thus the singularity on the disclination line can be removed. This process is depicted in figure 3.

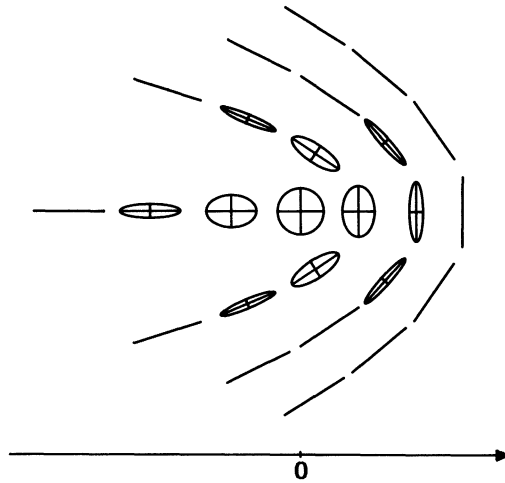


Fig. 3. — A 180°-disclination line of a uniaxial nematic liquid can be eliminated, if the phase escapes to biaxiality close to the singularity.

In the present work we want to demonstrate that also the singular cores of the hedgehog can be removed by escape to the biaxial phase.

Starting from the usual tensor order parameter field for such a defect :

$$\mathbf{R} = \sqrt{\frac{3}{2}} Q_0 \left(\hat{\mathbf{e}}_r \otimes \hat{\mathbf{e}}_r - \frac{1}{3} I \right) \quad (17)$$

we construct a biaxial core by broadening the point defect to a 180°-disclination ring (Fig. 2), and then relaxing the disclination to the biaxial state according to figure 3.

4. Analytic model.

An order parameter field describing the situation of figure 3 is provided by the following cylindrical *ansatz* :

$$\mathbf{H}(r, \theta, \phi) = \sqrt{\frac{3}{2}} Q_0 \left[\left(A(r, \theta) \left\{ \mathbf{e}_r \otimes \mathbf{e}_r - \frac{1}{3} I \right\} + B(r, \theta) \left\{ \mathbf{e}_z \otimes \mathbf{e}_z - \frac{1}{3} I \right\} \right) \right]. \quad (18)$$

\mathbf{e}_z is the unit vector in z -direction, (r, θ, ϕ) are polar coordinates of the position vector, Q_0 is given as in equation (11).

In (18) the homogeneous phase is superposed to the hedgehog. At the origin the uniaxial homogeneous phase is weighted strongly, at infinity the uniaxial hedgehog. The weight functions A and B have to satisfy the boundary conditions :

$$\begin{aligned} \lim_{r \rightarrow \infty} A &= 1 & \lim_{r \rightarrow 0} A &= 0 \\ \lim_{r \rightarrow \infty} B &= 0 & \lim_{r \rightarrow 0} B &= 1. \end{aligned} \quad (19)$$

5. Scaling of the free hedgehog.

The functions A and B are determined by minimizing the free energy of the singularity (preserving the boundary conditions). Since the energy of the whole system diverges we only vary the energy difference between the hedgehog with biaxial core and the overall uniaxial hedgehog :

$$\Delta f = f(\mathbf{H}) - f(\mathbf{R}). \quad (20)$$

This energy difference is a functional of A and B :

$$\Delta F[A, B] = \int_0^{2\pi} \int_0^\pi \int_0^\infty \Delta f[A, \partial_r A, \partial_\theta A, B, \partial_r B, \partial_\theta B, r, \theta] r^2 \sin \theta \, dr \, d\theta \, d\phi. \quad (21)$$

In principle the variational problem could be transformed into a system of coupled nonlinear differential equations for A and B (these turning into the equation of Schopohl and Sluckin [6] for $B = 0$). Because we only want to prove that a nonsingular biaxial core can have less energy than the singular core of figure 1, we start from a variational principle in only one parameter.

Apart from conditions (19) the weight functions A and B are also restricted by the requirement : $\text{Tr } \mathbf{H}^2 = Q_0^2$, which leads to a relation :

$$A^2 + B^2 + AB(3 \cos^2 \theta - 1) = 1. \quad (22)$$

Suitable functions satisfying (19) and (22) are :

$$A = \frac{r^2}{\sqrt{r^4 + r^2(3 \cos^2 \theta - 1) + 1}} \quad (23)$$

$$B = \frac{1}{\sqrt{r^4 + r^2(3 \cos^2 \theta - 1) + 1}}. \quad (24)$$

The uniaxial hedgehog (Fig. 1) is invariant under radial scaling, but not the hedgehog with biaxial core. Scaling changes the diameter of the disclination ring of figure 2. Below we will show that the points of the ring are to be interpreted as loci, where the tensor ellipsoid has changed its shape from prolate to oblate (for $b \geq 0$) and hence the cubic bulk term is maximum. As variational parameter we use the scaling length only and hence minimize the free energy difference (20) with respect to a scaling parameter λ .

$$\Delta F = 2 \pi \int_0^\pi \int_0^\infty \Delta f [A^\lambda, \partial_r A^\lambda, \partial_\theta A^\lambda, B^\lambda, \partial_r B^\lambda, \partial_\theta B^\lambda, r, \theta] r^2 \sin \theta \, dr \, d\theta \quad (25)$$

where

$$A^\lambda(r, \theta) := A \left(\frac{r}{\lambda}, \theta \right) \quad (26)$$

$$B^\lambda(r, \theta) := B \left(\frac{r}{\lambda}, \theta \right). \quad (27)$$

By the substitution $r \rightarrow r\lambda$ the integral (25) becomes :

$$\Delta F = 2 \pi \int_0^\pi \int_0^\infty \Delta f \left[A, \frac{1}{\lambda} \partial_r A, \partial_\theta A, B, \frac{1}{\lambda} \partial_r B, \partial_\theta B, \lambda r, \theta \right] \lambda^3 r^2 \sin \theta \, dr \, d\theta. \quad (28)$$

Inserting **H** and **R** into the free energy (3), we obtain a variational function :

$$\Delta F(\lambda) = -\lambda \frac{b}{3} T + \lambda^3 \left(\frac{L_1}{2} G + \frac{L_2}{2} D \right) \quad (29)$$

where

$$T = \int [\text{Tr } \mathbf{H}^3 - \text{Tr } \mathbf{R}^3] \, dV \quad (30)$$

$$G = \int [(\text{grad } \mathbf{H})^2 - (\text{grad } \mathbf{R})^2] \, dV \quad (31)$$

$$D = \int [(\text{div } \mathbf{H})^2 - (\text{div } \mathbf{R})^2] \, dV \quad (32)$$

are the volume energy difference, the gradient energy difference and the divergence energy difference for $\lambda = 1$ respectively. Variation with respect to λ yields the equilibrium value for the free energy of the biaxial hedgehog relative to the uniaxial hedgehog :

$$\lambda_0 = \sqrt{\frac{\frac{L_1}{2} G + \frac{L_2}{2} D}{bT}}. \quad (33)$$

To calculate these integrals analytically, we used the software-package MACSYMA, and arrived at the result :

$$G = -\frac{1}{3} \pi^2 [30 - 5 \sqrt{3} \text{arsinh}(\sqrt{3})] Q_0^2 = -61.17 Q_0^2 \quad (34)$$

$$D = -\frac{1}{48} \pi^2 [354 - 61 \sqrt{3} \text{arsinh}(\sqrt{3})] Q_0^2 = -44.18 Q_0^2 \quad (35)$$

$$T = -\frac{3}{4} \sqrt{\frac{3}{2}} \pi^2 Q_0^3 = -9.03 Q_0^3. \quad (36)$$

We shall estimate the free energy for a typical nematic, MBBA. The elastic constants are [16] :

$$L_1 = 1.33 \times 10^{-12} Q_0^2 [\text{N}] \quad (37)$$

$$L_2 = 1.33 \times 10^{-12} Q_0^2 [\text{N}]. \quad (38)$$

Using the same values for b and Q_0 as [10] and inserting $b = 6 \times 10^4 \frac{\text{J}}{\text{m}^3}$ and $Q_0 = 0.6$ in (33), the calculated equilibrium scaling parameter then is $\lambda_0 \approx 250 \text{ \AA}$. The energies are :

$$\Delta F(\lambda) = 3.9 \times 10^4 \lambda^3 - 7 \times 10^{-11} \lambda \text{ [J]} \quad (39)$$

$$\Delta F(\lambda_0) = -1.2 \times 10^{-18} \text{ [J]}. \quad (40)$$

The behavior of $\Delta F(\lambda)$ is shown in figure 4. The hedgehog with biaxial core has a lower energy and therefore is more stable than the uniaxial one.

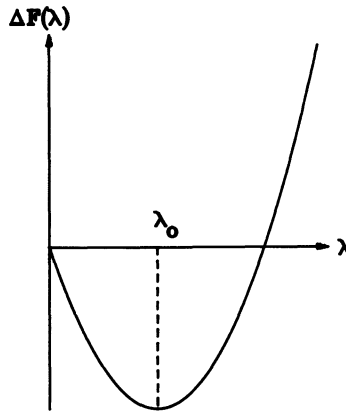


Fig. 4. — Free energy difference between the hedgehog with biaxial core and the uniaxial hedgehog as function of a scaling parameter.

6. The tensor field of the biaxial hedgehog.

Looking at the eigenvalues of the tensor order parameter (18) for unscaled functions ($\lambda = 1$) and variable $\theta < 90^\circ$ (Fig. 5), we recognize, that for increasing θ the eigenvalues deviate more and more from the uniaxial (constant) values $-\frac{1}{3}$, $-\frac{1}{3}$ and $\frac{2}{3}$. The greater the distortion, the more the system converts to biaxiality. In figure 6 the behavior of the eigenvalues at $\theta = 90^\circ$ is plotted. At $r = 1$ where the ring is to be located the two largest eigenvalues are degenerate, the tensor order parameter is oblate uniaxial ; a director cannot be defined in a consistent way. Therefore in the director picture the ring is a disclination line. For scaled functions the ring radius is equal to the equilibrium scaling factor λ_0 .

7. Linear topological solitons.

Linear topological solitons in a uniaxial nematic liquid crystal are director fields, which far away from a line are constant. A characteristic representation is the *fountain* (Fig. 7), where \hat{n} points down along the z -axis, and up at the mantle of a cylinder at infinity. Due to these boundary conditions, this soliton cannot be deformed to the uniform ground state, unless the system intermediately leaves the uniaxial phase.

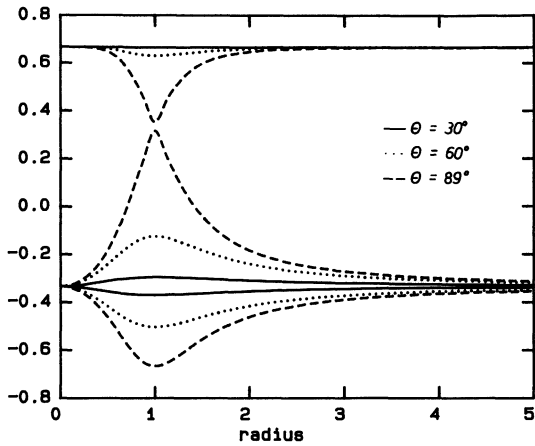


Fig. 5.

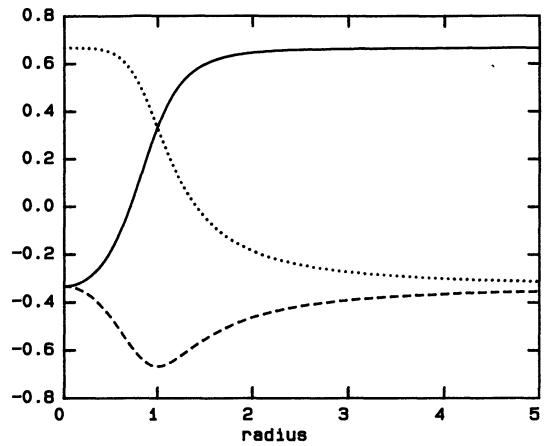


Fig. 6.

Fig. 5. — Eigenvalues of the biaxial order parameter along a ray for different angles θ .

Fig. 6. — Eigenvalues of the biaxial order parameter along the ray for $\theta = 90^\circ$.

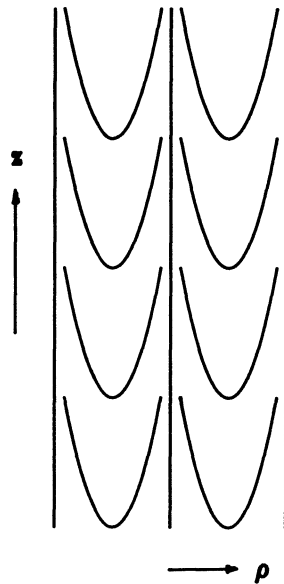


Fig. 7. — A cross-section through the field lines of the director, forming a linear topological soliton of a nematic liquid crystal. At infinity the director points up at the mantle of the cylinder, at the origin the director points down along the z -axis.

Now we search for a director field, which has translational symmetry along the z -axis, and minimizes the free energy in the one-constant-approximation [15] :

$$f = \frac{1}{2} K (\partial_i n_j) (\partial_i n_j) . \tag{41}$$

As model field we take cylinder coordinates (ρ, ϕ, z) in the physical space and spherical coordinates (Θ, Φ) for the director :

$$\hat{\mathbf{n}}(\rho, \phi, z) = (\Theta(\rho, \phi, z), \Phi(\rho, \phi, z)) \quad (42)$$

$$\text{with } \Theta(\rho, \phi, z) = \Theta(\rho) \quad (43)$$

$$\Phi(\rho, \phi, z) = \Phi(\rho, \phi). \quad (44)$$

The boundary conditions are :

$$\Theta(0) = \pi \quad (45)$$

$$\Theta(\infty) = 0. \quad (46)$$

The variation principle $\delta F = \delta \int f dV = 0$ leads to the Euler-Lagrange equation [13] :

$$\partial_{\rho\rho}\Theta + \rho^{-1}\partial_{\rho}\Theta = \frac{1}{2}\rho^{-2}\sin 2\Theta. \quad (47)$$

By substituing $\rho = e^s$ and $y = 2\Theta$, one arrives at the Sine-Gordon equation [13] :

$$\partial_{ss}y + \sin y = 0. \quad (48)$$

Equation (48) has the kink solution

$$y = \arctan \left[\exp \left(\frac{s}{\lambda} \right) \right] \quad (49)$$

where λ is an arbitrary constant reflecting the scale invariance of the differential equation. Taking the boundary conditions into account after resubstitution one obtains :

$$\Theta(\rho) = \pi - 2 \arctan \left(\frac{\rho}{\lambda} \right). \quad (50)$$

8. Topological solitons and the uniaxial hedgehog.

The linear topological soliton described by equation (50) is also obtained by unfolding the uniaxial hedgehog. Put a sphere of radius α around the uniaxial hedgehog and cut out a small disk at the north pole, then unfold the sphere to a disk of radius $\pi\alpha$ and stretch the radius to infinity keeping the directions of the directors fixed. This means, that only the position space is being *peeled off* (Fig. 8).

We describe the hedgehog by spherical coordinates (Θ, Φ) in order parameter space and (r, θ, ϕ) in physical space :

$$\hat{\mathbf{n}}_h = (\Theta(r, \theta, \phi), \Phi(r, \theta, \phi)) \quad (51)$$

with

$$\Theta(r, \theta, \phi) = \theta \quad (52)$$

$$\Phi(r, \theta, \phi) = \phi. \quad (53)$$

The unfolded hedgehog is specified in the order parameter space again by (Θ, Φ) , but in position space by cylindric coordinates (ρ, ϕ, z) :

$$\hat{\mathbf{n}}_{\text{unfold}} = (\Theta(\rho, \phi, z), \Phi(\rho, \phi, z)) \quad (54)$$

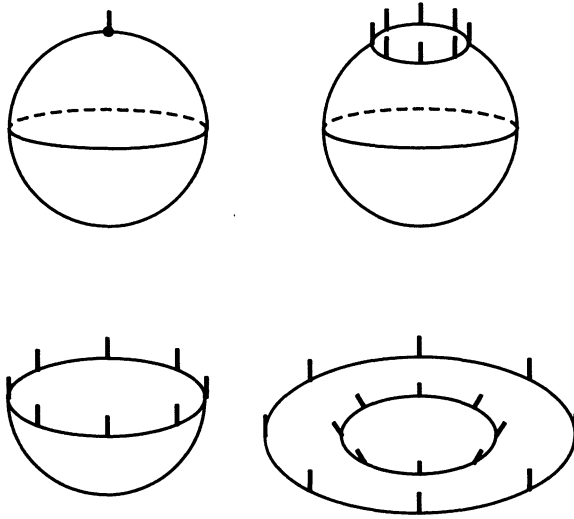


Fig. 8. — The hedgehog of the uniaxial phase is *peeled* as described in the text. The result is a linear topological soliton.

with

$$\Theta(\rho, \phi, z) = \pi - 2 \arctan (\rho) \tag{55}$$

$$\Phi(\rho, \phi, z) = \phi . \tag{56}$$

The rule for *peeling* the position space is :

$$\theta(\rho) = \pi - 2 \arctan (\rho) . \tag{57}$$

Unfolding the hedgehog for every α yields a vector field that has the same structure as the topological soliton shown in (Fig. 7), independent of the radius α .

9. Energy barriers and intermediate biaxial phase.

The process of unfolding is now applied to the hedgehog with biaxial core. For $\alpha \rightarrow \infty$ we obtain the linear topological soliton, for $\alpha = 0$ the uniform nematic state and for $0 < \alpha < \infty$ an intermediate biaxial phase.

By changing the parameter α (*time evolution parameter*) from infinity to zero, we establish a sequence of fields that describes the relaxation of the soliton into the uniform nematic state. We will study the free energy for every time α and look whether there are energy barriers.

The uniaxial hedgehog is characterised by the tensor order parameter :

$$\mathbf{R}(r, \theta, \phi) = \sqrt{\frac{3}{2}} Q_0 \left(\hat{\mathbf{e}}_r \otimes \hat{\mathbf{e}}_r - \frac{1}{3} I \right) \quad \text{with} \quad \hat{\mathbf{e}}_r = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix} . \tag{58}$$

For the unfolded hedgehog (topological soliton) corresponding to the kink solution (49) with $\lambda = 1$, the tensor field is :

$$\mathbf{P}_\infty(\rho, \phi, z) = \sqrt{\frac{3}{2}} Q_0 \left(\hat{\mathbf{g}}_r \otimes \hat{\mathbf{g}}_r - \frac{1}{3} I \right) \quad \text{with} \quad \hat{\mathbf{g}}_r = \begin{pmatrix} \sin \theta(\rho) \cos \phi \\ \sin \theta(\rho) \sin \phi \\ \cos \theta(\rho) \end{pmatrix} \tag{59}$$

$\theta(\rho)$ as in (57). The uniform uniaxial nematic state correspond to :

$$\mathbf{P}_0 = \sqrt{\frac{3}{2}} Q_0 \left(\hat{\mathbf{e}}_z \otimes \hat{\mathbf{e}}_z - \frac{1}{3} I \right) . \tag{60}$$

The shell of radius α of the biaxial hedgehog, if projected to the plane and stretched, is a superposition of \mathbf{P}_∞ and \mathbf{P}_0 with the same weight functions A (26) and B (27) as in section 5. Only θ is substituted by $\pi - 2 \arctan(\rho)$ and r by α :

$$\mathbf{G}_\alpha(\rho) = \sqrt{\frac{3}{2}} Q_0 \left[A_\alpha(\rho) \left\{ \hat{\mathbf{g}}_r \otimes \hat{\mathbf{g}}_r - \frac{1}{3} I \right\} + B_\alpha(\rho) \left\{ \hat{\mathbf{e}}_z \otimes \hat{\mathbf{e}}_z - \frac{1}{3} I \right\} \right] \tag{61}$$

$$A_\alpha(\rho) := A(\alpha, \theta(\rho)) \tag{62}$$

$$B_\alpha(\rho) := B(\alpha, \theta(\rho)) . \tag{63}$$

In figure 9 the tensor field \mathbf{G}_α is represented by ellipsoids for different α ($\phi = 0$).

The scaled tensor field $\mathbf{G}_\alpha \left(\frac{\rho}{\lambda} \right)$ corresponds to the kink solution (50) of radius λ , at time $\alpha = \infty$. We follow its energy if α goes to 0, and obtain for the energy per unit length by the same scaling procedure as in section 5 :

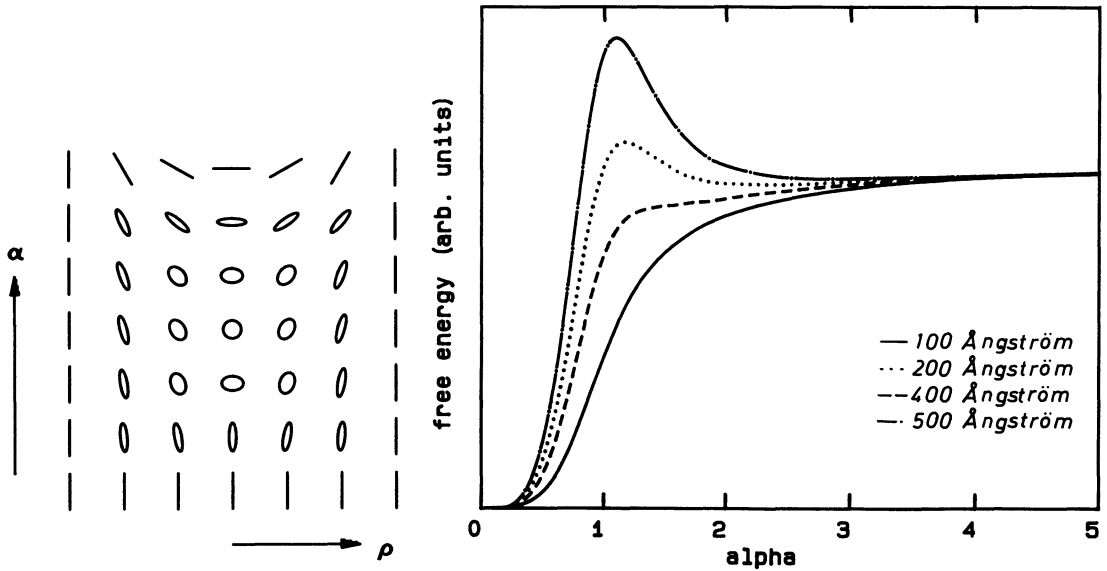


Fig. 9.

Fig. 10.

Fig. 9. — Cross-sections of the biaxial hedgehog plotted *versus* the *time evolution* parameter α . Coming from a linear topological soliton (uppermost row) one traverses a biaxial phase (indicated by ellipsoids) and arrives at the uniform phase. The picture has to be rotated about the right vertical axis.

Fig. 10. — Free energy of a decaying topological soliton for different diameters. At *time* $\alpha \rightarrow \infty$ the soliton is fully developed in a uniaxial phase, at $\alpha = 0$ it is relaxed into the uniform ground state. In between parts of the soliton become biaxial. If the soliton has a diameter of more than 200 Å (approximately the biaxial coherence length) the decay is obstructed by a barrier, which is absent for smaller diameters.

$$F_\alpha(\lambda) = \int_0^\infty \int_0^{2\pi} \Delta f \left[A_\alpha, B_\alpha, \frac{1}{\lambda} \partial_\rho A_\alpha, \frac{1}{\lambda} \partial_\rho B_\alpha, \lambda \rho \right] \lambda^2 \rho \, d\phi \, d\rho \quad (64)$$

$$F_\alpha(\lambda) = -\frac{1}{3} b \lambda^2 t_\alpha + \frac{L_1}{2} g_\alpha + \frac{L_2}{2} d_\alpha \quad (65)$$

where

$$t_\alpha = 2\pi \int_0^\infty (\text{Tr } \mathbf{G}_\alpha^3 - \text{Tr } \mathbf{P}_0^3) \rho \, d\rho \quad (66)$$

$$g_\alpha = 2\pi \int_0^\infty (\text{grad } \mathbf{G}_\alpha)^2 \rho \, d\rho \quad (67)$$

$$d_\alpha = 2\pi \int_0^\infty (\text{div } \mathbf{G}_\alpha)^2 \rho \, d\rho . \quad (68)$$

Because the energy is referred to the uniform ground state, there are no terms of second and quartic order in the bulk free energy.

In the process of scaling the area of a cross-section behaves like λ^2 , the elastic energy density (being quadratic in the gradient) like λ^{-2} . Therefore the total elastic energy is scale-invariant. However, the cubic term of the bulk energy, which becomes finite with every deviation from uniaxiality, scales like λ^2 and builds an energy barrier with increasing λ . In figure 10 the energy is plotted *versus* decay time α for different radii λ , the material parameter values being chosen for MBBA. The energy barrier arises for $\lambda = 200 \text{ \AA}$, which is comparable to the biaxial coherence length. But below this critical size, the soliton can turn quasistatically into the homogenous ground state without hindrance.

10. Summary and discussion.

We have investigated the core structure of a nematic hedgehog by minimizing the Landau-de Gennes free energy with radial boundary conditions and a simple variational *ansatz*. In smectic-A liquid crystals the point singularities observed are focal conic textures, which far away from their center display a hedgehog director configuration, but close to the core can be interpreted as a hyperbolic point. In reference [17] it was proved with Morse-theory, that in the transition region a 360° -disclination ring must form. This ring of diameter of about $50\,000 \text{ \AA}$ has been observed by Lavrentovich and Terentev [9] when the bend and twist constants were enhanced in the nematic phase close to the smectic-A transition. However it is not this type of ring, which has been described in the present paper. Here we analysed the fine structure of core regions yielding 180° -disclination rings of diameter of 250 \AA . Also the hyperbolic point should have a ringlike core. We have calculated its radius with the same variational procedure, but different boundary conditions, reflecting $\hat{\mathbf{e}}_r = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ on the z-axis to $\hat{\mathbf{e}}_{\text{th}} = (-\sin \theta \cos \phi, -\sin \theta \sin \phi, \cos \theta)$. Due to a reduced divergence elastic energy this radius was smaller by 10%. Thus, if Lavrentovich and Terentev had a better resolution, they would observe two rings in their system.

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