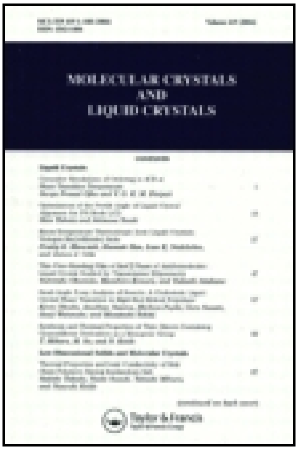

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Energetics of Disclinations in Liquid Crystals

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Energetics of Disclinations in Liquid Crystals†

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Continuum mechanics has been used to work out the structure and properties of disclinations in nematic and cholesteric liquid crystals. After a brief review of the earlier works on the energetics of disclinations in the one constant approximation, we consider the effect of elastic anisotropy. Elastic anisotropy not only alters the energies and director patterns of individual defects, but appears to favor the presence of wedge disclination in nematics in preference to twist disclinations. Disclination interactions are also considerably affected. The radial force of interaction can be worked out in terms of single defect solutions. In addition, there arise angular forces of interaction between defects in the presence of anisotropy.

We next consider cholesteric liquid crystals. Elastic anisotropy appears to favor helicoidal pairings between disclinations of the χ-screw type. We reanalyze the defect solutions in the coarse-grained approximation. It emerges that the χ-edge disclination should be like the smectic A edge disclination from the point of view of energetics.

The problem of slow motion of disclinations and disclination pairs has also been considered. Elastic anisotropy is found to increase the frictional coefficient. Like and unlike pairs behave differently in motion.

I. INTRODUCTION

Liquid crystals are readily characterized by the optical textures that they exhibit. The schlieren texture of the nematic, the finger-print texture of the cholesteric, the focal conic texture of smectic A—each represents a collection of defects which is peculiar to the state of molecular order prevailing in that particular mesophase.

The structure and properties of defects have been considered from the viewpoints of both topology[1–5] and continuum mechanics.[6–11] In this article

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we address ourselves to defects in nematic and cholesteric liquid crystals, within the framework of the Ericksen-Leslie[12,13] formalism. Here the mechanics is determined by three elastic constants and six viscosity coefficients.

II. NEMATIC LIQUID CRYSTALS

We describe the system in terms of a unit vector **n** referred to as the director. In an elastically distorted nematic **n** varies slowly and smoothly from point to point. The free energy density of such a distorted structure is given by

$$F = \frac{K_{11}}{2}(\nabla \cdot \mathbf{n})^2 + \frac{K_{22}}{2}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{K_{33}}{2}(\mathbf{n} \times \nabla \times \mathbf{n})^2 \tag{1}$$

The three terms represent the splay, the twist and the bend distortions respectively, the corresponding elastic constants being K_{11}, K_{22} and K_{33}. The total energy of the system is

$$E = \int F\, d\mathbf{r}$$

The allowed director distortions are obtained by minimizing E. This results[12,13] in the following set of differential equations:

$$\left[\frac{\partial F}{\partial n_{i,j}}\right]_{,j} - \frac{\partial F}{\partial n_i} = 0 \qquad i = 1, 2, 3 \tag{2}$$

where

$$n_{i,j} = \frac{\partial n_i}{\partial x_j}; \qquad [f]_{,j} = \frac{\partial f}{\partial x_j} \quad \text{etc.}$$

It is also a consequence of the theory that director distortions have stresses associated with them. The stress tensor σ_{ij} is in general asymmetric.

$$\sigma_{ij} = -p\delta_{ji} - \frac{\partial F}{\partial n_{k,i}} n_{k,j} \tag{3}$$

where p is the hydrostatic pressure $= -p_0 + F$, p_0 being an arbitrary constant.

The elasticity of nematics is completely described by Eqs. 1 to 3. We consider the following special cases.

A. One constant approximation

$$K_{11} = K_{22} = K_{33} = K$$

We seek planar solutions, i.e.,

$$n_x = \cos\varphi, \qquad n_y = \sin\varphi, \qquad n_z = 0.$$

Then the free energy F and the equations of equilibrium in Eq. (2) reduce to

$$F = \frac{K}{2}(\nabla\varphi)^2$$

and

$$\nabla^2\varphi = 0 \tag{4}$$

This admits the following types of singularities:

$$\varphi = S\tan^{-1}\frac{y}{x} + C$$

$$S = \pm\frac{1}{2}N, \qquad N = \text{integer}$$

$$C = \text{constant}. \tag{5}$$

The singular line referred to as a wedge disclination is along the z-axis, and the orientation of the director which is confined to the xy plane changes by an integral multiple of π as one goes round the line. S is called the strength of the defect. In fact the schlieren texture exhibited by nematics is due to a collection of such defects. Between crossed polaroids a defect of strength S appears with $4S$ dark brushes.

In many ways disclinations in nematics resemble[14–16] screw disclinations in crystals. Table I summarizes these similarities. However, there is one important difference. The stress field around a screw dislocation has only shear components with no hydrostatic stress. The stress field around a disclination, on the other hand, has only a hydrostatic stress and no shear components at all.

Disclinations have also been compared with superfluid vortex filaments.[17,18] These similarities have also been included in Table I. It has been claimed[18] that this analogy is better, but in reality there is again an important difference to be noticed. It is a consequence of the above theory and a fact of experiment that two like disclinations repel one another and two unlike disclinations attract one another. A pair of like vortex filaments, on the other hand, rotates about an axis through the center of the line joining the vortices. In the case of an unlike pair there is a translatory motion of the pair in a direction perpendicular to the line joining the singularities. In either case the distance separating the two singularities is unaltered. This important difference arises from the fact that disclination mechanics is

TABLE 1

	Disclinations	Screw Dislocations	Vortex Filaments
Solution	$\varphi = S \tan^{-1} \frac{y}{x}$	$u = b \tan^{-1} \frac{y}{x}$	$\chi = \nu \tan^{-1} \frac{y}{x}$
Energy	$S^2 \ln \frac{R}{r_c}$	$b^2 \ln \frac{R}{r_c}$	$\nu^2 \ln \frac{R}{r_c}$
Stresses	No shears $P = P_0 - \frac{KS^2}{2r^2}$	Only shears $P = 0$	No shears $P = P_0 - \frac{\rho\nu^2}{2r^2}$
Interaction	Like pair repel Unlike pair attract $f \propto \frac{S_1 S_2}{D}$	Like pair repel Unlike pair attract $f \propto \frac{b_1 b_2}{D}$	Like pair rotates Unlike pair bodily moves
Reaction	$S = S_1 + S_2$	$b = b_1 + b_2$	None

controlled by potential energy while vortex dynamics is due to the kinetic motion of the fluid particle. There is one other difference between vortices and disclinations. Though individual disclinations do not have shear stresses around them, a collection of such defects does have shear stresses. Indeed Eshelby[18] argues that the force of interaction between disclinations is real (unlike the pseudo force between screw dislocations) and arises from shear stresses in the medium. On the other hand under no circumstance are there hydrostatic shears in a collection of vortices.

In view of these facts it may be safe to assert that nematic disclinations are a class by themselves and that analogies with screw dislocations and vortices may lead to misleading conclusions.

B. Splay-bend anisotropy: $K_{11} \neq K_{33}$

In real systems the three elastic constants K_{11}, K_{22} and K_{33} do not have the same value. We work out in this section some interesting consequences of elastic anisotropy. We confine ourselves again to situations where the director is always in the xy plane and its orientation independent of z.

(a) *Single defects:*[8,19,20] The free energy density, Eq. 1, simplifies to

$$F = \frac{K}{2}\varphi_\alpha^2[1 + \varepsilon \cos 2(\varphi - \alpha)]\Big/\gamma^2 \tag{6}$$

$\varphi_\alpha = \partial\varphi/\partial\alpha$, $\alpha = \tan^{-1} y/x$, $K = (K_{11} + K_{33})/2$, $\varepsilon = (K_{11} - K_{33})/(K_{11} + K_{33})$. And the equation of equilibrium is given by

$$\varphi_{\alpha\alpha} = \varepsilon[\varphi_{\alpha\alpha} \cos 2(\varphi - \alpha) + \varphi_\alpha(2 - \varphi_\alpha) \sin 2(\varphi - \alpha)] \tag{7}$$

with $\varphi_{\alpha\alpha} = \partial^2\varphi/\partial\alpha^2$.

For any given value of ε, Eq. 7 can only be solved numerically. However, for small values of ε one can employ a perturbation technique[8] to obtain

$$\varphi = (S\alpha + C) + \varepsilon\left[\frac{S(2 - S)}{4(S - 1)^2} \sin[2(S - 1)\alpha + 2C] + C'\right]$$

with C and C' as constants. The energy of the singularity for $S \neq +1$ is

$$E = \pi K \ln \frac{R}{r_c}\left\{S^2 - \frac{\varepsilon^2}{2}\left[\frac{S(2 - S)}{2(S - 1)}\right]^2\right\}$$

In the case of $S = +1$ one gets the isotropic solution in Eq. 5 with $C = 0$ or $\pi/2$ to be a solution of Eq. 7 irrespective of ε. Similarly the isotropic solution $S = +2$ is also a solution of Eq. 7. Another interesting point to be noted is that $+S$ and $-S$ now have different types of solutions and energies. Equation 7 can be solved in the neighborhood of the extreme limit of $\varepsilon = 1$. Figure 1 gives the energies calculated[20] for $S = +½$ and $-½$, and Figure 2 the structure of $S = +½$ in the limit of $\varepsilon = +1$.

(b) Defect pairs: In the one constant approximation it is easy to work out the structure and properties of defect pairs[7,8] employing the superposition principle. For example a defect of strength S_1 at (x_1, y_1) and that of S_2 at (x_2, y_2) can be described by

$$\varphi = S_1 \tan^{-1}\frac{y - y_1}{x - x_1} + S_2 \tan^{-1}\frac{y - y_2}{x - x_2} \tag{8}$$

and the total energy per unit length

$$E = \frac{K}{2}\int (\nabla\varphi)^2\, dx\, dy \tag{9}$$

From this one can get the force of interaction between the two defects. This is given by[7,8]

$$f = 2\pi K\frac{S_1 S_2}{D} \tag{10}$$

where D is the distance separating the two disclinations. This is repulsive for a like pair and attractive for an unlike pair.

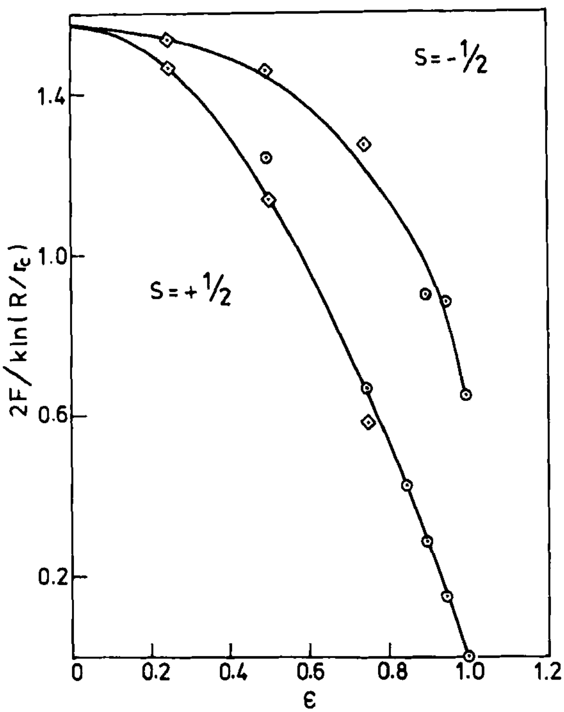

FIGURE 1 Dependence of energy on ε for ½ and −½. The squares are from the Nehring and Saupe approximation, circles from the perturbation in the neighborhood of $\varepsilon = 1$.

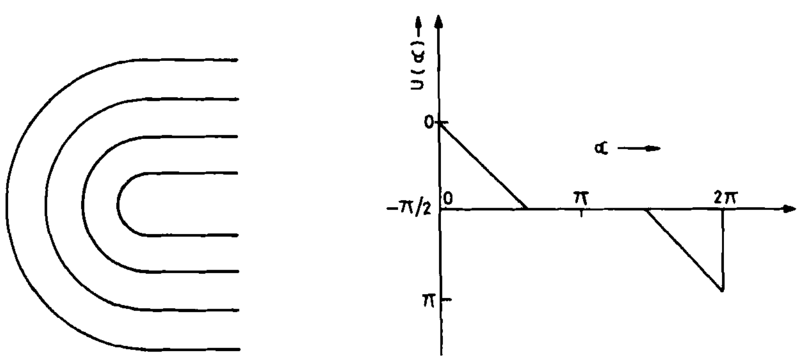

FIGURE 2 Structure of $s = ½$ in the extreme limit of $\varepsilon = 1$.

However, the superposition principle fails in the presence of elastic anisotropy. In this case the free energy density is

$$F = \frac{K}{2}\{\varphi_x^2 + \varphi_y^2 + \varepsilon[(\varphi_y^2 - \varphi_x^2)\cos 2\varphi - 2\varphi_x\varphi_y \sin 2\varphi]\} \quad (11)$$

and the equation of equilibrium is

$$\varphi_{xx} + \varphi_{yy} = \varepsilon[(\varphi_{xx} - \varphi_{yy} + 2\varphi_x\varphi_y)\cos 2\varphi - (\varphi_x^2 - \varphi_y^2 - 2\varphi_{xy})\sin 2\varphi] \quad (12)$$

where

$$\varphi_x = \partial\varphi/\partial x, \qquad \varphi_{xx} = \partial^2\varphi/\partial x^2, \quad \text{etc.}$$

(i) Radial force: It is not easy to solve Eq. 12, but it has an interesting scaling property[9,20] which can be used here. If $\varphi(x,y)$ is a solution then it is easy to verify that $\varphi(x/\lambda, y/\lambda)$ is also a solution. This is equivalent to scaling the coordinate system by a factor λ. Let two defects of strength S_1 and S_2 be respectively at $(+D/2, 0)$ and $(-D/2, 0)$. Near $(+D/2, 0)$ the director pattern reduces to that of S_1 and near $(-D/2, 0)$ to that of S_2. At distances large compared to D one may assume that the pattern becomes that of a defect of strength $S_1 + S_2$. To find the interaction between defects one needs only to find the change in energy as D changes. We illustrate in Figure 3 the two operations of scaling and shifting of defects. It can be shown that scaling does not alter the total energy E. It only alters the core sizes the distance D and the boundary at $r = R$. On the other hand if we shift the disclinations alone to a new separation λD, the total energy changes. Now it is easy to see that the interaction energy is given by

$$\Delta E = E_1 + E_2 - E_3.$$

Here E_1 is the total elastic energy stored in the region r_c to λr_c around S_1. E_2 is a similar energy around S_2. E_3 is the energy stored between R and λR. We have further assumed that shifting does not alter the core radius, which in principle is not correct.[9] Finally the force of interaction is found to be

$$f = -\frac{K}{2D}[I(S_1) + I(S_2) - I(S_1 + S_2)] \quad (13)$$

with

$$I(S) = \int_0^{2\pi} \varphi_\alpha^2[1 + \varepsilon \cos 2(\varphi - \alpha)]\,d\alpha \quad (14)$$

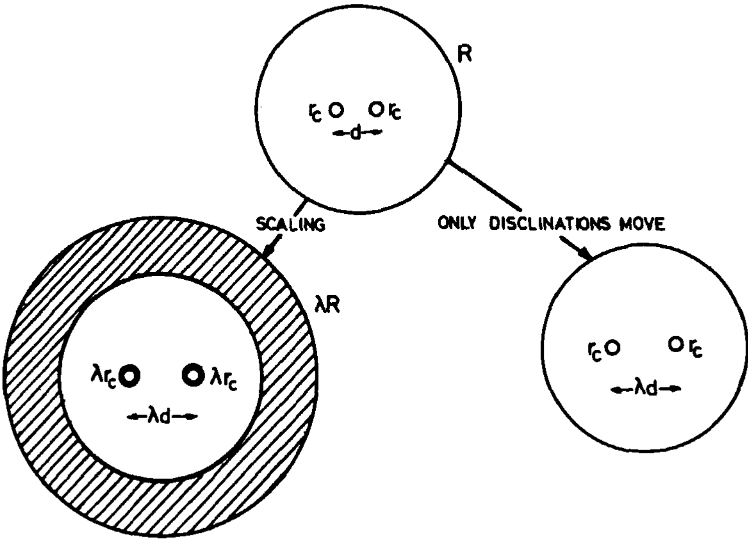

FIGURE 3 Schematic representation of scaling and disclination movement.

φ is the solution of Eq. 7 for a single defect of strength S in the presence of elastic anisotropy. When $\varepsilon = 0$ (Eq. 14), it reduces to Eq. 10.

(ii) Angular force:[21] There is one other consequence of ε which appears not to have been noticed. Figure 4 shows the director pattern for an unlike pair for two different situations. In one case ($C = 0$) the line joining the defects is parallel to the director orientation in the absence of defects. In the other case ($C = \pi/2$) it is perpendicular to the undistorted director. One could similarly draw the patterns for arbitrary orientations ($0 < C < \pi/2$). The total energy of all these configurations will be the same if $K_{11} = K_{33}$. However, the situation is dramatically altered when ε is present. For the ($+\frac{1}{2}, -\frac{1}{2}$) pair, though the director pattern in the neighborhood of the defects is the same for $C = 0$ as well as $\pi/2$, the intermediate regions are different. The pattern with $C = 0$ has the central region rich in bend while the pattern with $C = \pi/2$ is rich in splay. Therefore, in the presence of elastic anisotropy one or the other of the two patterns only will be allowed depending on the sign of ε. The patterns with intermediate values of C will experience an angular force which will ultimately take the configuration to the allowed value of C. Similar arguments can be invoked in cases where S_1 and/or $S_2 \neq +1$ or $S_1 + S_2 \neq +1$. In situations where this is not true we employ the following arguments. For any given ε depending on its sign, the $S = +1$ defect can have either $C = 0$ (pure radial) or $C = \pi/2$ (pure

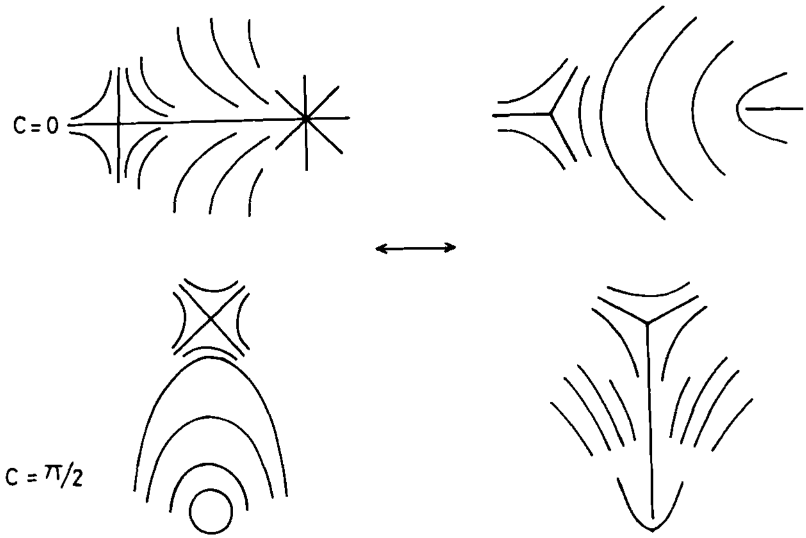

FIGURE 4 The director pattern for (+1, −1) and (+½, −½) pairs in two extreme situations of $C = 0$ and $\pi/2$ respectively.

circular) only. Structures with intermediate C values are forbidden. Thus in a combination of defects one again finds that only $C = 0$ or $\pi/2$ is allowed.

It is possible to calculate the angular force to a first order in ε. In the absence of elastic anisotropy the solution is given by Eq. 8. When $\varepsilon \neq 0$ but small we assume the solution to be

$$\psi = \varphi + \varepsilon\theta$$

Then

$$\nabla^2\theta = [(\varphi_{xx} - \varphi_{yy} + 2\varphi_x\varphi_y) \cos 2\varphi - (\varphi_x^2 - \varphi_y^2 - 2\varphi_{xy}) \sin 2\varphi] \tag{15}$$

And the total energy per unit length to a first order in ε is

$$E = \frac{K}{2}\int \{(\nabla\varphi)^2 - \varepsilon[(\varphi_x^2 - \varphi_y^2) \cos 2\varphi + 2\varphi_x\varphi_y \sin 2\varphi] + 2\varepsilon(\nabla\varphi \cdot \nabla\theta)\}\, dx\, dy \tag{16}$$

It can be shown that the last term does not contribute to E. The first term is independent of C. The angular part is therefore given by the second term. For an unlike pair this can be simplified to

$$E' = -\frac{K_{11} - K_{33}}{2} I \cos 2C \tag{17}$$

with

$$I = \int [(\varphi_x^2 - \varphi_y^2) \cos 2\varphi + 2\varphi_x\varphi_y \sin 2\varphi]\, dx\, dy \tag{18}$$

$$\varphi = s\left[\tan^{-1}\frac{y}{x + D} - \tan^{-1}\frac{y}{x - D}\right] \tag{19}$$

The resulting angular force $g = \partial E'/\partial C$ simplifies to

$$g = I(K_{11} - K_{33}) \sin 2C \tag{20}$$

C. Twist disclinations

Equation 4 admits one other type of singular solution, where φ is now a function of x and z and the singular line is along the y-axis. Again the director is confined to the x-y plane. This solution, referred to as a twist disclination, is given by

$$\varphi = S \tan^{-1}\frac{z}{x} + C \tag{21}$$

$S = \pm N/2$, N = Integer, C = Constant.

The energy of these solutions is exactly the same as that for the wedge disclinations. Yet experimentally they are not observed in nematics. One reason is perhaps the lack of proper anchoring mechanisms. But an interesting result follows by introducing elastic anisotropy to this problem.[19,22] Anisimov and Dzyaloshinskii showed[19] that twist disclinations have a lower or a higher energy than wedge disclinations depending upon whether K_{22} is smaller or greater than $(K_{11} + K_{33})/2$. Since K_{22} is generally smaller than $(K_{11} + K_{33})/2$ this theory favors twist disclinations to exist with greater probability, a fact not supported by experiments. However, if $K_{22} = (K_{11} + K_{33})/2$ but there is a splay-bend anisotropy we[22] get a very different answer. The first order perturbation calculation for a single defect at low ε values shows that the total energy is independent of the sign of S. [This should be compared with $+S$ and $-S$ having different energies in the case of wedge disclinations for $\varepsilon \neq 0$.] For a twist disclination with $S = \pm ½$ the total energy is

$$E_T = \frac{\pi K}{4}\left[1 - \frac{\varepsilon^2}{2}\frac{250}{576}\right] \ln\frac{R}{r_c} \tag{22}$$

On the other hand for a wedge disclination

$$E_W = \frac{\pi K}{4}\left[1 - \frac{\varepsilon^2}{2}\frac{4.5}{2}\right]\ln\frac{R}{r_c} \qquad \text{for } S = +\tfrac{1}{2}$$

$$= \frac{\pi K}{4}\left[1 - \frac{\varepsilon^2}{2}\frac{1.4}{2}\right]\ln\frac{R}{r_c} \qquad \text{for } S = -\tfrac{1}{2} \tag{23}$$

From Eqs. 22 and 23 we see that a twist disclination has higher energy than a wedge disclination in the presence of elastic anisotropy. This may also be one of the reasons why twist disclinations are not found in nematics.

It should be remarked that throughout we have confined the director to the x-y plane. This in principle is not true.[9,19] Detailed calculations allowing for a tilt out of the plane do not appear to have been made.

D. Escape in the third dimension

In the analysis presented so far we have only planar distortions. This results in $|S| = \tfrac{1}{2}$ having the lowest energy. Thus every high strength defect must ultimately dissociate into ½ singularities. But experimentally it is observed that $S = \pm 1$ defects exist with exceptional stability and without dissociating themselves into ½ singularities. This has now been explained[23,24] by allowing the director to escape in the z-direction also, over a region $0 < r < r_0$. Detailed calculations result in structures of the type

$$\left.\begin{aligned} n_x &= \cos \alpha S \sin \theta \\ n_y &= \sin \alpha S \sin \theta \\ n_z &= \cos \theta \end{aligned}\right\} S = \pm 1$$

$$\theta = 2\tan^{-1}\frac{r}{r_0}, \qquad r^2 = x^2 + y^2, \qquad \alpha = \tan^{-1}\frac{y}{x}$$

with an energy $E = 3\pi K$ for $S = +1$ and πK for $S = -1$. This is energetically favorable compared to a planar structure which gives an energy of $\pi K \ln r_0/r_c$.

III. CHOLESTERIC LIQUID CRYSTALS

For the purposes of continuum theory we can look upon a cholesteric as a spontaneously twisted nematic with a director pattern given by

$$n_x = \cos\theta, \qquad n_y = \sin\theta, \qquad n_z = 0$$

with

$$\theta = qz, \qquad q = 2\pi/P \tag{24}$$

P being the cholesteric pitch. The free energy density is

$$F = \frac{K_{11}}{2}(\nabla\cdot\mathbf{n})^2 + \frac{K_{22}}{2}(q + \mathbf{n}\cdot\nabla\times\mathbf{n})^2 + \frac{K_{33}}{2}(\mathbf{n}\times\nabla\times\mathbf{n})^2 \tag{25}$$

As in the case of nematics we can get singular solutions. In the one constant approximation we find

$$F = \frac{K}{2}\left[\left(\frac{\partial\theta}{\partial x}\right)^2 + \left(\frac{\partial\theta}{\partial y}\right)^2 + \left(\frac{\partial\theta}{\partial z} - q\right)^2\right].$$

A. χ-Screw disclinations

Just as in nematics we can again have a singular line along the z-axis (parallel to the twist) with the director pattern given by

$$n_x = \cos\theta, \qquad n_y = \sin\theta, \qquad n_z = 0$$

$$\theta = S\tan^{-1}\frac{y}{x} + qz \tag{26}$$

$$S = \pm N/2, \qquad N = \text{integer}$$

These are referred to as χ-screw disclinations and they are exactly like the nematic wedge disclinations. Many of the conclusions arrived at in nematics can be taken over to this case. In particular the consequences of elastic anisotropy has some interesting implications. For example, we have just seen that disclination pairs have angular forces in the presence of ε. For all practical purposes the solution that was obtained for nematics will hold for each nematic-like cholesteric layer, excepting for a continuous twist in the medium. Thus in the case of a pair of disclinations angular forces will lock the line joining the disclinations at the same orientation with respect to the local director **n** (of the defect free sample) in all the layers. Thus pairs of disclinations in a cholesteric should always be in a helical state while individual disclinations can be straight. For a pair of like disclinations the stable state is a double helix. Mutual repulsion increases the separation between the disclinations. In the helical state this increase is opposed by the line tension in the disclinations. In the end the two opposing processes compensate one another to result in a stable helical state. If the individual disclinations of the pair have different line tensions (as in the case of $+1$ and -1 collapsed structures) then the disclination with the lower tension should wind around the other with the higher tension. All these results are in agreement with the experimental observations of Rault[25] and Cladis *et al.*[26]

B. χ-Edge disclinations

There is another type of defect (referred to as the χ-edge) in cholesterics. Here the singular line is perpendicular to the twist axis. On going round this singular line, one gains or loses an integral number of half-pitches. The director pattern around such defects were first worked out by de Gennes,[10] who proposed a nematic twist disclination type solution:

$$n_x = \cos\theta, \qquad n_y = \sin\theta, \qquad n_z = 0$$

$$\theta = S \tan^{-1}\frac{z}{x} + qz \tag{27}$$

$$S = \pm N/2, \qquad N = \text{integer}$$

This results in an energy which logarithmically increases with the sample size. Though more refined solutions have been proposed,[27] they all result in a line tension increasing with sample size.

In this context it is necessary to point out that in many respects cholesterics simulate smectic A like behavior. Both of them exhibit focal conic textures. Under an external electric or magnetic field or an uniaxial tension parallel to the optic axis both develop instabilities.[28] In a capillary flow parallel to the optic axis both of them exhibit enormous viscosities.[29] All these features have been interpreted on the basis of a coarse-grained approximation. In all these situations the cholesteric distortions are slow and small over a pitch and the medium behaves as though it is layered,[30] each layer being a half-pitch. In this approximation the free energy can be worked out in terms of layer displacements 'u' parallel to the twist axis:

$$F' = \frac{B}{2}\left(\frac{\partial u}{\partial z}\right)^2 + \frac{\overline{K}}{2}\left[\left(\frac{\partial^2 u}{\partial x^2}\right) + \left(\frac{\partial^2 u}{\partial y^2}\right)\right]^2 \tag{28}$$

Identification with Eq. 25 yields $B = K_{22}q^2$, $\overline{K} = 3/8\, K_{33}$. This free energy is identical to that of smectic A.[31] Thus smectic A defects[10,32] must have their counterparts in cholesterics. The allowed singularities are:[33]

(i) Screw dislocation

$$u = \frac{NP}{4\pi}\tan^{-1}\frac{y}{x}$$

$$N = \pm\text{integer} \tag{29}$$

Here the singular line is along the twist axis. A circuit around the singular line results in a displacement of the layer along the helical axis by an integral number of half-pitches. Equation 29 can be recast to indicate the director orientation in the neighborhood of the singularity; it goes exactly over to Eq. 26 the χ-screw.

(ii) Edge dislocation: The singular line is perpendicular to twist axis; there is a gain of integral multiples of $P/2$ on going round the singular line. The distortion u in the neighborhood is given by

$$u = \frac{P}{8}\left\{1 + \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{dk}{ik}\exp[-k^2 z\sqrt{(\bar{k}/B)} + ikx]\right\} \tag{30}$$

This does not reduce to Eq. 27 and the implications of such a solution are entirely different. First, even in an infinite sample the energy W of the defect remains finite. In the one constant approximation,

$$W \approx \frac{0.6\pi KP}{4\xi} \tag{31}$$

ξ being the core radius which is of the order of $P/2$. This energy is smaller than that derived from Eq. 27. Thus energetics seem to favor a smectic A type edge dislocation solution. Also, like edge dislocations described by Eq. 30, they can attract one another and result in a small angle grain boundary.[32] This appears to account for the experimental observation of Bouligand and Kleman.[34] Even Grandjean-Cano wedge solution of equally spaced edge dislocations at a separation decided by the wedge angle is an allowed solution. Finally this solution appears to be closer to the topological model proposed by Kleman and Friedel.[35]

IV. MOTIONS OF DISCLINATIONS

A dislocation in a crystal can move with a finite velocity without dissipation.[36] However, the motion of a disclination is always associated with dissipation. A complete solution to the problem of disclination motion is difficult, but as a first approximation one may assume that the disclination velocities are so small that no real fluid velocity is excited and that the director inertia is negligible. Then the governing equations are:[12,13]

$$\left[\frac{\partial F}{\partial n_{i,j}}\right]_{,j} - \frac{\partial F}{\partial n_i} = \lambda_1 \dot{n}_i \qquad i = 1, 2, 3 \tag{32}$$

The density of entropy generated in the process for uniform motion is given by

$$s = \lambda_1 \sum_i \dot{n}_i^2 \tag{33}$$

Here $\lambda_1(=\alpha_3 - \alpha_2)$ is the twist viscosity coefficient. In the case of planar distortions in the xy plane and in the one constant approximation Eqs. 32 and 33 reduce to

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} = \frac{\lambda_1}{K}\frac{\partial\varphi}{\partial t} \tag{34}$$

and

$$s = \lambda_1\left(\frac{\partial\varphi}{\partial t}\right)^2 \tag{35}$$

In spite of these simplifying assumptions it does not seem possible to get an exact solution of Eq. 34. Let velocity **V** of the disclination be small enough, i.e.,

$$|\mathbf{V}| \ll (K/\lambda_1\tau)^{1/2} \tag{36}$$

where τ is the characteristic time involved in disclination motion. Then $\varphi(x - V_x t, y - V_y t)$ is to a good approximation a solution of Eq. 34 with $\varphi(x,y)$ representing the static solution.

We shall apply this theory to a single disclination motion.[37,38] The orientation φ is given by

$$\varphi \approx S\tan^{-1}\frac{y}{x - ut} \tag{37}$$

for a uniform motion along x-axis with a velocity u. And the total entropy production per unit length is

$$\begin{aligned} Q &= \int s\,dx\,dy \\ &= \left[\lambda_1 S^2 \frac{y^2}{[(x-ut)^2+y^2]^2}dx\,dy\right]u^2 \end{aligned} \tag{38}$$

since ut is small compared to distances over which effects of the singularity prevail we can approximate Eq. 38 to

$$Q \approx \left[S^2\lambda_1 \int \frac{y^2}{r^4}dx\,dy\right]u^2 \tag{39}$$

This gives for the frictional coefficient[37,38]

$$\eta = \frac{Q}{u^2} = \pi\lambda_1 S^2 \ln\frac{R}{r_c} \tag{40}$$

Most of the discussions on disclination motions appear to be on single defects. We show below that the presence of other defects markedly influences the results for the single defect.

A. Disclination pairs

As a simple example of the effect of one disclination on another we shall consider disclination pairs. The static solution is given by

$$\varphi = S_1 \tan^{-1}\frac{y}{x-D} + S_2 \tan^{-1}\frac{y}{x+D}. \tag{41}$$

There are two possible types of motions to be considered. In one case the pair moves bodily preserving the separation 2D, and in the other D varies with time resulting in relative motion of the two defects.

(i) As regards the bodily motion of the disclination pair, we consider the two cases of motion along or perpendicular to the line joining the defects. In the first case the solution is

$$\varphi = S_1 \tan^{-1}\frac{y}{x-ut-D} + S_2 \tan^{-1}\frac{y}{x-ut+D} \tag{42}$$

The entropy generated (calculated with the framework of the approximations already indicated) is found to be

$$\eta_\perp = \pi\lambda_1\left[(S_1^2 + S_2^2)\ln\frac{R}{r_c} + 2S_1S_2\ln\frac{R}{2D\sqrt{e}}\right] \tag{45}$$

yielding a frictional coefficient

$$\eta_\parallel = \pi\lambda_1\left[(S_1^2 + S_2^2)\ln\frac{R}{r_c} + 2S_1S_2\ln\frac{R\sqrt{e}}{2D}\right] \tag{44}$$

A similar calculation for the perpendicular motion yields

$$\eta_\perp = \pi_1\left[(S_1^2 + S_2^2)\ln\frac{R}{r_c} + 2S_1S_2\ln\frac{R}{2D\sqrt{e}}\right] \tag{45}$$

Therefore the frictional coefficient is anisotropic. From Eqs. 44 and 45 we get

$$\eta_\parallel - \eta_\perp = \pi\lambda_1 2S_1S_2 \tag{46}$$

showing that the anisotropy is dependent only on S_1 and S_2. It can also be shown from Eqs. 44 and 45 that for an unlike pair, i.e., $S_1 = -S_2$ both $\eta_\parallel$ and $\eta_\perp$ are dependent only on D and not on sample size R. Finally both $\eta_\parallel$ and $\eta_\perp$ for a like pair are greater than the values for an unlike pair.

(ii) Now we consider the second case where the disclinations have a relative motion due to variation in D. If $\partial D/\partial t = u$ is the velocity at which the disclinations approach or recede from one another, then the entropy generated can again be calculated using the same procedure and we find

$$Q = \pi\lambda_1\left[(S_1^2 + S_2^2)\ln\frac{R}{r_c} - 2S_1S_2\ln\frac{R\sqrt{e}}{2D}\right]u^2 \tag{47}$$

Defining the frictional coefficient as $\eta = Q/u^2$ we have for this relative motion:

$$\eta_R = \pi\lambda_1\left[(S_1^2 + S_2^2)\ln\frac{R}{r_c} - 2S_1S_2\ln\frac{R\sqrt{e}}{2D}\right], \tag{48}$$

from which we come to the interesting conclusion that as unlike defects more towards each other or as like defects recede from one another the frictional coefficient increases. It is as though friction opposes what elasticity dictates.

B. Elastic anisotropy

In the case of a +1 or +2 wedge disclination elastic anisotropy ε does not alter the director pattern given by the one constant approximation. To see the effect of elastic anisotropy we consider one simple example.

from which we come to the interesting conclusion that as unlike defects move towards each other or as like defects recede from one another the

$$\varphi = S\tan^{-1}\frac{y}{x} + \frac{(2-S)S}{4(S-1)^2}\varepsilon\sin\left[2(S-1)\tan^{-1}\frac{y}{x}\right] \tag{49}$$

We assume this to be moving along x-direction with a uniform velocity u. The frictional coefficient can be worked out employing the method indicated. It turns out that

$$\eta = \pi\lambda_1\left(S^2 + k\varepsilon^2\frac{(2-S)^2}{(S-1)^2}\right)\ln\frac{R}{r_c}$$

k being +1 for $S = +½$ and +2 for $S = -1$ and $-½$. Therefore elastic anisotropy increases the frictional coefficient. It can be shown similarly that ε increases η for twist disclinations.

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