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Dipoles of Disclination Lines of Half-Integer Strength in Nematics

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The equilibrium equation for the director field in the presence of a pair of parallel disclination lines of strength $\pm 1/2$ is considered. A perturbation procedure is employed, where the expansion parameter is the difference between the two elastic constants that play a role in this planar problem. It is demonstrated that the total energy, truncated to the first order, is minimized by one or the other of two special configurations, i.e., the problem generally admits only two possible orientations of the dipole axis with respect to the undistorted background. Between these two configurations, the "true" one is determined by the relative values of the elastic moduli.

Keywords: disclination lines, nematic disclinations, strength one half disclinations

1. INTRODUCTION

In the continuum theory of liquid crystals,[1] the equilibrium configurations of the director field $\mathbf{n}(\mathbf{r})$ are determined by minimization of the well-known Frank free-energy[2]; in the case of a nematic phase, this energy contains three independent constants—the k_is in Equation (1)—which measure the elastic response of the material to three basic types of distortion called splay, twist and bending.

Unfortunately, however, the full form of the Frank energy leads to an almost intractable equilibrium equation (see Equations (11), (12)). Moreover, the experimental values of all the constants are seldom known. As a consequence, the approximation of assuming that all these constants are equal is often made (one-constant approximation). The corresponding equilibrium equation is simply a Laplace equation: its solutions provide a first guess concerning the real distortion field.

Another source of difficulties is that in actual physical situations $\mathbf{n}(\mathbf{r})$ is not a smooth function of $\mathbf{r}$. There exist various kinds of "defects," known as disclinations: orientation cannot be defined on these lines (or points), the director field being discontinuous on them.

Since Frank free energy is obtained under the assumption of "slow variations" of $\mathbf{n}$, its use in close proximity to these discontinuities is certainly incorrect: indeed,

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the energy density at these point or line singularities is infinite. This last difficulty is, however, simply overcome by forbidding access into the disclination "cores."

Within this limitation, i.e., by disregarding local divergencies, configurations attained in the presence of a single disclination point or line have been determined.[3-5] In particular, for the case of a line, exact solutions have been found by Dzyaloshinskij.[5] The physical significance of single disclination line solutions is very limited, however, for the following reasons:

i) The energy of an isolated singularity in an infinite medium is infinite: this occurs because the director field does not approach uniformity at infinity, whatever the strength of the defect.

ii) For the case of a disclination of the integer type, a stability analysis[4] shows that a configuration containing two point singularities replaces the line discontinuity: this has been vividly described as an "escape in the third dimension."

In connection with point i), Ericksen[6] noticed that the energy of a finite number of disclinations is finite as long as the sum of their strengths is zero. So, the simplest realistic configuration consists in a pair of lines of opposite strength, each line being kept in a fixed position, i.e., a disclination dipole. By taking the strength S of these lines to be $\pm 1/2$, the complications mentioned in point ii) are also avoided.

In this work, the configurations determined by a pair of parallel lines with $S = \pm 1/2$ are considered. The $\mathbf{n}$ distortion is assumed to occur only in the planes perpendicular to the lines, so we really have a two-dimensional, or planar, problem. This case can be experimentally observed in liquid crystal films where disclination lines end on the plates enclosing the sample (a "sandwich" disposition). It is well known that disclinations of $S = \pm 1/2$ are dominant in liquid crystalline polymers.[7]

The general equation of statics and the boundary conditions for the disclination dipole are presented in Sections 2 and 3 of this paper, and a perturbation procedure is worked out, where the expansion parameter is the difference between the bend and splay constants. In Section 4, the first correction to the ground energy is evaluated, and minimum energy considerations are thereby developed. The results obtained are discussed in view of the predicted connection between optical and mechanical observations.

2. EQUILIBRIUM EQUATION AND BOUNDARY CONDITIONS

In the statics of liquid crystals (see, e.g., References 1 and 8), the free energy density e for a nematic phase is given by:

$$2e = k_1 (\nabla \cdot \mathbf{n})^2 + k_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + k_3 (\mathbf{n} \times \nabla \times \mathbf{n})^2 \tag{1}$$

As stated in the Introduction, we consider configurations of the director field such that:

$$\begin{aligned} n_z &= 0 \\ n_i &\text{ independent of } z \end{aligned} \tag{2}$$

the z axis being parallel to the disclination lines. Then, Equation (1) becomes:

$$2e' = k_1 (\nabla \cdot \mathbf{n})^2 + k_3 (\nabla \times \mathbf{n})^2 \tag{3}$$

By defining the "anisotropy parameter" α:

$$\frac{k_3 - k_1}{k_3 + k_1} = \alpha \qquad (|\alpha| \leq 1) \tag{4}$$

Equation (3) is rewritten in the form:

$$\frac{4e'}{k_3 + k_1} = \epsilon_{\mathrm{TOT}} = (1 - \alpha) (\nabla \cdot \mathbf{n})^2 + (1 + \alpha) (\nabla \times \mathbf{n})^2 \tag{5}$$

or, equivalently:

$$\epsilon_{\mathrm{TOT}} = \epsilon_0 + \alpha \epsilon_\alpha \tag{6}$$

with:

$$\begin{aligned} \epsilon_0 &= (\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2 \\ \epsilon_\alpha &= (\nabla \times \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2 \end{aligned} \tag{7}$$

To obtain the equilibrium equation we will now minimize the total distortion energy E (i.e., the surface integral of (6)) in the class of all the variations $\delta\mathbf{n}$ of the director field which keep $|\mathbf{n}| = 1$. To this end, we put:

$$\begin{aligned} n_x &= \cos\varphi \\ n_y &= \sin\varphi \end{aligned} \tag{8}$$

where φ is the angle between $\mathbf{n}$ and the dipole axis. By using Equation (8), Equation (7) becomes:

$$\begin{aligned} \epsilon_0(\varphi) &= (\varphi_{,x})^2 + (\varphi_{,y})^2 \\ \epsilon_\alpha(\varphi) &= D(\varphi)\cos 2\varphi + P(\varphi)\sin 2\varphi \end{aligned} \tag{9}$$

where:

$$\begin{aligned} D(\varphi) &= (\varphi_{,x})^2 - (\varphi_{,y})^2 \\ P(\varphi) &= (\varphi_{,x})\,(\varphi_{,y}) \end{aligned} \tag{10}$$

Minimization of E with respect to all variations in φ gives:

$$\nabla^2\varphi + \alpha A(\varphi) = 0 \tag{11}$$

with the following definition for the non-linear operator $A(\varphi)$:

$$A(\varphi) = (2P(\varphi) + (\varphi_{,xx} - \varphi_{,yy}))\cos 2\varphi - (D(\varphi) - (\varphi_{,xy} + \varphi_{,yx}))\sin 2\varphi \quad (12)$$

Of course, all preceding expressions do not hold very close to disclination centers where the energy density diverges; as mentioned in the Introduction, we define an "inaccessible core" for each disclination (see the end of this Section for the shape of this core), and assume that all equations are valid only outside of it.

In the infinite medium under consideration, boundary conditions supplementing Equation (11) emerge only from the requirement that the director field is uniform sufficiently far from the defect dipole, i.e., φ must approach a constant value K at infinity.

By analogy with the single disclination case, where a cylindrical symmetry is natural, a "bicylindrical symmetry" can be here inferred. In other words, we choose to use bipolar coordinates defined as (see Figure 1):

$$\begin{aligned} u &= \alpha_1 - \alpha_2 \\ v &= \ln(r_1/r_2) \end{aligned} \quad (13)$$

with:

$$\begin{aligned} \alpha_1 &= tg^{-1}(y/(x + L)) \\ \alpha_2 &= tg^{-1}(y/(x - L)) \\ r_1 &= ((x + L)^2 + y^2)^{1/2} \\ r_2 &= ((x - L)^2 + y^2)^{1/2} \end{aligned} \quad (14)$$

where $2L$ is the distance between the disclinations.

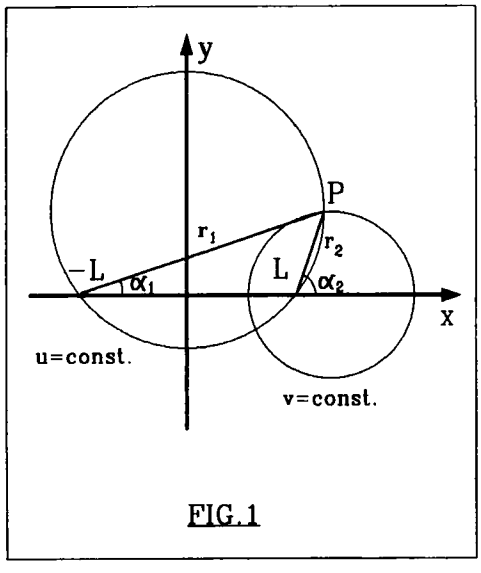

FIGURE 1 Cartesian coordinate system fixed to a disclination dipole (disclinations are at points $-L$, L on the x-axis) and definitions of r_1, r_2, α_1, α_2 needed to determine bipolar coordinates (see Equations (13), (14)). The circles shown are coordinate curves in bipolar coordinates.

As shown in Figure 1, coordinate curves in the bipolar system are circles, either through the singularities (u = const), or around them (v = const).

Since in bipolar coordinates the "origin" ($u = 0$, $v = 0$) is at infinity, the boundary condition becomes:

$$\varphi = K \quad \text{at} \quad u = 0, v = 0 \tag{15}$$

Definition of the disclination cores is now made by using the simplest choice in the coordinates adopted. Since $|v| \to \infty$ when approaching the disclinations, we limit the validity of the equations to the region $|v| \leq v_{MAX}$, where v_{MAX} is linked (logarithmically) to some characteristic molecular dimension.[1] Thus, $v = \pm v_{MAX}$ is the core boundary. This boundary is made up of two circles, the centers of which are somewhat displaced with respect to the disclinations (see Figure 2).

3. PERTURBATIVE APPROACH. ZEROTH ORDER SOLUTION AND FIRST ORDER ENERGY CORRECTION

We cannot solve Equation (11) for an arbitrary value of α; then we assume that the "anisotropy parameter" is small, i.e., $|\alpha| << 1$. Experiments show that this is the case for both low-molecular mass and polymeric liquid crystals (see References 1 and 9). With this hypothesis, we consider the perturbation expansion:

$$\varphi = \varphi^{(0)} + \alpha\varphi^{(1)} + \alpha^2\varphi^{(2)} + \ldots \tag{16}$$

where the $\varphi^{(i)}s$ ($i \neq 0$) are the "corrections" to the ground state function $\varphi^{(0)}$.

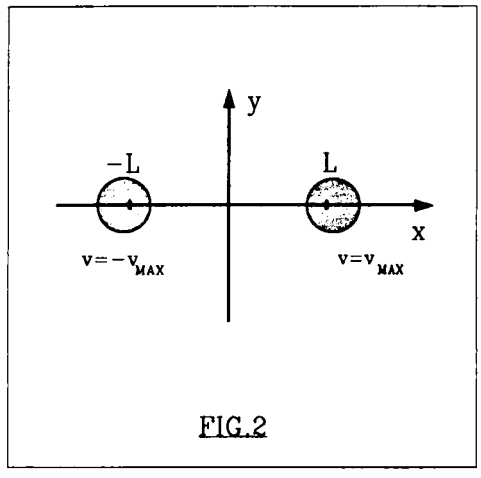

FIGURE 2 Disclination cores: the hatched region is "inaccessible," i.e., the continuum equations are not valid in it.

Substitution of Equation (16) into the exact equation, Equation (11), gives a sequence of differential equations for the $\varphi^{(i)}s$. Up to first order in α we have:

$$\nabla^2\varphi^{(0)} = 0 \tag{17}$$

$$\nabla^2\varphi^{(1)} = -A(\varphi^{(0)}) \tag{18}$$

The boundary condition (15) correspondingly becomes:

$$\varphi^{(0)} = K \quad \text{and} \quad \varphi^{(i)} = 0 \quad \text{at} \quad u = 0, v = 0 \tag{19}$$

Notice that Equation (19) implies:

$$\varphi = \varphi^{(0)} \quad \text{at} \quad u = 0, v = 0 \tag{20}$$

i.e., the zeroth order solution and the exact solution coincide on the boundary (the boundary being at infinity, this can be seen as an "asymptotic identity").

The zeroth order equation, Equation (17), is simply a Laplace equation, whereas Equation (18) for $\varphi^{(1)}$ is a Poisson equation whose "charge density" is determined by $\varphi^{(0)}$. Of course, Equation (17) could have been obtained also by putting $\alpha = 0$ in Equation (11), i.e., by using the so-called "one-constant approximation."

For the problem at hand (isolated dipole of disclinations $\pm 1/2$ at a distance $2L$), a solution $\varphi^{(0)}$ of Equation (17) is obtained by superposition of two single disclination solutions (see Reference 2), because of linearity of the Laplace equation:

$$\varphi^{(0)} = (1/2)(\alpha_1 - \alpha_2) + K = (1/2)u + K \tag{21}$$

(Notice that Equation (21) already accounts for the boundary condition).

All other solutions of Equation (17) can be excluded for the following reasons. In the first place, the physical situation requires that, whenever either α_1 or α_2 are separately increased by 2π (i.e., when a turn is made around only one of the two disclinations), φ must change by a multiple of π. This condition, while excluding a class of solutions of Equation (17), also sets the coefficient of $(\alpha_1 - \alpha_2)$ to be an integer multiple of 1/2 (thus defining the disclination strength S).

It can then be shown that all remaining solutions have the form:

$$\varphi^{(0)} = Su + Av + K + \sum_n \{[A_n \cos(nu) + B_n \sin(nu)]\, e^{nv}\} \tag{22}$$

where n must be a non-zero relative integer.

Now, for any non-zero A, A_n, B_n values, the director would make an infinite number of windings while approaching the disclination lines, i.e., for $|v| \to \infty$. These configurations, although physically acceptable solutions of Equation (17), certainly have a much larger energy than those represented by Equation (21). This argument remains essentially valid also in the presence of a finite size "core" associated to each disclination, in the sense that any possible v-dependence anyhow increases the energy of the solution. We are thus allowed to limit attention to solutions (21) only.

All these remaining solutions, i.e., by varying K, give rise to the same value of $\epsilon_0(\varphi^{(0)})$. Since $\epsilon_0(\varphi^{(0)})$ is recognized as the zeroth order term of the energy density expansion (see Equations (23), (24)), we are compelled to consider higher order terms in this expansion. Substitution of Equation (16) into Equations (6), (9) for the energy density gives:

$$\epsilon_{\mathrm{TOT}} = \epsilon^{(0)} + \alpha\epsilon^{(1)} + \alpha^2\epsilon^{(2)} + \ldots \tag{23}$$

where (up to first order in α):

$$\epsilon^{(0)} = \epsilon_0(\varphi^{(0)}) \tag{24}$$

$$\epsilon^{(1)} = \Omega_{01} + \epsilon_\alpha(\varphi^{(0)}) \tag{25}$$

and Ω_{01} is given by:

$$\Omega_{01} = 2\,\nabla\varphi^{(0)}\cdot\nabla\varphi^{(1)} \tag{26}$$

From Equation (25) one might be led to conclude that the first order correction to the energy depends on $\varphi^{(1)}$, i.e., on the solution of Equation (18), due to the presence of the "cross-term," Equation (26). However, we can readily show that:

$$C_{01} \equiv \int_S \Omega_{01}\,\mathrm{d}S = 0 \tag{27}$$

where, as described in the previous Section, S is the entire plane less the circles identified by $|\nu| \geq \nu_{\mathrm{MAX}}$.

Indeed, the integral C_{01} defined in Equation (27) can be rewritten as:

$$C_{01} = \int_S \nabla\cdot(\varphi^{(1)}\nabla\varphi^{(0)})\mathrm{d}S - \int_S \varphi^{(1)}\nabla^2\varphi^{(0)}\mathrm{d}S \tag{28}$$

The rightmost integral in Equation (28) is zero because of Equation (17). The remaining integral in Equation (28) can be transformed to a contour integral by use of the two-dimensional Green's theorem:

$$\int_S \nabla\cdot(\varphi^{(1)}\nabla\varphi^{(0)})\mathrm{d}S = \oint_l \varphi^{(1)}\nabla\varphi^{(0)}\cdot\mathbf{N}\,\mathrm{d}l \tag{29}$$

In Equation (29), l is the contour of S and $\mathbf{N}$ is the external normal to this contour. Region S is multiply connected; its contour l is made up of the projected line plus the circles $|\nu| = \nu_{\mathrm{MAX}}$. The part "at infinity" of the line integral in Equation (29) is zero, because of the boundary condition, Equation (19). The part at $|\nu| = \nu_{\mathrm{MAX}}$ is also zero. In fact, the normal $\mathbf{N}$ to the circles $|\nu| = \nu_{\mathrm{MAX}}$ is the unit vector of the coordinate u; on the other hand, it is:

$$\nabla\varphi^{(0)} = (1/2)\,\nabla u \tag{30}$$

So, $\nabla\varphi^{(0)}$ is perpendicular to any coordinate curve $u = \text{const}$. Then it follows:

$$\nabla\varphi^{(0)} \cdot \mathbf{N} = 0 \qquad \text{at} \qquad |\nu| = \nu_{MAX} \tag{31}$$

and this, in turn, demonstrates Equation (27).

In conclusion, the integral of the first order correction, Equation (25), to the energy density is obtained by considering only the perturbation ϵ_α operating on the unperturbed state $\varphi^{(0)}$. Although this is a standard result in ordinary perturbation theory, i.e., in the case of linear operators, it is remarkable that we find a similar result for the non-linear operator involved in our problem.

4. TOTAL ENERGY TO FIRST ORDER. MINIMIZATION

As we have shown in Section 3, the only relevant zeroth order solutions are in the form given by Equation (21). Moreover, only these zeroth order solutions are needed to calculate the first-order correction to the unperturbed energy. In the present Section, we will find out that the first order corrections to the total energy associated with these functions are indeed different, and that, consequently, energy minimization imposes a specific α-dependent value for K.

Let us define:

$$\begin{aligned} \varphi_0^{(0)} &= (1/2)u \\ \varphi_K^{(0)} &= (1/2)u + K \end{aligned} \tag{32}$$

Now, since ϵ_0, D, P are all differential operators, it is:

$$\begin{aligned} \epsilon_0(\varphi_K^{(0)}) &= \epsilon_0(\varphi_0^{(0)}) \\ D(\varphi_K^{(0)}) &= D(\varphi_0^{(0)}) \\ P(\varphi_K^{(0)}) &= P(\varphi_0^{(0)}) \end{aligned} \tag{33}$$

By using the second and third of Equations (33) we find:

$$\begin{aligned} \epsilon_\alpha(\varphi_K^{(0)}) \equiv\ & D(\varphi_K^{(0)})\cos 2(\varphi_K^{(0)}) + P(\varphi_K^{(0)})2\sin 2(\varphi_K^{(0)}) = \\ =\ & \cos 2K\,[D(\varphi_0^{(0)})\cos 2(\varphi_0^{(0)}) + P(\varphi_0^{(0)})2\sin 2(\varphi_0^{(0)})] + \\ & \sin 2K\,[-D(\varphi_0^{(0)})\sin 2(\varphi_0^{(0)}) + P(\varphi_0^{(0)})2\cos 2(\varphi_0^{(0)})] = \\ =\ & \cos 2K\,\epsilon_\alpha(\varphi_0^{(0)}) + \sin 2K\,b(\varphi_0^{(0)}) \end{aligned} \tag{34}$$

Integration of Equation (34) over S gives for the first order correction to the total energy:

$$E_\alpha(\varphi_K^{(0)}) = \cos 2K\, E_\alpha(\varphi_0^{(0)}) + \sin 2K\, B(\varphi_0^{(0)}) \tag{35}$$

where:

$$B(\varphi_0^{(0)}) = \int_S b(\varphi_0^{(0)})\mathrm{d}S \tag{36}$$

$$E_\alpha(\varphi_0^{(0)}) = \int_S \epsilon_\alpha(\varphi_0^{(0)})\mathrm{d}S \tag{37}$$

Now since:

$$E_{\mathrm{TOT}} = E_0 + \alpha E_\alpha(\varphi_K^{(0)}) \tag{38}$$

where E_0 is the ground energy, the conditions for E_{TOT} to be a minimum become:

$$\sin 2K\, E_\alpha(\varphi_0^{(0)}) - \cos 2K\, B(\varphi_0^{(0)}) = 0 \tag{39}$$

$$\alpha\,[\cos 2K\, E_\alpha(\varphi_0^{(0)}) + \sin 2K\, B(\varphi_0^{(0)})] < 0 \tag{40}$$

Symmetry considerations greatly simplify the evaluation of the integrals in Equations (36), and (37). Indeed, with respect to Cartesian coordinates we find the following parities:

$$\begin{aligned} \varphi_0^{(0)}(x, y) &= \varphi_0^{(0)}(-x, y) = -\varphi_0^{(0)}(x, -y) \\ D(\varphi_0^{(0)}) &= D(x, y) = D(-x, y) = D(x, -y) \\ P(\varphi_0^{(0)}) &= P(x, y) = -P(-x, y) = -P(x, -y) \end{aligned} \tag{41}$$

We then find:

$$B(\varphi_0^{(0)}) = 0 \tag{42}$$

$$E_\alpha(\varphi_0^{(0)}) = 4\int_{S'} D(\varphi_0^{(0)})\cos 2\varphi_0^{(0)}\mathrm{d}S \tag{43}$$

where S' is the part of S contained in the first quadrant ($x \geq 0$, $y \geq 0$). The latter integral has been evaluated numerically. Although the value of this integral depends on the arbitrary choice of ν_{MAX}, it is always found that:

$$E_\alpha(\varphi_0^{(0)}) > 0 \tag{44}$$

By using Equations (42), (44), Equations (39), (40) become:

$$\begin{aligned} \sin 2K &= 0 \\ \alpha \cos 2K &< 0 \end{aligned} \tag{45}$$

Equation (45) is our main result.

The first of Equations (45) limits K to two values:

$$K = 0, \pi/2 \tag{46}$$

Correspondingly, there are two "ground functions" for our problem:

$$\varphi_0^{(0)} = \alpha_1 - \alpha_2 \qquad \text{and} \qquad \varphi_{\pi/2}^{(0)} = \alpha_1 - \alpha_2 + \pi/2 \tag{47}$$

The director fields corresponding to these solutions are drawn in Figure 3. In one of them, the director at infinity and the dipole axis are perpendicular; in the other case they have the same direction. Which of the two possibilities is the actual

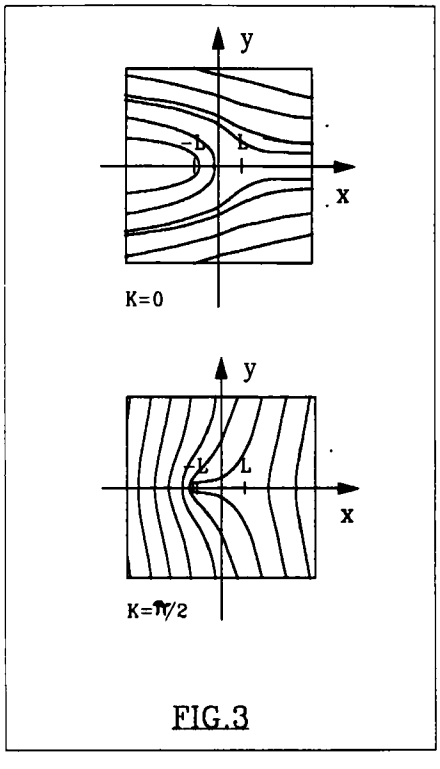

FIGURE 3 The two possible director fields for the dipole, corresponding to $K = 0$, $K = \pi/2$ (see Equation (47)).

solution is determined by the inequality in Equation (45), i.e., by the sign of α. The following correspondence applies:

$$\begin{aligned} \alpha > 0 &\leftrightarrow K = \pi/2 \\ \alpha < 0 &\leftrightarrow K = 0 \end{aligned} \tag{48}$$

It may be of interest to examine, in the two cases, how the total energy splits into the respective contributions of the relevant elastic modes, i.e., splay and bend. Using Equation (7) we find:

$$\begin{aligned} M &= \int_S (\nabla \cdot n)^2 dS = \int_S (1/2)(\epsilon_0 - \epsilon_\alpha) dS = (1/2)(E_0 - E_\alpha) \\ N &= \int_S (\nabla \times n)^2 dS = \int_S (1/2)(\epsilon_0 + \epsilon_\alpha) dS = (1/2)(E_0 + E_\alpha) \end{aligned} \tag{49}$$

Then, since from Equation (35) it is found that

$$E_\alpha(\varphi_K^{(0)}) = -E_\alpha(\varphi_0^{(0)}) \tag{50}$$

from Equations (44) and (50), Equations (49) give:

$$\begin{aligned} K = 0 &\leftrightarrow N > M, \quad M \text{ is minimum} \\ K = \pi/2 &\leftrightarrow M > N, \quad N \text{ is minimum} \end{aligned} \tag{51}$$

On the other hand, the splay and bend contributions are given by (see Equation (5)):

$$\begin{aligned} E_S &= (1 - \alpha)M \\ E_B &= (1 + \alpha)N \end{aligned} \tag{52}$$

Thus, from Equations (48), (51), (52) we find:

$$\begin{aligned} \alpha > 0 &\leftrightarrow K = \pi/2 \leftrightarrow E_B \text{ is minimum} \\ \alpha < 0 &\leftrightarrow K = 0 \leftrightarrow E_S \text{ is minimum} \end{aligned} \tag{53}$$

In other words, the configuration minimizing the total energy also minimizes the contribution of the "harder" elastic mode (i.e., the mode with the larger elastic constant k), as one might have expected.

It is experimentally known that for low-molecular mass liquid crystals, the bend constant is larger than the splay one, so that it always is the case that $\alpha > 0$. However, disclinations of strength $\pm 1/2$ are more frequently encountered in polymeric liquid crystals which can present both signs for α.

Quite recently Thomas *et al.*[10,11] have obtained electron micrographs of the molecular director pattern by means of the "lamellar decoration" technique. These authors always find the configuration corresponding to $K = 0$ for the isolated dipoles in their liquid-crystalline polymers (thermotropic polyesters). The results of this work would then indicate that $k_3 < k_1$ for the materials used in these experiments.

5. CONCLUSIONS

We have discussed the statics of a $\pm 1/2$ disclination dipole in nematic liquid crystals without the assumption that the elastic constants are equal. An expansion parameter α has been used, defined as the (normalized) difference of the relevant elastic constants.

A perturbation expansion in powers of α has been carried out, leading to a hierarchy of partial differential equations. The same perturbation procedure has been used to calculate corrections to the energy. It has been shown that the first-order correction is just the value of the perturbation energy operating on the "ground state."

Minimization of the total energy (up to first order) has then the following consequences: i) The dipole axis can form only two angles $(0, \pi/2)$ with respect to the homogeneous director field at infinity, i.e., there exist two preferential configurations; ii) The sign of α determines which of these two configurations is the right one.

Together with the total energy, the two configurations also minimize the "individual" energy content of either the bend or the splay elastic mode, depending on which of the two is the harder one.

These results imply that from the experimental observation of a configuration, we can predict which of the two elastic constants prevails, and vice-versa.

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