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## NON-SINGULAR DISCLINATIONS OF STRENGTH $S = +1$ IN NEMATICS (\*)

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**Résumé.** — On montre que les lignes de singularité de rang  $+1$  dans les nématiques ( $S = +1$  correspondent à une rotation de  $2\pi$  du directeur autour de la ligne) sont d'énergie minimale lorsque le directeur a une composante hors du plan perpendiculaire à la ligne et se trouve parallèle à la ligne le long de celle-ci. On fait le calcul de la configuration et de l'énergie dans les cas des déformations purement astrales (splay-flexion) et purement circulaires (torsion-flexion), en tenant compte de l'anisotropie des constantes élastiques. Ces solutions satisfont à la condition de champ moléculaire de de Gennes. L'énergie de la ligne ne dépend pas de la taille  $R$  de l'échantillon (supposé cylindrique). Pour  $R$  inférieur à une valeur critique de l'ordre de quelques longueurs moléculaires, la solution de Franck avec cœur (isotrope ou nématique) est préférable.

**Abstract.** — It is shown that the energy of a screw disclination of strength  $+1$  [ $2\pi$  rotation of the director around the line) is reduced if the molecules are allowed to relax out of the plane perpendicular to the line. This solution has no singularity on the axis,  $r = 0$ . The calculation is done in the case of the anisotropic elasticity [2] for the pure splay-bend and twist-bend cases. It satisfies de Gennes' [3] molecular field. The line energy of the solution does not depend upon the size  $R$  of the specimen. When  $R$  becomes smaller than a critical value of the order of several molecular lengths, the Frank solution with an isotropic (or nematic) core is preferable.

**I. Introduction.** — Screw disclination lines in nematic liquid crystals were first proposed by Frank [1]. His solutions are of the form :

$$\psi = S\theta + \psi_0 \quad (1)$$

where  $\psi$  is the angle of the director with a given axis in the plane perpendicular to the line ;  $\theta$  is the polar angle and  $S$ , the strength of the line (on a closed path around the line, the molecular inclination changes by  $2\pi S$ ), is an integral multiple of  $\pm \frac{1}{2}$ . The validity of eq. (1) depends upon two basic assumptions :

- a) the director lies in a plane perpendicular to the line,
- b) the elastic constants of bend ( $K_{33}$ ), splay ( $K_{11}$ ) and twist ( $K_{22}$ ) are equal (isotropic elasticity or the one constant approximation).

In a recent calculation, Dzyaloshinskii [2] has studied the Frank screw disclinations without assumption (b). He found that, qualitatively, the molecular orientation close to the line is the same as in the case of isotropic elasticity except for the case  $S = 1$ . For this case, he found that the only solutions which « survive » anisotropic elasticity are the purely radial ( $\psi = \theta$ ) and the

purely circular ( $\psi = \theta + \pi/2$ ) configurations. We have verified Dzyaloshinskii's result using a molecular field argument [3] that the  $S = 1$  planar configuration correctly gives an extremum to the free energy if (and only if)  $\psi = \theta$  and  $\psi = \theta + \pi/2$ .

We show, however, that the nature of this extremum depends upon assumption (a) and is in fact a saddle-point for macroscopic samples.

A characteristic of the planar solutions of Frank and Dzyaloshinskii is that the strain energy increases logarithmically as  $r$ , the radial distance from the line, approaches zero. This necessitates the presence of a core (i. e. a central region in which the elastic solution breaks down) to maintain a finite total energy. However, in the case of screw disclinations of strength  $S = 1$ , we have found that the total energy may be reduced and the core dispensed with, by allowing the molecules to relax out of the plane. Assumption (a) is thus removed. For these non-planar solutions, the line energy does not necessarily diverge as  $r \rightarrow 0$  and the total energy per unit length of line is finite and smaller than the planar solution, at least for cylindrical samples of radius,  $R$ , large. As  $R \rightarrow 0$ , the planar solution becomes again the least energetic one, even though a core is necessary.

Before presenting our results for the isotropic nematic ( $K_{11} = K_{22} = K_{33}$ ) (for which case we discuss in detail the problem of the core) and the anisotropic nematic ( $K_{11} \neq K_{22} \neq K_{33}$ ), we discuss

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the general problem of the existence of solutions of the screw type using de Gennes' molecular field argument [3].

## II. Molecular field of screw disclinations in nematics.

— The free energy density of a nematic is [1]

$$f = \frac{1}{2} \{ K_{11}(\text{div } \mathbf{n})^2 + K_{22}(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 + K_{33}(\mathbf{n} \times \text{curl } \mathbf{n})^2 \}; \quad (2)$$

where  $\mathbf{n}$  is the director and

$$n_1^2 + n_2^2 + n_3^2 = 1. \quad (3)$$

The correct minimization [3] of the total energy,

$$\mathcal{F} = \int f dV \text{ subject to the constraint eq. (3) is}$$

$$h_i = \frac{\partial f}{\partial n_i} - \frac{\partial}{\partial x_j} \frac{\partial f}{\partial n_{i,j}} = -\lambda n_i, \quad i = 1, 2, 3, \quad (4)$$

where  $n_{i,j} = \partial n_i / \partial x_j$  and  $\lambda$  is a Lagrange multiplier, i. e.  $\mathbf{h}$ , which de Gennes [3] calls a « molecular field » in analogy with magnetism, must be parallel to  $\mathbf{n}$ . Eq. (4) is then equivalent to  $\mathbf{h} \wedge \mathbf{n} = 0$ . Assuming  $\mathbf{n}$  constrained before hand and minimizing eq. (2) does not necessarily lead to stable solutions for the free energy.

For example, we consider the Frank configurations, constrained to be planar

$$\begin{aligned} n_r &= \cos \{ (S-1)\theta + \theta_0 \} \\ n_\theta &= \sin \{ (S-1)\theta + \theta_0 \} \\ n_z &= 0. \end{aligned} \quad (5)$$

From eq. (4), the molecular field has components

$$-h_r = \{ K_{11} S + K_{33}(S^2 n_\theta^2 + S(S-1)) \} \frac{n_r}{r^2} \quad (6a)$$

$$-h_\theta = \{ K_{11}(S-1)S + K_{33}(S^2 n_\theta^2 + S) \} \frac{n_\theta}{r^2}. \quad (6b)$$

Comparing (6a) and (6b), we see that we can only define a  $\lambda$ , such that  $-\mathbf{h} = \lambda \mathbf{n}$ , if one of the following applies.

- a)  $K_{11} = K_{33}$ ; any value of  $S$  allowed;
- b)  $S = 2$ , arbitrary  $K_{ii}$ ;
- c) if (and only if),  $n_\theta = 0$  ( $S = 1, \psi = \theta$ ) or

$$n_r = 0 \quad \left\{ S = 1, \psi = \theta + \frac{\pi}{2} \right\} \text{ (arbitrary } K_{ii} \text{)}.$$

More generally, considering the general planar solution  $\chi = \psi - \theta$  to be a function of the polar angle only, we find  $\mathbf{h}$  to have components (here  $\chi$  is the angle of  $\mathbf{n}$  with the radial vector)

$$-h_r = \frac{\cos \chi}{r} \left\{ K_{11} \left( 1 + \frac{d\chi}{d\theta} \right) + K_{33} \left\{ (\sin^2 \chi + 1) \left( \frac{d\chi}{d\theta} \right)^2 + (2 \sin^2 \chi + 1) \frac{d\chi}{d\theta} + \frac{\sin \chi}{\cos \chi} \frac{d^2 \chi}{d\theta^2} + \sin^2 \chi \right\} \right\} \quad (7a)$$

$$-h_\theta = \frac{\sin \chi}{r} \left\{ K_{11} \left\{ \left( 1 + \frac{d\chi}{d\theta} \right) \frac{d\chi}{d\theta} - \frac{\cos \chi}{\sin \chi} \frac{d^2 \chi}{d\theta^2} \right\} + K_{33} \left\{ \sin^2 \chi + \frac{d\chi}{d\theta} (2 \sin^2 \chi + 1) + \left( \frac{d\chi}{d\theta} \right)^2 \sin^2 \chi + 1 \right\} \right\}. \quad (7b)$$

Particular solutions for eq. (7) which satisfy the molecular field criterion are one of the following :

$$a) \quad K_{11} = K_{33} \quad \text{and} \quad \frac{d^2 \chi}{d\theta^2} = 0, \quad \text{i. e.} \quad \psi = S\theta + \psi_0$$

$$b) \quad \left( \frac{d\chi}{d\theta} \right)^2 = 0 \quad \text{and} \quad \frac{d^2 \chi}{d\theta^2} = 0 \quad \text{arbitrary } K_{ii} \quad \text{i. e.} \quad \begin{cases} \psi = \psi_0 & (S = 0) \\ \psi = 2\theta + \psi_0 & (S = 2) \end{cases}$$

$$c) \quad \left( \frac{d\chi}{d\theta} \right) = 0 \quad \text{but} \quad \psi = \theta \quad \text{or} \quad \psi = \theta + \frac{\pi}{2} \quad \text{(arbitrary } K_{ii} \text{)}.$$

There are just the conclusions we came to for the Frank planar model. However, most generally, to define a  $\lambda$  we require :

$$\begin{aligned} K_{11} + K_{33} \left\{ \left( \frac{d\chi}{d\theta} \right)^2 + \frac{\sin \chi}{\cos \chi} \frac{d^2 \chi}{d\theta^2} \right\} &= \\ &= K_{11} \left\{ \left( \frac{d\chi}{d\theta} \right)^2 - \frac{\cos \chi}{\sin \chi} \frac{d^2 \chi}{d\theta^2} \right\} + K_{33} \end{aligned} \quad (8a)$$

which may be written :

$$-\frac{d^2 \chi}{d\theta^2} \{ 1 - \alpha \cos 2\chi \} = \sin 2\chi \left\{ \left( \frac{d\chi}{d\theta} \right)^2 - 1 \right\} \alpha \quad (8b)$$

where  $\alpha = \frac{K_{33} - K_{11}}{K_{33} + K_{11}}$ . Eq. (8b) is the Euler-Lagrange

equation of Dzyaloshinskii. Consequently, all his solutions are stable solutions [4]. We use stable here in the sense that these solutions exist. In the next section we show that even though these solutions exist and are derivable from a minimization process, the corresponding energy is not an absolute minimum.

Releasing the planar constraint so that  $\chi$  is now a function of  $r$  (as well as  $\theta$ ), leads to a topologically similar configuration but one for which the total free energy is less. We have studied the case  $S = 1$  in some detail and we consider first the isotropic case  $K_{11} = K_{33} = K_{22}$  in the next section.

**III. The one constant calculation ( $K_{11} = K_{22} = K_{33}$ ).**

— In this limit,  $K_{11} = K_{22} = K_{33} = K$ , the cases pure splay ( $\psi = \theta$ ) and pure bend ( $\psi = \theta + \frac{\pi}{2}$ ) are described by the same free energy,

$$\frac{\mathcal{F}}{\pi K} = \int_{r_c}^R \left\{ \frac{\cos^2 \varphi}{r} - 2 \cos \varphi \sin \varphi \frac{d\varphi}{dr} + r \left( \frac{d\varphi}{dr} \right)^2 \right\} \times dr + \frac{E_c}{\pi K} \quad (9)$$

where  $r_c$  is the anticipated core radius and  $E_c$  is the core energy.  $\varphi$  is defined in figure (1a') and (b').

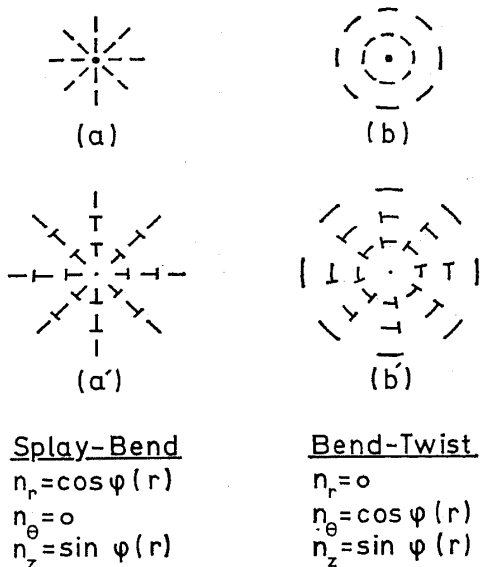


FIG. 1. — The Frank disclinations [1] of strength  $S = 1$  for the case of pure splay (a) and pure bend (b). The top two figures present the disclination as they appeared in ref [1]. The bottom two figures show how the nematic may relax the strains imposed by the disclination. In the figure, we show the components of the director for these two cases.  $\varphi$  is the angle between the director and the plane.

The Euler Lagrange equation for eq. (9) is

$$\frac{d}{dr} \left( r \frac{d\varphi}{dr} \right) = - \frac{\sin \varphi \cos \varphi}{r} \quad (10)$$

The trivial planar solution  $\varphi = 0, d\varphi/dr = 0$  exists, indicating that it also is an extremum of  $\mathcal{F}$ . The first integral of eq. (10) is :

$$\left( r \frac{d\varphi}{dr} \right)^2 = A^2 - \sin^2 \varphi \quad (11)$$

where  $A$  is the constant of integration. The molecular field condition is satisfied with a value of  $\lambda$  ( $\mathbf{h} = -\lambda \mathbf{n}$ )

$$\lambda = \frac{1}{r^2} \{ A^2 + \cos^2 \varphi \} \quad (12)$$

**A. CONFIGURATION OUTSIDE THE CORE.** — We now investigate the behaviour of the solution for eq. (11) for different values of  $A^2$ , given a cylinder of

radius  $R$  with the condition  $\varphi(R) = 0$ . We assume that  $\varphi$  increases as  $r$  decreases.

1.  $A^2 \geq 1$ . — If  $A^2 \geq 1$ , put  $A^2 = \frac{1}{\sin^2 \alpha}$ . The solution of eq. (11) is

$$r = R \exp \{ - \sin \alpha F(\varphi, \sin \alpha) \} \quad (13)$$

where  $F$  is the elliptic function of the first kind. Eq. (13) describes a molecular configuration which rotates infinitely fast as  $r \rightarrow 0$ . The period of rotation decreases exponentially as

$$\frac{r(\varphi)}{r(\varphi + \pi)} = \exp \{ 2 \sin \alpha K(\alpha) \} \quad (14)$$

where  $K(\alpha)$  is the complete elliptic integral of the first kind. The director is singular near the axis and the configuration must be cut off by a core region.

An interesting property of the solution is that the energy of the region between  $r(\varphi)$  and  $r(\varphi + \pi)$  does not depend on  $r$  and is given by

$$\frac{\mathcal{F}}{\pi K} = \frac{2}{\sin \alpha} \{ 2 E(\alpha) - \cos^2 \alpha K(\alpha) \} \quad (15)$$

It increases as  $A$  increases ( $E(\alpha)$  is the complete elliptic integral of the second kind).

When  $A^2 = 1$ , the solution of eq. (11) may be written

$$\frac{r}{R} = \cot \left( \frac{\pi}{4} + \frac{\varphi}{2} \right) = \left( \frac{1 - \sin \varphi}{1 + \sin \varphi} \right)^{1/2} \quad (16)$$

and  $r \rightarrow 0$  when  $\varphi \rightarrow \pi/2$ . A solution exists with no core, which is of smaller energy than any solution of the type  $A^2 > 1$ . For  $A^2 \geq 1$

$$\frac{\mathcal{F}}{\pi K} = \frac{1}{\sin \alpha} \{ 2 E(\alpha) - \cos^2 \alpha K(\alpha) \} + 1 \quad (17)$$

and when  $A^2 = 1, \mathcal{F}/\pi K = 3$ ; (see Fig. 2).

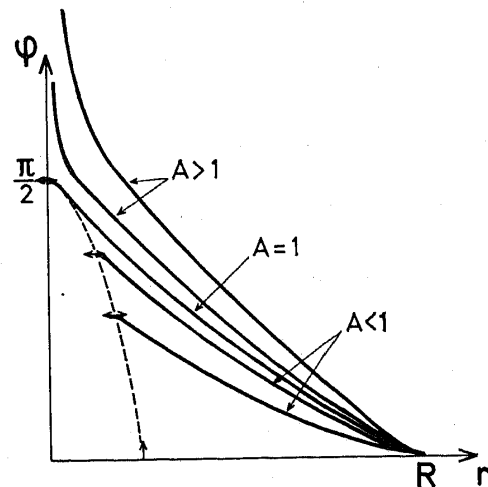


FIG. 2. — Solutions of eq. (11) for different values of constant  $A$ .  $A > 1$ : the director rotates an infinite number of times near the axis.  $A < 1$ : the solution is defined in the range

$$\{ \varphi = \sin^{-1} A, \varphi = 0 \}.$$

Note the horizontal tangents for  $A < 1$ , at  $\varphi = \sin^{-1} A$ .

2.  $A^2 \leq 1$ . — Put  $A^2 = \sin^2 \alpha$ , eq. (11) becomes :

$$\left( r \frac{d\varphi}{dr} \right)^2 = \sin^2 \alpha - \sin^2 \varphi \quad (18)$$

and  $\varphi \leq \alpha$ .

The solution of eq. (18) is

$$r = R \exp \left\{ - F \left( \sin^{-1} \left( \frac{\sin \varphi}{\sin \alpha} \right), \sin \alpha \right) \right\} \quad (19)$$

and  $r$  reaches the value  $r_0$ ,

$$r_0 = R \exp \{ - K(\alpha) \} \quad (20)$$

when  $\varphi = \alpha$ . From eq. (18) this implies  $\left( r \frac{d\varphi}{dr} \right)_{r_0} = 0$ .

We show later (in section III C.1) that  $\left( r \frac{d\varphi}{dr} \right)_{r_0} = 0$  permits us to complete the solution (eq. 19) with a core for  $0 \leq r \leq r_0$ .

$\frac{\mathcal{F}}{\pi K}(\sin \alpha)$  is shown in figure 5 and is given by

$$\frac{\mathcal{F}}{\pi K}(\sin \alpha) = \sin^2 \alpha - \cos^2 \alpha K(\alpha) + 2 E(\alpha). \quad (21)$$

$\mathcal{F}$  decreases when  $A = \sin \alpha$  decreases and is independent of  $R$ . For  $\alpha = 0$ , we get as limiting solution the Frank solution but restricted to the range  $r > R \exp - \pi/2$  (Fig. 2).

**B. GENERAL CONSIDERATIONS ABOUT A CORE.** — The above results state that there is a solution,  $A = 1$  which allows a non-singular distribution of the director from  $r = 0$ , where  $\mathbf{n}$  is parallel to the  $Z$ -axis, to the outside region where  $\mathbf{n}$  is in the plane (eq. 10). The energy,  $\mathcal{F}/\pi K$  is smaller than the energy of any distribution extending on the same angular range for  $A > 1$  but bigger than the energy of any distribution permitted in the permitted angular range for  $A < 1$ .

Three questions arise :

1. Does a core region completing the solution  $A < 1$  lead to a total energy smaller than the solution  $A = 1$  ? We discuss this in section D.

2. What are the boundary conditions at  $r = r_0$  in the core required to complete the solution  $A < 1$  with a core ? We discuss this in section C.

3. Does a core superimposed on the  $A = 1$  solution decrease the total energy of that solution ?

Two types of core require attention; a core consisting of isotropic liquid, or a core perfectly nematic, with the director along the axis of the line. In the first case, the core energy, if we neglect the latent heat, is of the order of  $K_B \Delta T_c$  per molecule ;  $K_B$  is the Boltzmann's constant and  $\Delta T_c$  the temperature difference between the clearing point  $T_c$  and the temperature of observation. We shall introduce later on a dimension

$r_p = \sqrt{K/2E}$  ( $E = K_B \Delta T_c N$ ,  $N$  number of molecules per unit volume), of the order of the core radius. Typically  $r_p$  is of the order of 55 Å ( $\Delta T_c = 10^\circ$ ,  $K \sim 10^{-6}$  cgs, density  $\sim 1$ , molecular weight  $\sim 250$ ). In the second case, the core energy is due to the surface tension  $\gamma$ . We estimate  $\gamma$  to be of the order of  $K/a \cos^2 \varphi_0$ , where  $a$  is a molecular length and  $\varphi_0$  the value of  $\varphi$  at the boundary in the outside region (i. e. at  $r = r_0$ ).

In principle the conditions of equilibrium are not satisfied in the region of the core since the presence of the core means that the Frank energy density is not minimized everywhere; indeed, a correct representation of a small region as the core usually is, would necessitate the introduction of second order elasticity coefficients or of an order parameter  $S$  which varies continuously. This latter description has been attempted by Fan [5]. Here we are concerned with the limitations of our description, which corresponds to the cases when the order parameter is large (nematic core) or small (isotropic core).

In order to solve the question raised in 1, above, we need to know the necessary boundary condition at the interface  $r = r_0$ , where the solution  $A < 1$  ends. Boundary conditions are of two types; balance of torques and balance of forces. In the following we assume that forces are entirely balanced by anchoring forces; this may not be true, but we prefer to limit ourselves here to the simplest case where only the torques have to be balanced (no anchoring torques, no surface tension effects).

In general, we shall find that for arbitrary  $\varphi$ ,  $d\varphi/dr = 0$  at  $r = r_0$  gives the stable solution (no torques). This enables us to answer question 3, here.

For the solution  $A = 1$ ,  $\left( r \frac{d\varphi}{dr} \right) = \cos \varphi$ . This is only zero when  $\varphi = \pi/2$  (i. e. at  $r = 0$ ). To place a core at  $r \neq 0$ , results in an unstable interface. However, if we ignore this condition and compute the resulting energies of an  $A^2 = 1$  solution with a superimposed core we find that for large  $R$  the solution has larger energy than the no core solution and for small  $R$  ( $\sim$  several molecular lengths) it has a smaller total energy.

**C. STABILITY OF SURFACES.** — We investigate the surface torques,  $\Gamma$ , present on the two surfaces  $r = R$  and  $r = r_0$ , and on sections  $Z = \pm d$  perpendicular to the line: According to de Gennes [3], and using Parodi's notations [6], per unit area of surface,

$$\Gamma = \mathbf{r} \wedge \mathbf{v} \cdot \boldsymbol{\sigma} + \mathbf{n} \wedge \boldsymbol{\pi} \cdot \mathbf{v} \quad (22)$$

where  $\boldsymbol{\pi}$  has components

$$\pi_{ij} = \frac{\delta f}{\delta n_{i,j}} = K n_{i,j} \quad (23)$$

taking  $f$ , the Frank Free Energy to be

$$f = \frac{K}{2} (n_{i,j} n_{i,j}) + \text{surface terms}.$$

From eq. 23, we see that  $\pi = K \nabla \mathbf{n}$ , (Parodi's convention, dyadic notation). In the formalism of de Gennes,  $\pi = (\nabla \mathbf{n})^T$  where  $T$  refers to the matrix  $\nabla \mathbf{n}$  transposed.  $\mathbf{v}$  is the unit vector normal to the surface in question.  $\pi$  is the radius vector to the surface,  $\sigma$  is the distortion stress tensor and is defined by

$$\sigma = - K(\nabla \mathbf{n})^T (\nabla \mathbf{n}) \quad (24)$$

in the one constant approximation. It is evident from eq. (24) that  $\sigma$  is symmetric in the one constant limit. In order to compute  $\pi$ , we neglect the surface terms in  $f$ .

In the case of splay-bend, and in cylindrical coordinates

$$\pi = K \nabla \mathbf{n} = K \begin{bmatrix} \frac{dn_r}{dr} & 0 & 0 \\ 0 & \frac{n_r}{r} & 0 \\ \frac{dn_z}{dr} & 0 & 0 \end{bmatrix}. \quad (25)$$

In the case of bend-twist

$$\pi = K \nabla \mathbf{n} = K \begin{bmatrix} 0 & -\frac{\cos \varphi}{r} & 0 \\ -\sin \varphi \frac{d\varphi}{dr} & 0 & 0 \\ \cos \varphi \frac{d\varphi}{dr} & 0 & 0 \end{bmatrix}. \quad (26)$$

1. On the surface  $r = r_0$  and  $r = R$ . — On these surfaces,  $\mathbf{v}$  is radial. For  $r = r_0$ ,  $\mathbf{v} = (-1, 0, 0)$  and for  $r = R$ ,  $\mathbf{v} = (1, 0, 0)$ . Computing  $\Gamma$ , we find for the case of splaybend,  $\Gamma_r = \Gamma_z = 0$  but

$$\Gamma_\theta = -v \left( \frac{d\varphi}{dr} \right) K. \quad (27)$$

Evaluating eq. (27) at  $r = r_0$ ,

$$\Gamma_\theta = \frac{K}{r_0} \sqrt{\sin^2 \alpha - \sin^2 \varphi_0} = 0$$

if  $\varphi(r_0) = \varphi_0 = \alpha$  (eq. 18). If  $\Gamma_\theta \neq 0$  at  $r = r_0$ , we would not be able to complete the solution  $A^2 < 1$  by filling the cylinder  $r \leq r_0$  with nematic.

At

$$r = R, \Gamma_\theta = -\frac{K \sin \alpha}{R}.$$

There is a net torque which per unit length of outside surface =  $-2 \pi K \sin \alpha$ . However, at  $r = R$ , the interface may be nematic-solid so that the torques at this surface may be balanced by an external source.

In the case of bend-twist, we have a similar result ;  $\Gamma_\theta = \Gamma_z = 0$  but

$$\Gamma_r = v \left( \frac{d\varphi}{dr} \right) K. \quad (28)$$

2. On the surface  $Z = \pm d$ . — On this surface  $\pi \cdot \mathbf{v} = 0$  and  $\sigma \cdot \mathbf{v} = 0$  so there are no torques at all on a planar surface even if we allow  $\mathbf{n}$  to vary freely.

D. CONFIGURATION IN THE CORE ( $A^2 \leq 1$ ). — 1) *Isotropic core*. — We assume eq. (19) to give the molecular configuration for  $r_0 \leq r \leq R$  where  $r_0$  is given by eq. (20). At  $r = r_0$ ,  $\varphi = \alpha$  and  $\sin^2 \alpha = A^2$  (see § III.A.2). For  $r_c \leq r \leq r_0$ , we put  $\varphi = \alpha$ . An isotropic core [8], [9] is supposed to be contained in the cylinder  $r \leq r_c$ . The case  $\alpha = 0$  corresponds to the planar case with an isotropic core radius  $r_p = \sqrt{K/2E}$  where we have estimated  $E$  in § III.B.

With a core as described above, we compute the total energy.  $\partial \mathcal{F} / \partial r_c = 0$  implies

$$r_c = (\cos \alpha) r_p. \quad (29)$$

In the limit  $\alpha = \pi/2$ , we see  $r_c = 0$ . The total energy is

$$\frac{\mathcal{F}_I}{\pi K} = 2 \left\{ E \left( \frac{\pi}{2}, \sin \alpha \right) - \cos^2 \alpha K \left( \frac{\pi}{2}, \sin \alpha \right) \right\} + \sin^2 \alpha + \cos^2 \alpha \left\{ \ln \frac{R}{r_p} + \ln \cos \alpha + \frac{1}{2} \right\}. \quad (30)$$

Eq. (30) is shown in figure 3, for different values of  $\ln R/r_p + \frac{1}{2}$ . From figure 3, it is evident that for  $\ln R/r_p \geq 6.5$  (i. e.  $R \geq 3.6 \mu$ ),  $A = 1$  represents a true minimum for our model. However for  $\ln R/r_p \sim 4.5$  (i. e.  $R \sim 0.25 \mu$ ) we note  $\alpha = 0$  (i. e. the Frank solution) becomes metastable. When  $\ln R/r_p \leq 2.5$  (i. e.  $R \sim 550 \text{ \AA}$ )  $\alpha = 0$  represents a stable solution. The solution  $A = 1$ , then is a true minimum for large  $R$  ( $\ln R/r_p \geq 6.5$ ) and it corresponds to a solution for which we do not need any core.

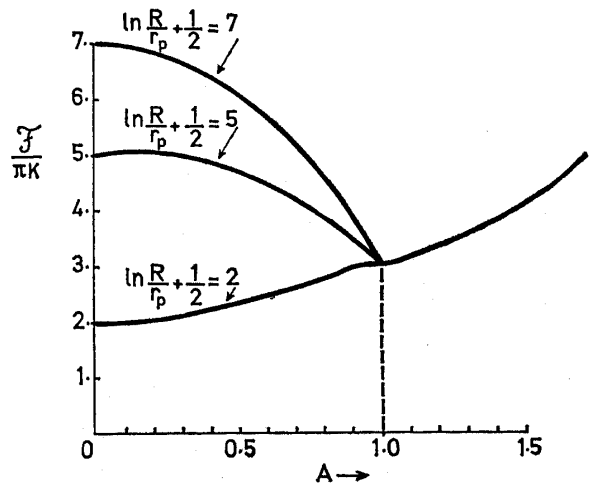


FIG. 3. — The effect of varying the constant of integration on the total free energy  $\mathcal{F}$  is shown.  $A > 1$ : the plotted value corresponds to eq. (17), which assumes that the core is nematic and of zero energy.  $A < 1$ : the core is assumed to be isotropic. When  $\ln R/r_p + \frac{1}{2} < 3$ , a minimum to  $\mathcal{F}$  is found for a constant of integration = 0. When  $\ln R/r_p + \frac{1}{2} \sim 7$ ,  $A = 1$  is seen to give an absolute minimum to  $\mathcal{F}$ .

2) *Nematic core* ( $A^2 \leq 1$ ). — This calculation as we present it would also apply to a hollow core. For reasons of stability, (§ III.C), we take at  $r = r_0$ ,  $d\varphi/dr = 0$ . For  $r < r_0$ , we put undistorted nematic with director  $\mathbf{n} = (0, 0, 1)$ . The energy to create a unit length of cylindrical surface, radius  $r_0$  is

$$E_c = 2 \pi r_0 \gamma \cos^2 \alpha \quad (31)$$

where  $\gamma$  is a surface tension  $\sim K/a$  (« $a$ » a molecular length). The  $\cos^2 \alpha$  factor indicates that molecules parallel to each other have zero surface energy.

The total energy is

$$\begin{aligned} \frac{\mathcal{F}_N}{\pi K} &= 2 E(\alpha) - \cos^2 \alpha K(\alpha) + \sin^2 \alpha + \\ &+ \frac{2R}{a} \cos^2 \alpha \exp \{ -K(\alpha) \}. \end{aligned} \quad (32)$$

The surface energy is seen to be quite large. If we resort to a core constructed similarly as in III.D.1 then we reduce the surface we must construct. The results are similar as for the isotropic core, except  $r_n = a/2$  and  $E_c/\pi K = 1$ .  $r_n$  is the equivalent of  $r_p$  in § III.D. In particular we note for macroscopic  $R$

$$\mathcal{F}_N - \mathcal{F}_I \geq 0 \quad (33)$$

where the equality pertains when  $\alpha = \pi/2$ . Note however, when  $R \rightarrow 0$ ,  $\mathcal{F}_N - \mathcal{F}_I < 0$ .

3) *Remark on the Frank solution.* — The core radius,  $r'$  of the Frank solution (where  $r'$  is either  $r_p$  of § D.1 or  $r_n$  of § D.2) is smaller than the limiting value  $r_0 = R \exp(-\pi/2)$  of the dashed curve for  $\varphi = 0$  (fig. 2) for macroscopic values of  $R$ . Our solution for  $A \leq 1$  does not satisfy the molecular field for

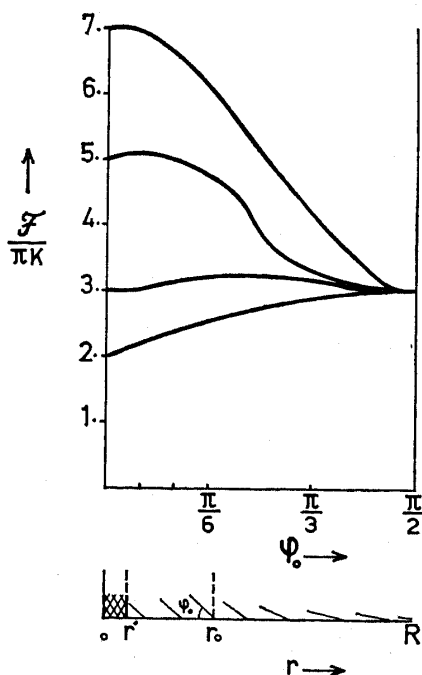


FIG. 4. — Total Free energy as a function of  $\varphi_0$  for the core as drawn in the lower part of the figure, for different values of  $\ln R/r_p + \frac{1}{2}$  ( $= 2, 3, 5, 7$ ). (Calculation for an isotropic core).

$r' \cos \alpha \leq r \leq r_0$  unless  $A = 0$  (the Frank case) or  $A = 1$  (the no core non-planar case). If we consider neighbouring solutions in the vicinity  $A = 0$ ,  $r_c = r'$ , for all samples a small variation of  $r_c$  increases  $\mathcal{F}$ . For large samples ( $\ln R_{\max}/r_c > 7$ ) varying  $A$  about zero leads to a decrease in  $\mathcal{F}$  (Fig. 4). The Frank solution is then a saddlepoint. When  $\ln R_{\max}/r_c < 7$ , it becomes a relative minimum and is a true minimum only for samples of the order of a few molecular lengths.

IV. **The anisotropic cases**  $K_{11} \neq K_{22} \neq K_{33}$ . — Here we must consider separately the cases of splay-bend (Fig. 1a') and bend-twist (Fig. 1b').

A. **THE CASE OF SPLAY-BEND FOR WHICH**  $K_{11} \neq K_{33}$ . — The free energy density is

$$2f = \frac{K_{11}}{r} \left\{ \cos \varphi - r \sin \varphi \frac{d\varphi}{dr} \right\}^2 + K_{33} \left\{ r \cos^2 \varphi \left( \frac{d\varphi}{dr} \right)^2 \right\}. \quad (34)$$

The Euler-Lagrange equation for eq. (34) yields as a first integral

$$\left( r \frac{d\varphi}{dr} \right)^2 = \frac{K_{11} \cos^2 \varphi + A_{SB}}{K_{11} \sin^2 \varphi + K_{33} \cos^2 \varphi}. \quad (35)$$

We have demonstrated the existence of a solution to eq. (35) with  $\varphi = \pi/2$  on the line, i. e. a coreless solution,  $A_{SB} = 0$ .

The result is tabulated in Table I for the two cases  $K_{11} < K_{33}$  and  $K_{11} > K_{33}$ . Also in Table I, we have tabulated the molecular configuration  $r(\varphi)/R$  where our boundary condition for  $r = R$  is  $\varphi = 0$ .

From the Table we see that for  $K_{11} < K_{33}$ ,  $\varphi(r)$  has an exponential behaviour as  $r \rightarrow 0$ . This approaches a more nearly core like behaviour. As  $K_{11} \rightarrow 0$ , without considering the addition of higher order terms to the expansion of the free energy  $\mathcal{F}/\pi \rightarrow 0$ . For  $K_{11} \rightarrow K_{33}$ ,  $\mathcal{F}/\pi$  tends to the isotropic limit of  $3K$ .

The molecular field is satisfied and we find

$$-\lambda = \left\{ \left( \frac{\partial \varphi}{\partial r} \right)^2 \times \left( 1 + \cos^2 \varphi + \frac{K_{11}}{K_{11} \sin^2 \varphi + K_{33} \cos^2 \varphi} \right) \right\}. \quad (36)$$

B. **THE CASE OF BEND-TWIST FOR WHICH**  $K_{22} \neq K_{33}$ . — The free energy density is

$$2f = \frac{K_{22}}{r} \left\{ \cos \varphi \sin \varphi - r \frac{d\varphi}{dr} \right\}^2 + \frac{K_{33}}{r} \cos^4 \varphi. \quad (37)$$

The first integral to the Euler-Lagrange equation is

$$\begin{aligned} \left( r \frac{d\varphi}{dr} \right)^2 &= \\ &= \frac{K_{33}}{K_{22}} \cos^2 \varphi \left\{ 1 + \left( \frac{K_{22}}{K_{33}} - 1 \right) \sin^2 \varphi \right\} + A_{BT} \end{aligned} \quad (38)$$

TABLE I

Summary of solutions of the minimization criteria for the free energy of a nematic in the presence of an  $S = + 1$  disclination

|                                 | $\frac{r}{R}$   | $\frac{\mathcal{F}}{\pi} \left( \alpha = \frac{\pi}{2} \right)$ | $k$  |
|---------------------------------|---|---|--|
| $K_{11} = K_{22} = K_{33} = K$  | $\cot \left( \frac{\pi}{4} + \frac{\varphi}{2} \right) = \left( \frac{1 - \sin \varphi}{1 + \sin \varphi} \right)^{1/2}$  | $3K$  | $k = 0$                                      |
| SPLAY-BEND<br>$K_{11} < K_{33}$ | $\left  \frac{\cos k \sin \varphi - \sqrt{1 - \sin^2 k \sin^2 \varphi}}{\cos k \sin \varphi + \sqrt{1 - \sin^2 k \sin^2 \varphi}} \right ^{1/2} \times \exp \{ -\psi \tan k \}$<br>where $\sin \psi = \sin k \sin \varphi$        | $2K_{11} + K_{33} \frac{k}{\tan k}$                             | $\tan^2 k = \frac{K_{33} - K_{11}}{K_{11}}$  |
|                                 | $\left  \frac{\coth k \sin \varphi - \sqrt{1 + \sin^2 \varphi \sinh^2 k}}{\coth k \sin \varphi + \sqrt{1 + \sin^2 \varphi \sinh^2 k}} \right ^{1/2} \times \exp \{ -\psi \tanh k \}$<br>where $\sinh \psi = \sinh k \sin \varphi$ | $2K_{11} + K_{33} \frac{k}{\tanh k}$                            | $\sin^2 k = \frac{K_{11} - K_{33}}{K_{33}}$  |
| BEND-TWIST<br>$K_{22} < K_{33}$ | $\left  \frac{\cos k \sin \varphi - \sqrt{1 - \sin^2 k \sin^2 \varphi}}{\cos k \sin \varphi + \sqrt{1 - \sin^2 k \sin^2 \varphi}} \right ^{1/2}$  | $2K_{22} + K_{33} \frac{k}{\sin k}$                             | $\sin^2 k = \frac{K_{33} - K_{22}}{K_{33}}$  |
|                                 | $\left  \frac{\coth k \sin \varphi - \sqrt{1 + \sinh^2 k \sin^2 \varphi}}{\coth k \sin \varphi + \sqrt{1 + \sinh^2 k \sin^2 \varphi}} \right ^{1/2}$  | $2K_{22} + K_{33} \frac{k}{\tanh k}$                            | $\sinh^2 k = \frac{K_{22} - K_{33}}{K_{33}}$ |

where  $A_{BT}$  is the constant of integration. We have calculated  $\mathcal{F}$  and  $r(\varphi)/R$  for the boundary conditions  $\varphi(R) = 0$  and  $\varphi(0) = \pi/2$  (summarized on Table I), i. e.  $A_{BT} = 0$ .

We see that the isotropic limit is  $3K$ . In the case  $K_{33} < K_{22}$ , we find the limit as  $K_{33} \rightarrow 0$  (neglecting higher order derivatives to the expansion of  $\mathcal{F}$ )  $\mathcal{F} \rightarrow 2K_{22}$  and not zero. This suggests that for sufficiently small  $K_{33}$  (we know of no nematic for which  $K_{33} < K_{22}$ ) the planar configuration would be the stable one. To estimate how small  $K_{33}$  must be would require the neglected higher order derivatives.

The molecular field condition is satisfied and  $\lambda$  can be defined as

$$-\lambda = \left\{ K_{22} \left( \frac{d\varphi}{dr} \right)^2 + (K_{33} - 2K_{22}) \frac{\cos \varphi \sin \varphi}{r} \frac{d\varphi}{dr} \right\} + \frac{\cos^2 \varphi}{r^2} \{ K_{22} \sin^2 \varphi + K_{33} \cos^2 \varphi \}. \quad (39)$$

**V. Discussion.** — We have demonstrated the existence of non-singular coreless solutions for the case  $S = 1$ . Such solutions seem to be experimentally verified, since a characteristic of  $S = 1$  disclinations is fringes of decreasing birefringence at  $r \rightarrow 0$ . This would correspond to a scheme such as figure 1a' or 1b'. It has also been proposed that coreless solutions exist for  $S = 1$  in cholesterics [12], [13], and this seems to have been verified experimentally [13].

We are unable to construct a «coreless» solution (see Fig. 6) for the  $S = + \frac{1}{2}$ . Consequently we expect disclinations of type  $S = \frac{1}{2}$  to be more energetic than the coreless  $S = 1$  variety (keeping in mind  $R$  large).

In fact, we have observed [10] two disclinations of type  $S = + \frac{1}{2}$  «associate» to form a  $+ 1$  which was subsequently observed to annihilate with an  $S = - 1$ . Such a situation is improbable if one insists upon a planar constraint for the  $+ 1$ , in this case, the energy  $\mathcal{F} \sim S^2$  predicts a «dissociation» of the

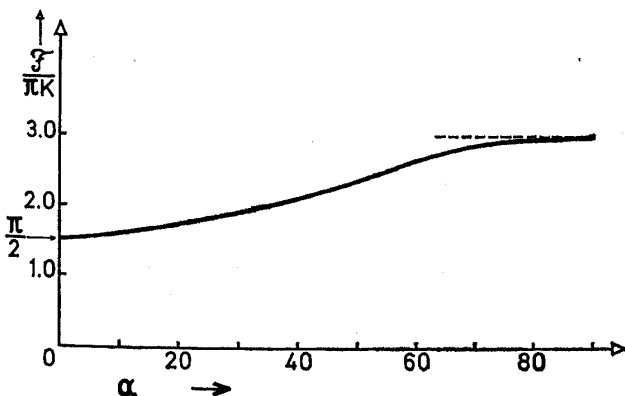


FIG. 5. —  $A < 1$ . Energy of the range allowed to the solution of eq. (11).

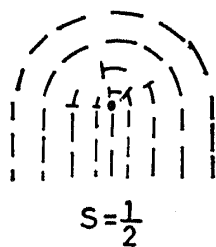


FIG. 6. — Topological scheme to demonstrate the necessity of a core for an  $S = +\frac{1}{2}$ .

$S = 1$ . Certainly disclinations of type  $S = 1$  appear to be far more abundant in samples of M. B. B. A. (p-n-methoxy benzilidene-p-butylaniline) sample thickness  $\sim 20 \mu$  than those of type  $S = +\frac{1}{2}$ . This again, does not accord with the relative energies of the lines assigned by the planar constraint.

**VI. Conclusion.** — When  $R$  is large compared to a molecular dimension, a non-planar, coreless solution has a lower free energy than the planar solution of Frank for the  $S = +1$ . The coreless solution is not singular (there are no logarithmic divergences in the

free energy) and exists irrespective of the relative values of the constants  $K_{11}$ ,  $K_{22}$  and  $K_{33}$ .

We consider our non-singular solution to represent a disclination, whose core has been dispersed throughout the sample in a manner reminiscent of the Peierls-Nabarro [11] model for dislocations. This implies that the molecular array may be described as a set of infinitesimal disclinations,  $d\Omega$ . A way of considering it is to take a circuit of constant radius around the line; the « change in inclination » of the director around this circuit is  $\Omega = \cos \varphi(r)$ . Therefore

$$d\Omega = -\sin \varphi d\varphi.$$

The total strength  $S$ , is given by

$$\begin{aligned} 2\pi S &= 2\pi \int_0^R d\Omega = -2\pi \int_0^R \sin \varphi \frac{d\varphi}{dr} dr \\ &= -2\pi \int_{\pi/2}^0 \sin \varphi d\varphi = 2\pi \quad \text{or} \quad S = 1. \end{aligned} \quad (46)$$

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