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Some Features of a Continuum Description of Disclination Lines in Nematic Liquid Crystals†

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Abstract—This paper employs continuum theory to investigate orientation patterns in a nematic liquid crystal in a long circular cylinder when a disclination line is coincident with the tube axis. Accepting Ericksen's hypothesis⁽¹⁾ that the disclination consists of a cylindrical core of isotropic fluid, it is of some interest to investigate the implications of associating an anisotropic surface energy with the nematic liquid crystal-isotropic core interface. To fix ideas, we consider the situation in which a radial orientation obtains at the cylinder wall while the surface energy dictates a parallel orientation at the interface, and examine particular forms of solution of the field equations appropriate to this arrangement. For each form discussed, more than one solution exists satisfying the boundary conditions employed, provided the tube radius is greater than a certain critical value. To distinguish between the various possibilities, we compare their energies anticipating that the solution with least energy is the one likely to occur.

1. Introduction

In this paper we consider the situation in which a sample of nematic liquid crystal is contained in a long circular cylinder, the orientation of the molecules being fixed and radial at the surface of the cylinder. For this arrangement, the Frank disclination pattern⁽²⁾ is a possible solution of the appropriate field equations and boundary conditions, but this solution is unsatisfactory in that it requires an infinite energy on the cylinder axis. To overcome this difficulty, Ericksen⁽¹⁾ has suggested that the disclination consists of a cylindrical core of isotropic fluid, and he assumes at the interface that the isotropic fluid exerts upon the liquid crystal only a normal pressure and no couple. In this event, the uniform radial pattern remains a solution. Also,

† Presented at the Fourth International Liquid Crystal Conference, Kent State University, August 21-25, 1972.

employing these conditions, Currie⁽³⁾ examines the possibility of distorted configurations, having in mind that solutions involving phase change may be relevant to the problem of flow through a pipe. However, as Ericksen⁽¹⁾ mentions, it is possible that the effects of surface energy at liquid crystal-isotropic fluid interfaces are important. Hence, it is of interest to associate an anisotropic surface energy with the nematic liquid crystal-isotropic core interface, and to investigate its influence. This has a precedent in the work of Dubois-Violette and Parodi,⁽⁴⁾ who include such a surface energy density in their analysis of the equilibrium shape and internal director configuration of small droplets of nematic liquid crystal suspended in an isotropic liquid which is at rest.

To fix ideas, we consider that the surface energy tends to orientate the molecules parallel to the interface, this presumably being of greater interest since in this case the orienting influence of the interface and that of the cylinder wall are in competition. In this event, the cylindrical symmetry of the situation suggests that one examines two particular forms of solution. Taking cylindrical polar coordinates (r, ϕ, z) , the z -axis being coincident with the tube axis, one is a distortion in the (r, ϕ) -plane which we call the planar solution, and the other is a distortion in the (r, z) -plane which we call the non-planar solution. Similar solutions with core structures have been investigated in recent papers by Cladis and Kléman⁽⁵⁾ and Meyer,⁽⁶⁾ but these authors employ interfacial conditions different from those used here.

2. The Continuum Theory

We employ the continuum theory proposed by Oseen,⁽⁷⁾ Frank,⁽²⁾ Ericksen⁽⁸⁾ and Leslie⁽⁹⁾ to consider static, isothermal states of an incompressible nematic liquid crystal. In this theory, one denotes the preferred direction of the molecular axis by a unit vector \mathbf{n} , called the director, and assumes that \mathbf{n} and $-\mathbf{n}$ are physically indistinguishable. The field equations to be satisfied throughout the liquid crystal are in Cartesian tensor notation

$$\left(\frac{\partial W}{\partial n_{i,j}} \right)_{,j} - \frac{\partial W}{\partial n_i} + \gamma n_i = 0, \quad (2.1)$$

where the scalar γ arises from the constraint upon the magnitude of

the director, and W is the Helmholtz free energy per unit volume. In general W may be any isotropic function of the director and its gradients, which is independent of the sign of \mathbf{n} , and here we adopt the form proposed by Frank⁽²⁾

$$2W = \alpha_2 n_{i,j} n_{i,j} + \alpha_4 n_{i,j} n_{j,i} + (\alpha_1 - \alpha_2 - \alpha_4) n_{i,i} n_{j,j} + (\alpha_3 - \alpha_2) n_i n_j n_{k,i} n_{k,j}, \quad (2.2)$$

where the α_i 's are constant for isothermal states. Assuming that W is a minimum when all director gradients are zero, Ericksen⁽¹⁰⁾ has shown that

$$\alpha_1 \geq 0, \quad \alpha_2 \geq 0, \quad \alpha_3 \geq 0, \quad |\alpha_1 - \alpha_2 - \alpha_4| \leq \alpha_1. \quad (2.3)$$

An immediate consequence of equations (2.2) and (2.3) is that W is always positive.

Following Ericksen,⁽¹⁾ we assume that a phase change occurs when the free energy of the liquid crystal exceeds a critical value W_c , the nematic liquid crystal changing into the isotropic liquid without change of density. To determine the radius of the isotropic core, one therefore uses the criterion that the free energy is equal to W_c at the interface.

Further, we endow a liquid crystal-isotropic fluid interface with a free energy w per unit area and assume that it is a function of the director and the unit outward surface normal \mathbf{v} ,† so that

$$w = w(\mathbf{n}, \mathbf{v}). \quad (2.4)$$

Using invariance arguments, it can be shown that

$$w = w[(\mathbf{v} \cdot \mathbf{n})^2]. \quad (2.5)$$

Since our present interest is to consider the case in which the surface energy strives for a parallel orientation at the interface, we assume that $w(0)$ is a minimum and that w increases monotonically with $(\mathbf{v} \cdot \mathbf{n})^2$ to a maximum $w(1)$.

The Eqs. (2.1) are second order non-linear differential equations, and in general it is reasonable to assume that certain specified conditions on the cylinder and at the interface must be satisfied. It is well known (Zocher and Coper,⁽¹¹⁾ Chatelain⁽¹²⁾) that solid

† Dubois-Violette and Parodi⁽⁴⁾ employ a more general expression for the surface energy density. However we prefer in the first instance to use the simpler form of Eq. (2.4), since non-trivial results are obtained.

boundaries may be treated to obtain, at least in a sample of nematic liquid crystal, a definite orientation of the molecular axis at the boundary. Hence we assume that the director orientation is fixed and radial at the surface of the cylinder. At the interface, it is natural to ask that there is a balance of forces and couples. The former is satisfied trivially, but the latter requires (see Jenkins and Barratt⁽¹³⁾)

$$\frac{\partial W}{\partial n_{i,k}} \nu_k + \frac{\partial w}{\partial n_i} = \beta n_i, \quad (2.6)$$

where β is an arbitrary scalar.

3. The Planar Solution

Here we examine solutions in which the preferred direction has physical components

$$n_r = \cos \theta(r), \quad n_\phi = \sin \theta(r), \quad n_z = 0, \quad (3.1)$$

where θ is the angle between the director and the radial direction. For this form of solution, one obtains the volume free energy density as

$$W = \frac{1}{2r^2} \left\{ f(\theta) \left(r \frac{d\theta}{dr} \right)^2 - \frac{df(\theta)}{d\theta} \cdot r \frac{d\theta}{dr} + g(\theta) \right\}, \quad (3.2)$$

with

$$f(\theta) = \alpha_3 \cos^2 \theta + \alpha_1 \sin^2 \theta, \quad g(\theta) = \alpha_1 \cos^2 \theta + \alpha_3 \sin^2 \theta. \quad (3.3)$$

From (2.2_{1,3}), $f(\theta)$ and $g(\theta)$ are obviously positive, and in this paper we exclude the possibility that either can be zero. Also it is found that the surface energy density has the functional form

$$w = w(\cos^2 \theta), \quad (3.4)$$

where $w(1)$ is a maximum and w decreases monotonically with $\cos^2 \theta$, to a minimum $w(0)$.

Eliminating γ from the field Eqs. (2.1), the equation for θ becomes

$$f(\theta) \frac{d^2 \theta}{dr^2} + \frac{1}{2} \frac{df(\theta)}{d\theta} \left(\frac{d\theta}{dr} \right)^2 + \frac{1}{r} f(\theta) \frac{d\theta}{dr} + \frac{1}{2r^2} \frac{df}{d\theta} = 0, \quad (3.5)$$

and we assume that

$$\theta = 0 \quad \text{on} \quad r = R, \quad (3.6)$$

R being the radius of the cylinder. After some manipulation employing (2.2), (2.6) and (3.1), one finds the expression representing balance of couple at the interface (see Jenkins and Barratt⁽¹³⁾) to be given by

$$\bar{f}\Theta - \frac{1}{2}\frac{d\bar{f}}{d\theta} + \bar{w}\bar{r}\sin 2\bar{\theta} = 0, \quad \Theta \equiv r\frac{d\theta}{dr}\bigg|_{r=\bar{r}}, \quad (3.7)$$

where \bar{r} is the radius of the circular isotropic core, a dot denotes differentiation with respect to $\cos^2 \theta$, and overbars denote quantities evaluated at the interface. The expression

$$W_c = \frac{1}{2\bar{r}^2} \left\{ \bar{f}\Theta^2 - \frac{d\bar{f}}{d\theta}\Theta + \bar{g} \right\} \quad (3.8)$$

determines the radius of the isotropic core, and using the interfacial boundary condition (3.7₁), one obtains \bar{r} as

$$\bar{r}^2 = \frac{\alpha_1\alpha_3}{2W_c\bar{f} - \bar{w}^2\sin^2 2\bar{\theta}}, \quad (3.9)$$

where the various parameters are assumed to be such that

$$2W_c\bar{f} - \bar{w}^2\sin^2 2\bar{\theta} > 0. \quad (3.10)$$

It is immediately obvious that the uniform radial orientation pattern, with an isotropic core of radius \bar{r}_0 given by

$$\bar{r}_0 = \left(\frac{\alpha_1}{2W_c} \right)^{1/2}, \quad (3.11)$$

is one possible solution of (3.5) subject to (3.6) and (3.7₁). However we investigate the possibility of a distorted configuration. Employing the change of variable

$$r = \bar{r}e^s, \quad (3.12)$$

one requires solutions of

$$f(\theta)\frac{d^2\theta}{ds^2} + \frac{1}{2}\frac{df}{d\theta}\left(\frac{d\theta}{ds}\right)^2 + \frac{1}{2}\frac{df}{d\theta} = 0 \quad (3.13)$$

subject to

$$\bar{f}\frac{d\bar{\theta}}{ds} - \frac{1}{2}\frac{d\bar{f}}{d\theta} + \bar{w}\bar{r}\sin 2\bar{\theta} = 0 \quad \text{on} \quad s = 0 \quad (3.14)$$

and

$$\theta = 0 \quad \text{on} \quad s = l, \quad (3.15)$$

where

$$l = \log_e (R/\bar{r}). \quad (3.16)$$

Using (3.14), (3.13) integrates to yield

$$(1 + m \sin^2 \theta) \left(\frac{d\theta}{ds} \right)^2 = \bar{h}^2 - m \sin^2 \theta, \quad (3.17)$$

where

$$\bar{h}^2 = \frac{1}{f\alpha_3} \{ (\alpha_1 - \alpha_3 - 2\bar{w}\bar{r})^2 \cos^2 \bar{\theta} + m \} \sin^2 \bar{\theta}, \quad m = \frac{\alpha_1}{\alpha_3} - 1. \quad (3.18)$$

To avoid making the remainder of this section unnecessarily long and complex, attention is restricted to the case

$$\alpha_1 = \alpha_3 = \alpha. \quad (3.19)$$

Since we assume $\dot{w} > 0$, it follows that the monotonic distortion

$$l - s = \frac{\alpha \theta}{\bar{w}\bar{r} \sin 2\bar{\theta}}, \quad |\theta| \leq \frac{\pi}{2}, \quad (3.20)$$

with

$$l = l_1(\bar{\theta}) \equiv \frac{\alpha \bar{\theta}}{\bar{w}\bar{r} \sin 2\bar{\theta}} \quad \text{and} \quad \lim_{|\bar{\theta}| \rightarrow \pi/2} l_1(\bar{\theta}) = \infty, \quad (3.21)$$

is also a solution of (3.5) subject to (3.6) and (3.7₁). For $|\bar{\theta}|$ in the interval zero to $\pi/2$, the inverse relation to $l_1(\bar{\theta})$ giving $|\bar{\theta}|$ in terms of R will not be single valued in general, and hence more than one solution of the form (3.20) may be possible. Utilizing (3.21₁), one obtains a critical value R_1^c of the tube radius given by

$$R_1^c = \bar{r}_0 \exp \left\{ \frac{\alpha}{2\bar{r}_0 \dot{w}(1)} \right\}, \quad (3.22)$$

at which a smooth transition between the uniform radial pattern and a planar distortion is possible. In the event that

$$l_1(0) < l_1(\bar{\theta}) + \log_e(\bar{r}/\bar{r}_0), \quad 0 < |\bar{\theta}| \leq \frac{\pi}{2}, \quad (3.23)$$

the uniform radial configuration is the only possible solution when R is less than R_1^c , but for R greater than R_1^c , both the radial configura-

ration and the monotonic distortion (3.20) are solutions having the required form. However, even if $\bar{r}_0 \exp(l_1(0))$ is only a local minimum of the function $\bar{r} \exp(l_1(\bar{\theta}))$, there is a possibility that the threshold effect may still be observed. Further, under certain conditions it is possible that $\bar{r} \exp(l_1(\bar{\theta}))$ increases monotonically with $|\bar{\theta}|$ for all values of $|\bar{\theta}|$ less than $\pi/2$. In this event, there is only one value of $|\bar{\theta}|$ between zero and $\pi/2$ which satisfies (3.21₁), and hence only one distortion of the form (3.20) is possible.

To determine which of the possible configurations is the stable solution, a stability analysis of the dynamic equations would be desirable. At the moment such an analysis appears not to be possible, and so we follow Dafermos⁽¹⁴⁾ in comparing the total energies associated with each solution. Intuitively, one anticipates that the configuration having least energy is the one likely to occur, and hence we refer to that solution as the stable solution. However the possibility that a solution of a form not considered in this paper may have an even smaller energy must be admitted.

The total energies per unit length of cylinder associated with the distorted and uniform radial configurations are given by

$$\epsilon_1(\bar{\theta}) = W_0 \pi \bar{r}^2 + 2\pi \bar{r} \bar{w} + \pi \alpha \int_{\bar{r}}^R \frac{1}{r} \left\{ \left(r \frac{d\bar{\theta}}{dr} \right)^2 + 1 \right\} dr \quad (3.24)$$

and

$$\epsilon(0) = W_0 \pi \bar{r}_0^2 + 2\pi \bar{r}_0 w(1) + \pi \alpha \int_{\bar{r}_0}^R \frac{dr}{r} \quad (3.25)$$

respectively, where W_0 is the volume free energy density of the isotropic core. It therefore follows that the distortion is the stable solution whenever

$$\begin{aligned} \frac{2w(1)}{(2W_c \alpha)^{1/2}} - \frac{2\bar{w}}{(2W_c \alpha - \bar{w}^2 \sin^2 2\bar{\theta})^{1/2}} &> \frac{W_0 \bar{w}^2 \sin^2 2\bar{\theta}}{2W_c (2W_c \alpha - \bar{w}^2 \sin^2 2\bar{\theta})} \\ &+ \frac{\bar{\theta} \bar{w} \sin 2\bar{\theta}}{(2W_c \alpha - \bar{w}^2 \sin^2 2\bar{\theta})^{1/2}} + \frac{1}{2} \log_e \left(1 - \frac{\bar{w}^2 \sin^2 2\bar{\theta}}{2W_c \alpha} \right). \end{aligned} \quad (3.26)$$

In the event that w , W_0 and W_c were known, it would be possible to find those values of $\bar{\theta}$ for which (3.26) obtains. Since no such data is available, we assume that W_0 and W_c are equal and examine some special cases.

For sufficiently small $|\bar{\theta}|$, (3.26) can be satisfied only if $w(1)$ is

strictly negative, which seems unlikely. For example, if the surface energy has the form suggested by Cladis and Kléman⁽⁵⁾

$$w = \dot{w}(1) \cos^2 \theta, \quad \dot{w}(1) > 0, \quad (3.27)$$

(3.26) is never satisfied for small enough $|\bar{\theta}|$, and in such cases the radial pattern is the stable configuration. However for values of $|\bar{\theta}|$ in a neighbourhood of $\pi/2$, it is readily shown that (3.26) obtains and the distortion is the stable solution. These observations suggest that, although there are values of $\bar{\theta}$ for which the distortion has the smaller energy, no local planar distortion about the uniform radial configuration may occur. Also we note that $\epsilon_1(\bar{\theta})$ and R tend to infinity as $|\bar{\theta}|$ approaches $\pi/2$.

In the above analysis, θ is restricted to values between $-\pi/2$ and $\pi/2$, and it is assumed that α_1 and α_3 are equal. As in those cases discussed by Dafermos,⁽¹⁴⁾ we admit that solutions with $|\theta|$ greater than $\pi/2$ are possible. Although such solutions are not investigated here, the experience of Dafermos⁽¹⁴⁾ suggests that these solutions are associated with larger energies than the distortion for which θ lies in the interval $-\pi/2$ to $\pi/2$. Finally an analysis for the case when α_1 and α_3 are not equal, similar to that given here for equal coefficients, is possible and is given elsewhere.⁽¹⁵⁾

4. The Non-planar Solution

In this section, we consider solutions whose physical components of the preferred direction have the form

$$n_r = \cos \theta(r), \quad n_\phi = 0, \quad n_z = \sin \theta(r). \quad (4.1)$$

For such configurations, the volume energy density is

$$W = \frac{1}{2r^2} \left\{ f(\theta) \left(r \frac{d\theta}{dr} \right)^2 - \tau \sin 2\theta \left(r \frac{d\theta}{dr} \right) + \alpha_1 \cos^2 \theta \right\}, \quad (4.2)$$

where

$$\tau = \alpha_1 - \alpha_2 - \alpha_4, \quad |\tau| \leq \alpha_1, \quad (4.3)$$

and the surface energy density has the functional form

$$w = w(\cos^2 \theta). \quad (4.4)$$

Using (2.2) and (4.1) in (2.1), one obtains the equation for θ as

$$f(\theta) \frac{d^2 \theta}{dr^2} + \frac{1}{2} \frac{df}{d\theta} \left(\frac{d\theta}{dr} \right)^2 + \frac{1}{r} f(\theta) \frac{d\theta}{dr} + \frac{\alpha_1 \sin \theta \cos \theta}{r^2} = 0. \quad (4.5)$$

On the cylinder we assume that

$$\theta = 0, \quad (4.6)$$

and the condition for balance of couple at the interface⁽¹³⁾ yields

$$\bar{f} \bar{\theta} + (2\bar{w}\bar{r} - \tau) \cos \bar{\theta} \sin \bar{\theta} = 0. \quad (4.7)$$

Combining (4.7) with Eq. (4.2) at the interface, one obtains

$$\bar{r}^2 = \frac{(\bar{f}\alpha_1 - \tau^2 \sin^2 \bar{\theta}) \cos^2 \bar{\theta}}{2W_c \bar{f} - \bar{w}^2 \sin^2 2\bar{\theta}}, \quad (4.8)$$

and it is assumed that the various parameters satisfy the inequalities

$$2W_c \bar{f} - \bar{w}^2 \sin^2 2\bar{\theta} > 0 \quad \text{and} \quad \bar{f}\alpha_1 - \tau^2 \sin^2 \bar{\theta} > 0. \quad (4.9)$$

It is interesting to observe that \bar{r} tends to zero as $|\bar{\theta}|$ approaches $\pi/2$.

The uniform radial orientation pattern, with an isotropic core of radius \bar{r}_0 given by (3.11), is one solution of (4.5) subject to (4.6) and (4.7), but we examine the possibility of a distorted solution. Employing the change of variable (3.10) and the interfacial boundary condition (4.7), one may integrate (4.5) once to obtain

$$(1 + m \sin^2 \theta) \left(\frac{d\theta}{ds} \right)^2 + \sin^2 \theta = \bar{k}^2, \quad (4.10)$$

where

$$\bar{k}^2 = \left\{ \frac{-2\bar{w}\bar{r} + \tau}{\bar{f}\alpha_1} \cos^2 \bar{\theta} + 1 \right\} \sin^2 \bar{\theta}. \quad (4.11)$$

It is found that two types of distortion may occur, depending upon the sign of $-2\bar{w}\bar{r} + \tau$. This suggests that α_4 may be important in determining which type of distortion is possible.

In the event that

$$-2\bar{w}\bar{r} + \tau < 0, \quad (4.12)$$

the monotonic distortion

$$l - s = \text{sgn } \theta \int_0^\theta \left(\frac{\alpha_3}{\alpha_1} \right)^{1/2} \left(\frac{1 + m \sin^2 \psi}{\bar{k}^2 - \sin^2 \psi} \right)^{1/2} d\psi, \quad |\theta| \leq \frac{\pi}{2}, \quad (4.13)$$

with

$$l = l_2(\bar{\theta}) \equiv \operatorname{sgn} \bar{\theta} \int_0^{\bar{\theta}} \left(\frac{\alpha_3}{\alpha_1} \right)^{1/2} \left(\frac{1 + m \sin^2 \psi}{\bar{k}^2 - \sin^2 \psi} \right)^{1/2} d\psi, \quad (4.14)$$

is a solution of (4.5) subject to (4.6) and (4.7). Introducing the further change of variable

$$\sin \lambda = \frac{\sin \psi}{\bar{k}}, \quad (4.15)$$

one obtains the relationship between the tube radius and the interfacial angle as

$$\log_e(R/\bar{r}) = l_2(\bar{\theta}) \equiv \operatorname{sgn} \lambda_1 \int_0^{\lambda_1} \left(\frac{\alpha_3}{\alpha_1} \right)^{1/2} \left(\frac{1 + m \bar{k}^2 \sin^2 \lambda}{1 - \bar{k}^2 \sin^2 \lambda} \right)^{1/2} d\lambda, \quad (4.16)$$

where

$$\sin \lambda_1 = \frac{\sin \bar{\theta}}{\bar{k}}, \quad |\lambda_1| \leq \frac{\pi}{2}. \quad (4.17)$$

We note that there may be more than one solution of the form (4.13), since the inverse relation to $l_2(\bar{\theta})$ giving $|\bar{\theta}|$ in terms of R is not generally single valued, for $|\bar{\theta}|$ in the interval zero to $\pi/2$. Using (4.16), one determines a critical value R_2^c of the tube radius as

$$R_2^c = \bar{r}_0 \exp \left[\left(\frac{\alpha_3}{\alpha_1} \right)^{1/2} \sin^{-1} \left\{ \frac{(-2w(1)\bar{r}_0 + \tau)^2}{\alpha_1 \alpha_3} + 1 \right\}^{-1/2} \right], \quad (4.18)$$

at which a smooth transition between the uniform radial pattern and a non-planar monotonic distortion is possible. If

$$l_2(0) < l_2(\bar{\theta}) + \log_e(\bar{r}/\bar{r}_0), \quad 0 < |\bar{\theta}| \leq \frac{\pi}{2}, \quad (4.19)$$

the radial configuration is the only solution of the form (4.1) for R less than R_2^c , but when R exceeds R_2^c , both the radial pattern and the distortion (4.13) are possible solutions. As before, it is possible that the threshold effect may be observed, even if $\bar{r}_0 \exp(l_2(0))$ is only a local minimum of the function $\bar{r} \exp(l_2(\bar{\theta}))$. Further if $\bar{r} \exp(l_2(\bar{\theta}))$ increases monotonically with $|\bar{\theta}|$ for all values of $|\bar{\theta}|$ less than $\pi/2$, only one value of $|\bar{\theta}|$ between zero and $\pi/2$ exists satisfying (4.16), and therefore only one solution of the form (4.13) is possible.

The total energy per unit length of cylinder, $\epsilon_2(\bar{\theta})$, associated with the distortion (4.13) is given by

$$\epsilon_2(\bar{\theta}) = W_0 \pi \bar{r}^2 + 2\pi \bar{r} \bar{w} + \pi \tau \sin^2 \bar{\theta} + \pi \alpha_1 \int_0^{|\lambda_1|} G(\lambda; m; \bar{k}^2) d\lambda, \quad (4.20)$$

where

$$G(\lambda; m; \bar{k}^2) \equiv (1 + \bar{k}^2 \cos 2\lambda) \left(\frac{\alpha_3}{\alpha_1} \right)^{1/2} \left(\frac{1 + m \bar{k}^2 \sin^2 \lambda}{1 - \bar{k}^2 \sin^2 \lambda} \right)^{1/2}, \quad (4.21)$$

and the total energy per unit length of cylinder associated with the radial configuration is given by (3.25) with α replaced by α_1 . Thus the distortion is the stable solution provided the stability inequality

$$\begin{aligned} 2 \left\{ \left(\frac{(\bar{f} \alpha_1 - \tau^2 \sin^2 \bar{\theta}) \cos^2 \bar{\theta}}{2 W_c \bar{f} - \bar{w}^2 \sin^2 2\bar{\theta}} \right)^{1/2} \bar{w} - \left(\frac{\alpha_1}{2 W_c} \right)^{1/2} w(1) \right\} \\ > W_0 \left\{ \frac{(\bar{f} \alpha_1 - \tau^2 \sin^2 \bar{\theta}) \cos^2 \bar{\theta}}{2 W_c \bar{f} - \bar{w}^2 \sin^2 2\bar{\theta}} - \frac{\alpha_1}{2 W_c} \right\} + \tau \sin^2 \bar{\theta} \\ + \alpha_1 \left\{ \frac{1}{2} \log_e \left[\frac{\alpha_1}{2 W_c} \frac{2 W_c \bar{f} - \bar{w} \sin^2 2\bar{\theta}}{(\bar{f} \alpha_1 - \tau^2 \sin^2 \bar{\theta}) \cos^2 \bar{\theta}} \right] \right. \\ \left. + \left(\frac{\alpha_1}{\alpha_3} \right)^{1/2} \int_0^{|\lambda_1|} \left(\frac{1 + m \bar{k}^2 \sin^2 \lambda}{1 - \bar{k}^2 \sin^2 \lambda} \right)^{1/2} \bar{k}^2 \cos 2\lambda d\lambda \right\} \end{aligned} \quad (4.22)$$

is satisfied. Since insufficient information is available to determine those values of $\bar{\theta}$ for which (4.22) obtains, we examine the situation in which W_0 and W_c are equal and $w(1)$ is strictly positive. It is found that the distortion (4.13) has the smaller energy for sufficiently small $|\bar{\theta}|$, provided

$$W_c \alpha_3 > 2 \bar{w}^2(1). \quad (4.23)$$

This suggests that a local non-planar distortion about the radial orientation pattern may occur. Further, it may be shown that

$$\lim_{|\bar{\theta}| \rightarrow \pi/2} \epsilon_2(\bar{\theta}) = \begin{cases} \pi \tau + \pi \alpha_1 \left\{ 1 + \frac{\sin h^{-1} m^{1/2}}{m^{1/2} (1+m)^{1/2}} \right\}, & m > 0, \\ \pi \tau + \pi \alpha_1 \left\{ 1 + \frac{\sin^{-1} (-m)^{1/2}}{(-m)^{1/2} (1+m)^{1/2}} \right\}, & m < 0, \end{cases} \quad (4.24)$$

which is in agreement with the energy associated with the non-singular solution discussed by Cladis and Kléman⁽⁵⁾ and Meyer.⁽⁵⁾ If on the other hand

$$-2 \bar{w} \bar{r} + \tau > 0, \quad (4.25)$$

a second type of distortion is possible. Here θ' vanishes at least once

in the nematic material, and for distortions to exist one must have θ in the interval $-\pi/2$ to $\pi/2$. In this event, a possible solution is

$$l-s = \begin{cases} \operatorname{sgn} \theta \int_0^\theta \left(\frac{\alpha_3}{\alpha_1}\right)^{1/2} \left(\frac{1+m\sin^2\psi}{\sin^2\theta_m - \sin^2\psi}\right)^{1/2} d\psi, & (\theta^2)' < 0, \\ \operatorname{sgn} \theta \left\{ \int_0^{\theta_m} \left(\frac{\alpha_3}{\alpha_1}\right)^{1/2} \left(\frac{1+m\sin^2\psi}{\sin^2\theta_m - \sin^2\psi}\right)^{1/2} d\psi \right. \\ \quad \left. - \int_{\theta_m}^\theta \left(\frac{\alpha_3}{\alpha_1}\right)^{1/2} \left(\frac{1+m\sin^2\psi}{\sin^2\theta_m - \sin^2\psi}\right)^{1/2} d\psi \right\}, & (\theta^2)' > 0, \end{cases} \quad (4.26)$$

where

$$\sin^2 \theta_m \equiv \left\{ \frac{(-2\bar{w}\bar{r} + \tau)^2 \cos^2 \bar{\theta}}{f_{\alpha_1}} + 1 \right\} \sin^2 \bar{\theta}, \quad (4.27)$$

and θ_m has the physical significance of being the value attained by θ at its extremum. With the change of variable

$$\sin \lambda = \frac{\sin \psi}{\sin \theta_m}, \quad (4.28)$$

one obtains the relationship between the tube radius and the interfacial angle as

$$l_3(\bar{\theta}) = \log_e (R/\bar{r}) = \left(\frac{\alpha_3}{\alpha_1}\right)^{1/2} \left\{ \int_0^{\pi/2} \left(\frac{1+m\sin^2\theta_m \sin^2\lambda}{1-\sin^2\theta_m \sin^2\lambda}\right)^{1/2} d\lambda \right. \\ \left. + \int_{\lambda_2}^{\pi/2} \left(\frac{1+m\sin^2\theta_m \sin^2\lambda}{1-\sin^2\theta_m \sin^2\lambda}\right)^{1/2} d\lambda \right\}, \quad (4.29)$$

where

$$\sin \lambda_2 \equiv \frac{\sin \bar{\theta}}{\sin \theta_m}, \quad 0 \leq \lambda_2 \leq \frac{\pi}{2}. \quad (4.30)$$

The critical value of the tube radius R_3^c is given by

$$R_3^c = \bar{r}_0 \exp \left\{ \left(\frac{\alpha_3}{\alpha_1}\right)^{1/2} \left[\pi - \sin^{-1} \left\{ \frac{(-2\bar{w}(1)\bar{r}_0 + \tau)^2}{\alpha_1 \alpha_3} + 1 \right\}^{-1/2} \right] \right\}, \quad (4.31)$$

and here also one can state conditions for this tube radius to be a critical value.

The total energy per unit length of the tube, $\epsilon_3(\bar{\theta})$, associated with the distortion (4.26) is given by

$$\epsilon_3(\bar{\theta}) = W_0 \pi \bar{r} \bar{w}^2 + 2\pi \bar{r} + \pi \tau \sin^2 \bar{\theta} + \pi \alpha_1 \\ \times \left\{ \int_0^{\pi/2} F(\lambda; m; \sin^2 \theta_m) d\lambda + \int_{\lambda_2}^{\pi/2} F(\lambda; m; \sin^2 \theta_m) d\lambda \right\}, \quad (4.32)$$

where the function $F(\lambda; m; \sin^2 \theta_m)$ is equivalent to the right hand side of (4.21) with \bar{k}^2 replaced by $\sin^2 \theta_m$.

Assuming that W_0 and W_c are equal and $w(1)$ is strictly positive, one may again show that the distortion is the stable solution for sufficiently small $|\bar{\theta}|$, provided (4.23) obtains. Also it may be shown that

$$\lim_{|\bar{\theta}| \rightarrow \pi/2} \epsilon_3(\bar{\theta}) = \lim_{|\bar{\theta}| \rightarrow \pi/2} \epsilon_2(\bar{\theta}). \quad (4.33)$$

In closing this section, we admit that solutions with $|\theta|$ greater than $\pi/2$ are again possible. Also, in the event that (4.25) holds, distortions with more than one extremum are possible. However such solutions are not investigated here.

5. Discussion

Here our remarks are necessarily confined to the case when the coefficients α_1 and α_3 are equal. We have seen that the uniform radial configuration is a possible solution of the field equations and applied boundary conditions, for any value of R greater than \bar{r}_0 . However, if R exceeds certain critical values a variety of distorted configurations are also available. Of all the solutions considered in this paper, is it possible to predict which one will occur in a given situation? We have demonstrated that local non-planar distortions about the radial configurations are stable, whereas local planar distortions appear to be unstable. Also, when the surface energy effect is dominant at the interface, so that a nearly parallel orientation obtains there, the energy associated with a non-planar distortion remains finite, while that associated with a planar distortion becomes very large. These observations lead us to conjecture that the non-planar solution may be the stable solution whenever it is available.

Taking the estimate for the order of magnitude of the core radius to be that given by Cladis and Kléman⁽⁵⁾ and Meyer,⁽⁶⁾ the non-planar distortion is always available for any practical tube radius. This is not necessarily the case for the planar distortion, especially if the quantity $W_c \alpha / 2 \dot{w}^2(1)$ is very much larger than one. Further, since the radius of the core seems to be so small compared to any tube

radius, Meyer⁽⁶⁾ suggests that the cylinder wall has little or no effect upon the orientation at the nematic liquid crystal-isotropic core interface. In this event, one anticipates a nearly parallel orientation at the interface, and the non-planar distortion is the stable solution with the core radius tending to zero as $|\theta|$ approaches $\pi/2$. It is of interest to observe that the non-singular solution proposed by Cladis and Kléman⁽⁵⁾ and Meyer⁽⁶⁾ is the limiting case of our non-planar distortion, and that the results presented here are in general agreement with those obtained by these authors concerning the occurrence of a non-planar distortion. In addition, it appears that these theoretical predictions are compatible with the experimental observations reported by Williams, Pieránski and Cladis.⁽¹⁶⁾ In the apparent absence of any other relevant experimental results, it is felt that further experimentation might serve two useful purposes. One is naturally to test the validity of the model employed in the continuum theory, in particular the concept of an isotropic core and the association of an anisotropic surface energy with a liquid crystal-isotropic core interface. If the model proves to be incompatible with experiment, it would seem that one should either modify the surface energy density (2.4) or, more drastically, dispense with the isotropic core. In this event, one hopes that experimentation would fulfil a second purpose in yielding useful information as to how the model might be improved. On the other hand, if the model is shown to be a good one, the results presented here should help in the analysis of experimental observations.

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