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Interfacial effects in the magnetohydrostatic theory of nematic liquid crystals

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Abstract. In this paper, we associate an anisotropic surface energy with a nematic liquid crystal-isotropic fluid interface. Employing continuum theory, two sets of simple experimental situations are examined, in which a solid boundary, a nematic liquid crystal-isotropic fluid interface, and an applied magnetic field act as competing influences upon the orientation of the molecules in the liquid crystal.

1. Introduction

The idea of associating an anisotropic surface energy with a nematic liquid crystalisotropic fluid interface was apparently first suggested by Oseen (1933). For the interested reader, a detailed discussion concerning its motivation is given elsewhere (Jenkins and Barratt 1973). Chandrasekhar (1966) and Dubois-Violette and Parodi (1969) include various anisotropic surface energy densities in their analyses of the equilibrium shape, and internal director configurations of small droplets of nematic liquid crystal suspended in an isotropic fluid. In a recent paper, Jenkins and Barratt (1973) employ a variational principle to obtain the equations representing balance of traction and couple at the interface.

In their paper, Jenkins and Barratt (1973) also investigate two simple experimental situations. In each, a solid boundary and an interface act as competing influences upon the molecular orientation in a layer of nematic liquid crystal, bounded below by a horizontal solid surface and above by an isotropic fluid. In this paper, we examine two sets of similar experimental situations which utilize a magnetic field as an additional orientating influence. In one, the director orientation at the solid boundary is parallel to the surface, and the magnetic field is applied either parallel to or normal to this boundary. In the other, a perpendicular director orientation obtains at the solid boundary. If these experiments are practical, the analysis indicates that both qualitative and quantitative information concerning the anisotropic surface energy, associated with a particular interface, could be obtained.

2. The continuum theory

This section contains a brief summary of the continuum theory proposed by Oseen (1929) and developed by Frank (1958), Ericksen (1962) and Leslie (1968) to describe the

static, isothermal behaviour of incompressible nematic liquid crystals. For convenience, we choose a set of right-handed cartesian axes, and employ cartesian tensor notation.

As is customary, one associates with the molecular axis a director **n** of fixed magnitude, normalized by

$$n_i n_i = 1, (2.1)$$

and assumes that n and -n are physically indistinguishable. The field equations to be satisfied throughout the liquid crystal are

$$-p\delta_{ik} - \frac{\partial W}{\partial n_{l,k}} n_{l,i} \Big|_{,k} + f_i = 0$$
(2.2)

and

$$\left(\frac{\partial W}{\partial n_{i,k}}\right)_{,k} - \frac{\partial W}{\partial n_i} + \phi_i = \lambda n_i, \qquad (2.3)$$

where f_i is the body force per unit volume, ϕ_i is the director body force per unit volume, and the scalar fields p and λ arise from the assumed incompressibility of the material and the constraint upon the magnitude of the director respectively. Also W is the Helmholtz free energy per unit volume, and depends only upon the director and its gradients. A possible form for the Helmholtz free energy, which we adopt, is that proposed by Frank (1958):

$$2W = \alpha_2 n_{i,j} n_{i,j} + \alpha_4 n_{i,j} n_{j,i} + (\alpha_1 - \alpha_2 - \alpha_4) n_{i,i} n_{j,j} + (\alpha_3 - \alpha_2) n_i n_j n_{k,i} n_{k,j}.$$
 (2.4)

Under isothermal conditions the coefficients α_1 , α_2 , α_3 and α_4 are constants, and, if W is to be a minimum when the director gradients vanish, Ericksen (1966) has shown that they are restricted by the inequalities

$$\alpha_1 \ge 0, \quad \alpha_2 \ge 0, \quad \alpha_3 \ge 0, \quad |\alpha_4| \le \alpha_2, \quad \alpha_2 + \alpha_4 \le 2\alpha_1.$$

$$(2.5)$$

In this paper, it is assumed that the external body forces arise from an applied magnetic field H and gravity. Consequently, accepting the estimates of Ericksen (1962), the body force and director body force are given by

$$f_i = -\chi_{,i} + \{(\nu_1 - \nu_2)H_j n_j n_k + \nu_2 H_k\} H_{k,i}$$
(2.6)

and

$$\phi_i = (v_1 - v_2) H_j n_j H_i, \tag{2.7}$$

where χ is the gravitational potential, and v_1 and v_2 are the constant magnetic susceptibilities parallel and perpendicular to the molecular axis respectively. In this event, one is able to show that the overdeterminate system of seven equations (2.1), (2.2) and (2.3) for the unknown fields p, λ and n may be replaced by the four equations (2.1) and (2.3), and the relation

$$p = p_0 - \chi - W - \Theta \tag{2.8}$$

which determines the pressure. In (2.8), p_0 is an arbitrary constant and

$$\Theta \equiv -\frac{1}{2} \{ (v_1 - v_2) (H_k n_k)^2 + v_2 H_k H_k \}$$
(2.9)

is the magnetic energy per unit volume, associated with an external magnetic field H. Henceforth, we assume that

$$v_1 > v_2 > 0,$$
 (2.10)

which insures Θ is a minimum when the director is parallel to the applied magnetic field.

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 v. Using invariance arguments, it follows that

$$w = w((v, n)^2).$$
(2.11)

Hence, ignoring the energy associated with the interface between the liquid crystal and a solid (Rapini and Papoular 1969), the total energy E of a sample of nematic liquid crystal is given by

$$E = \int_{v} (W + \Theta) \, \mathrm{d}v + \int_{\bar{s}} w \, \mathrm{d}s, \qquad (2.12)$$

where v is the volume of the sample and \bar{s} is that part of its bounding surface which is in contact with an isotropic fluid. The rest of the surface bounding the sample is assumed to be in contact with a solid.

In the next section, we seek solutions of the second-order nonlinear differential equations (2.3) subject to boundary conditions at both the solid surface and the isotropic fluid interface. For a sample of nematic liquid crystal, it is well known (Zocher and Coper 1928, Chatelain 1943) that solid boundaries may be treated to obtain a definite orientation of the molecular axis at the boundary. Hence it seems reasonable to assume that there is a fixed director orientation at a liquid crystal–solid boundary. At a liquid crystal–isotropic fluid interface, it is natural to require that force and torque be balanced, and to assume that the isotropic fluid exerts only a normal force upon the liquid crystal. For the simple geometry and director configurations treated here, Jenkins and Barratt (1973) have shown that the force condition is trivially satisfied, while the balance of torque requires that in general

$$\frac{\partial W}{\partial n_{i,k}} v_k + \frac{\partial w}{\partial n_i} = \beta n_i, \qquad (2.13)$$

where β is an arbitrary scalar. Although there is no certainty that it is the case (Saupe 1960, Rapini and Papoular 1969), we follow the common practice of assuming that the boundary conditions are unaffected by the presence of an applied magnetic field.

3. The solutions

Here, we consider how an external magnetic field influences the director configuration in thin layers of nematic liquid crystal, bounded below by a plane solid boundary and above by a plane liquid crystal-isotropic fluid interface. Initially, we prescribe a parallel director orientation at the solid boundary, and determine director configurations for orientations of the applied magnetic field parallel to and perpendicular to this boundary. Next, we examine situations where a perpendicular director orientation is assumed at the solid boundary. If practical, one could perform these experiments to establish the relative importance of the orienting effects of the boundary terms derived from the interfacial surface energy compared to those resulting from the presence of solid boundaries and an applied magnetic field.

3.1. Parallel director orientation at the solid boundary

It is convenient to choose a set of cartesian coordinates (x, y, z) so that the solid boundary

and interface occupy the planes z = 0 and z = l respectively, and such that the orientation at the solid boundary is parallel to the x axis. First, we examine the situation in which a uniform magnetic field is applied normally to the bounding planes and has components

$$H_x = 0, \qquad H_y = 0, \qquad H_z = H.$$
 (3.1)

It seems reasonable to consider director fields of the form

$$n_x = \cos \theta(z), \qquad n_y = 0, \qquad n_z = \sin \theta(z),$$
 (3.2)

and initially we assume that

$$-\pi < \theta < \pi. \tag{3.3}$$

Utilizing the free energy density (2.4), (2.7), (3.1) and (3.2) in the field equations (2.3), one may eliminate λ to obtain the equation for θ as

$$f(\theta)\theta'' + \frac{1}{2}(\theta')^2 \frac{\mathrm{d}f}{\mathrm{d}\theta} + \nu H^2 \sin\theta \cos\theta = 0, \qquad (3.4)$$

where

$$f(\theta) = \alpha_1 \cos^2 \theta + \alpha_3 \sin^2 \theta, \qquad v = v_1 - v_2 > 0, \qquad (3.5)$$

and a prime denotes a derivative taken with respect to z. It follows from (2.5) that the function $f(\theta)$ is non-negative, and throughout this paper it is assumed to be strictly positive. After some manipulation employing (2.4), (2.13) and (3.2), one obtains the interfacial boundary condition (see Jenkins and Barratt 1973) as

$$f\theta' + \overline{w}\sin 2\overline{\theta} = 0$$
 on $z = l,$ (3.6)

where, for the director field (3.2), a dot denotes differentiation with respect to $\sin^2\theta$, and overbars indicate quantities evaluated at the interface. Also, at the solid boundary, one has

$$\theta = 0 \qquad \text{on} \qquad z = 0. \tag{3.7}$$

It is obvious that the uniform parallel orientation is one possible solution of equation (3.4) subject to the boundary conditions (3.6) and (3.7). However, there are other possible solutions of the form (3.2). Using (3.6), (3.4) integrates once to yield

$$f(\theta)(\theta')^2 = vH^2 \left(\sin^2 \bar{\theta} + \frac{\bar{w}^2}{vH^2 \bar{f}} \sin^2 2\bar{\theta} - \sin^2 \theta \right).$$
(3.8)

Two basic types of distortion are possible, depending upon the sign of $\bar{\theta}'$ relative to that of $\bar{\theta}$.

The first type of distortion we consider occurs when the form of w is such that the interfacial condition (3.6) requires $\overline{\theta}'$ and $\overline{\theta}$ to have the same sign. In this event, it is necessary that $\overline{w} < 0$ when $0 < |\overline{\theta}| < \frac{1}{2}\pi$, and $\overline{w} > 0$ when $\frac{1}{2}\pi < |\overline{\theta}| < \pi$. In the former case the applied magnetic field and the surface couple act together, and in the latter they act in opposition. Thus provided

$$\vec{w}\sin 2|\vec{\theta}| < 0,\tag{3.9}$$

a possible solution of (3.8) subject to (3.6) and (3.7) is the monotone distortion

$$z = \operatorname{sgn} \theta(\nu H^2)^{-1/2} \int_0^\theta \left(\frac{f(\psi)}{\bar{k}^2 - \sin^2 \psi} \right)^{1/2} d\psi, \qquad (3.10)$$

where

$$\bar{k}^2 = \frac{\bar{w}^2}{vH^2} \sin^2 2\bar{\theta} + \sin^2 \bar{\theta}.$$
(3.11)

For $0 < |\bar{\theta}| < \frac{1}{2}\pi$ it is necessary that

$$\bar{k}^2 > \sin^2 \bar{\theta},\tag{3.12}$$

while for $\frac{1}{2}\pi < |\bar{\theta}| < \pi$ one requires

$$\bar{k}^2 > 1.$$
 (3.13)

In addition, the angle at the interface is related to the layer thickness by

$$l = l_1(\bar{\theta}) = \operatorname{sgn} \bar{\theta}(\nu H^2)^{-1/2} \int_0^{\bar{\theta}} \left(\frac{f(\psi)}{\bar{k}^2 - \sin^2 \psi} \right)^{1/2} \mathrm{d}\psi.$$
(3.14)

In either case, given l and H, the relation inverse to (3.14) determining a nonzero $|\bar{\theta}|$ in terms of l and H need not be single valued. Thus, depending upon the nature of w, many solutions of the form (3.2) may be possible. Of all such solutions and the homogeneous orientation, we call that solution which involves the least total energy the stable solution.

With the change of variable

$$\sin \lambda = \frac{\sin \psi}{\bar{k}},\tag{3.15}$$

we rewrite (3.14) as

$$l_1(\bar{\theta}) = \operatorname{sgn} \lambda_0 (\nu H^2)^{-1/2} \int_0^{\lambda_0} \frac{f^{1/2}(\psi)}{\cos \psi} d\lambda, \qquad (3.16)$$

where λ_0 is defined by

$$\sin \lambda_0 \equiv \frac{\sin \bar{\theta}}{\bar{k}}, \qquad -\frac{1}{2}\pi < \lambda_0 < \frac{1}{2}\pi.$$
(3.17)

From (3.11) one obtains

$$\sin^2 \lambda_0 = \left(\frac{4\bar{w}^2}{vH^2\bar{f}}\cos^2\bar{\theta} + 1\right)^{-1}.$$
(3.18)

Assuming that $\overline{w} < 0$ in a neighbourhood of $\overline{\theta} = 0$, we find the critical layer thickness l_1^c , at which a smooth transition from the homogeneous orientation to the monotone distortion is possible, to be given by

$$l_{1}^{c} \equiv \lim_{\bar{\theta} \to 0} l_{1}(\bar{\theta}) = \left(\frac{\alpha_{1}}{\nu H^{2}}\right)^{1/2} \tan^{-1} \left(-\frac{(\alpha_{1}\nu H^{2})^{1/2}}{2\dot{w}(0)}\right).$$
(3.19)

Here, as elsewhere in this paper, the inverse tangent is restricted to take values between 0 and $\frac{1}{2}\pi$.

In the event that $\overline{w} < 0$ everywhere in $0 < |\overline{\theta}| < \frac{1}{2}\pi$, the surface energy certainly has its least value at a director orientation perpendicular to the interface. If, in addition, the functional form of w is such that $l_1(\overline{\theta})$ is an increasing function of $|\overline{\theta}|$ in $0 < |\overline{\theta}| < \frac{1}{2}\pi$, there is only one value of $|\overline{\theta}|$ which satisfies (3.14), whenever l exceeds l_1^c . When $l < l_1^c$,

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the only possible solution of the form (3.2) is the uniform parallel orientation. Alternatively, if the behaviour of w is such that the function $H(\bar{\theta})$, defined implicitly by (3.16), is a monotonic increasing function of $|\bar{\theta}|$ for a fixed layer thickness *l*, then both the distortion and homogeneous orientation are possible solutions, whenever the magnetic field strength *H* exceeds a critical value H_c given by

$$\tan H_{\rm c} \left(\frac{v l^2}{\alpha_1}\right)^{1/2} = -\frac{(\alpha_1 v)^{1/2} H_{\rm c}}{2\dot{w}(0)}.$$
(3.20)

To discriminate between the various solutions, a stability analysis of the dynamic equations would be desirable. However such an analysis does not seem possible at the moment, and so we follow Dafermos (1968) in comparing the total energies associated with each solution. Intuitively, one anticipates that the solution involving the least total energy is the one more likely to occur, and therefore we refer to that solution as the stable solution. However, we admit the possibility that a solution of a form not considered here may have an even smaller total energy.

The total energy E of the sample of nematic liquid crystal is given by (2.12), and one obtains the energy difference per unit area $\Delta E(\bar{\theta})$ between the total energy $E(\bar{\theta})$ of a monotonic distortion and the total energy E(0) of the uniform configuration as

$$\Delta E(\bar{\theta}) = \frac{1}{2} \int_0^l \left\{ f(\theta)(\theta')^2 - vH^2 \sin^2\theta \right\} dz + w(\sin^2\bar{\theta}) - w(0).$$
(3.21)

Utilizing (3.10) in (3.21) yields

$$\Delta E(\bar{\theta}) = \frac{1}{2} \operatorname{sgn} \bar{\theta} (vH^2)^{1/2} \int_0^{\bar{\theta}} (\bar{k}^2 - 2\sin^2\psi) \left(\frac{f(\psi)}{\bar{k}^2 - \sin^2\psi}\right)^{1/2} d\psi + w(\sin^2\bar{\theta}) - w(0).$$
(3.22)

In appendix 1, we show that the right-hand side of (3.22) is strictly negative for those values of $\bar{\theta}$ for which the surface energy function satisfies the inequality

$$\frac{w(\sin^2\bar{\theta}) - w(0)}{\bar{w}\sin 2\bar{\theta}} > \frac{1}{2} \frac{E(\bar{\theta}|m)}{(1 + m\sin^2\bar{\theta})},$$
(3.23)

where

$$m \equiv \left(\frac{\alpha_3}{\alpha_1} - 1\right) > -1 \qquad \text{and} \qquad E(\bar{\theta}|m) \equiv \int_0^{\bar{\theta}} (1 + m\sin^2\psi)^{1/2} \,\mathrm{d}\psi. \tag{3.24}$$

This stability inequality arises in the nonmagnetic case discussed by Jenkins and Barratt (1973). For example, for a fixed magnetic field, if $l_1(\bar{\theta})$ increases monotonically and the surface energy decreases monotonically with $|\bar{\theta}|$ in the interval $|\bar{\theta}| \leq \frac{1}{2}\pi$, we anticipate that the distortion (3.10) commences as the layer thickness exceeds l_1^c , provided (3.23) obtains in a neighbourhood of $\bar{\theta} = 0$, and persists so long as (3.23) is satisfied. Alternatively, if the layer thickness is fixed, we expect the distortion (3.10) to commence as the magnetic field exceeds the critical value given by (3.20), provided $H(\bar{\theta})$ increases monotonically with $|\bar{\theta}|$. One notes that under the above conditions

$$\lim_{|\bar{\theta}| \to \pm \pi} l_1(\bar{\theta}) = \infty \qquad \text{and} \qquad \lim_{|\bar{\theta}| \to \pm \pi} H(\bar{\theta}) = \infty, \tag{3.25}$$

and fixed H and l respectively.

When $\bar{k}^2 > 1$, solutions of the form (3.2) with $|\bar{\theta}| > \pi$ are also possible. For each of these there exists a solution within the interval $-\pi$ to π giving the same value to the surface energy. For fixed *l*, the former solutions are associated with larger distortional

energies. In order to exclude these, it is necessary to show that the increase in distortional energy is not compensated for by a sufficiently large decrease in magnetic energy. This is easily shown in the event that $k^2 > 2$.

For those values of $\bar{\theta}$ where the form of w requires that, in order to satisfy (3.6), $\bar{\theta}$ and $\bar{\theta}'$ are of opposite sign, a second type of distortion is possible. Here θ' vanishes at least once in the layer, and for distortions to exist one must have $0 < |\bar{\theta}| < \frac{1}{2}\pi$. Hence it follows that

$$\overline{w}\sin 2|\overline{\theta}| > 0. \tag{3.26}$$

In this event, a possible solution is

$$z = \begin{cases} \operatorname{sgn} \theta(\nu H^{2})^{-1/2} \int_{0}^{\theta} \left(\frac{f(\psi)}{\sin^{2}\theta_{m} - \sin^{2}\psi} \right)^{1/2} d\psi, & (\theta^{2})' > 0, \\ \operatorname{sgn} \theta(\nu H^{2})^{-1/2} \left\{ \int_{0}^{\theta_{m}} \left(\frac{f(\psi)}{\sin^{2}\theta_{m} - \sin^{2}\psi} \right)^{1/2} d\psi - \int_{\theta_{m}}^{\theta} \left(\frac{f(\psi)}{\sin^{2}\theta_{m} - \sin^{2}\psi} \right)^{1/2} d\psi \right\}, \\ (\theta^{2})' < 0, \end{cases}$$
(3.27)

where

$$\sin^2\theta_m \equiv \frac{\bar{w}^2}{vH^2}\sin^22\bar{\theta} + \sin^2\bar{\theta}.$$
(3.28)

In the above θ_m has the physical significance of being the value attained by θ at its extremum. The relationship between the layer thickness and the angle at the interface is

$$l = l_2(\bar{\theta}) \equiv \operatorname{sgn}\bar{\theta}(vH^2)^{-1/2} \left\{ \int_0^{\theta_m} \left(\frac{f(\psi)}{\sin^2\theta_m - \sin^2\psi} \right)^{1/2} d\psi - \int_{\theta_m}^{\bar{\theta}} \left(\frac{f(\psi)}{\sin^2\theta_m - \sin^2\psi} \right)^{1/2} d\psi \right\}.$$
(3.29)

With the change of variable

$$\sin \lambda = \frac{\sin \psi}{\sin \theta_m} \tag{3.30}$$

in (3.29), one obtains

$$l = l_2(\bar{\theta}) \equiv (\nu H^2)^{-1/2} \left(\int_0^{\pi/2} \frac{f^{1/2}(\psi)}{\cos \psi} d\lambda + \int_{\lambda_1}^{\pi/2} \frac{f^{1/2}(\psi)}{\cos \psi} d\lambda \right),$$
(3.31)

where

$$\sin \lambda_1 \equiv \frac{\sin \bar{\theta}}{\sin \theta_m}; \qquad \text{so } 0 \leq \lambda_1 \leq \frac{1}{2}\pi.$$
(3.32)

Assuming that $\overline{w} > 0$ in a neighbourhood containing $\overline{\theta} = 0$, we obtain

$$l_{2}^{c} \equiv \lim_{\bar{\theta} \to 0} l_{2}(\bar{\theta}) = \left(\frac{\alpha_{1}}{\nu H^{2}}\right)^{1/2} \left\{ \pi - \tan^{-1} \left(\frac{(\alpha_{1}\nu H^{2})^{1/2}}{2\dot{w}(0)}\right) \right\},$$
(3.33)

or

$$\tan\left\{H_{\rm c}\left(\frac{vl^2}{\alpha_1}\right)^{1/2} - \pi\right\} = \frac{(\alpha_1 v)^{1/2} H_{\rm c}}{2\dot{w}(0)}.$$
(3.34)

The difference per unit area $\Delta E(\bar{\theta})$ in the total energies associated with the distortion (3.27) and the uniform parallel orientation is given by

$$\Delta E(\bar{\theta}) = \frac{1}{2} \operatorname{sgn} \bar{\theta} (\nu H^2)^{1/2} \left\{ \int_0^{\theta_m} (\sin^2 \theta_m - 2\sin^2 \psi) \left(\frac{f(\psi)}{\sin^2 \theta_m - \sin^2 \psi} \right)^{1/2} d\psi - \int_{\theta_m}^{\bar{\theta}} (\sin^2 \theta_m - 2\sin^2 \psi) \left(\frac{f(\psi)}{\sin^2 \theta_m - \sin^2 \psi} \right)^{1/2} d\psi \right\} + w(\sin^2 \bar{\theta}) - w(0).$$
(3.35)

In appendix 2, it is shown that, for those values of $\bar{\theta}$ for which the surface energy function satisfies the inequality

$$w(\sin^2\bar{\theta}) - w(0) \leqslant \frac{\bar{w}\sin 2\bar{\theta}E(\bar{\theta}|-1)}{2\cos\bar{\theta}} = \bar{w}\sin^2\bar{\theta}, \qquad (3.36)$$

the right-hand side of (3.35) is strictly negative. In a similar fashion, one may show that distortions containing more than one extremum are associated with larger energies than the corresponding solution (3.27) having only a single turning point. Consequently, if $\overline{w} > 0$ in $|\overline{\theta}| \leq \frac{1}{2}\pi$ and (3.36) obtains in a neighbourhood of $\overline{\theta} = 0$, we anticipate that the distortion commences as the appropriate critical value is exceeded, provided that the corresponding monotonicity condition is satisfied.

In the above analysis, it has been assumed that \overline{w} is nonzero. However, the analysis may be suitably modified for the case when \overline{w} is zero, where the problem is essentially that considered by Dafermos (1968) and Leslie (1970). One observes that, if $\overline{\theta}$ tends to values where $\overline{w} = 0$, the distortions (3.10) and (3.27) smoothly approach the monotone solution found by these authors. Thus there exists the possibility of a smooth transition between the two distinct types of director configurations.

In closing this subsection, we consider the situation in which the applied magnetic field is parallel to the bounding planes and has components

$$H_x = H, \qquad H_y = 0, \qquad H_z = 0.$$
 (3.37)

For the director field (3.2), one obtains the differential equation governing θ as

$$f(\theta)\theta'' + \frac{1}{2}(\theta')^2 \frac{\mathrm{d}f}{\mathrm{d}\theta} - vH^2 \sin\theta \cos\theta = 0, \qquad (3.38)$$

and we assume that the boundary conditions (3.6) and (3.7) still apply. It is obvious that the uniform parallel orientation is a possible solution of (3.38) subject to (3.6) and (3.7). Also, it follows from (3.6) that a monotonic distortion is a possible solution of (3.38) subject to (3.6) and (3.7), provided that (3.9) is satisfied.

Using (3.6), one may integrate (3.38) to obtain

$$f(\theta)(\theta')^2 = \nu H^2(\bar{h} + \sin^2\theta), \qquad (3.39)$$

where

$$\bar{h} = h(\bar{\theta}) \equiv \frac{\bar{w}^2}{\nu H^2 \bar{f}} \sin^2 2\bar{\theta} - \sin^2 \bar{\theta}.$$
(3.40)

For a nontrivial solution of (3.38), (3.39) requires that

$$h(\bar{\theta}) > 0 \tag{3.41}$$

or, equivalently,

$$0 \leqslant \nu H^2 < \frac{4\bar{w}^2}{\bar{f}} \cos^2\bar{\theta}. \tag{3.42}$$

Integrating (3.39), one obtains the monotonic distortion

$$z = \operatorname{sgn} \theta(vH^2)^{-1/2} \int_0^{\theta} \left(\frac{f(\psi)}{\bar{h} + \sin^2 \psi} \right)^{1/2} d\psi.$$
(3.43)

Thus the relationship between the layer thickness and the angle at the interface is

$$l = l_3(\bar{\theta}) \equiv \operatorname{sgn} \bar{\theta}(\nu H^2)^{-1/2} \int_0^{\bar{\theta}} \left(\frac{f(\psi)}{\bar{h} + \sin^2\psi}\right)^{1/2} d\psi.$$
(3.44)

With the change of variable

$$\sinh \lambda = \frac{\sin \psi}{h^{1/2}},\tag{3.45}$$

(3.44) becomes

$$l_{3}(\bar{\theta}) = \operatorname{sgn} \lambda_{2} \left(\frac{\alpha_{1}}{\nu H^{2}} \right)^{1/2} \int_{0}^{\lambda_{2}} \left(\frac{1 + m\bar{h} \sinh^{2}\lambda}{1 - \bar{h} \sinh^{2}\lambda} \right)^{1/2} d\lambda, \qquad (3.46)$$

where $\hat{\lambda}_2$ is defined by

$$\sinh \lambda_2 \equiv \frac{\sin \bar{\theta}}{\bar{h}^{1/2}}.$$
(3.47)

Provided $\overline{w} < 0$ in a neighbourhood of $\overline{\theta} = 0$, the critical layer thickness and the critical magnetic field strength are given by

$$l_{3}^{c} \equiv \lim_{\bar{\theta} \to 0} l_{3}(\bar{\theta}) = \left(\frac{\alpha_{1}}{\nu H^{2}}\right)^{1/2} \sinh^{-1} \left(\frac{4\dot{w}^{2}(0)}{\alpha_{1}\nu H^{2}} - 1\right)^{-1/2}$$
(3.48)

and

$$\left(\frac{\nu l^2}{\alpha_1}\right)^{1/2} H_{\rm c} = \sinh^{-1} \left(\frac{4\dot{w}^2(0)}{\alpha_1 \nu H_{\rm c}^2} - 1\right)^{-1/2} \tag{3.49}$$

respectively. So, for example, with appropriate monotonicity conditions on \overline{w} and $l(\overline{\theta})$ or $H(\overline{\theta})$, both the homogeneous parallel orientation and the monotonic distortion (3.43) are possible solutions of the differential equation (3.38) subject to the boundary conditions (3.6) and (3.7), provided that either

$$l > l_3^c$$
 (3.50)

for fixed H or

$$vH^2 < vH_c^2 < \frac{4\overline{w}^2}{\overline{f}}\cos^2\overline{\theta}, \qquad |\overline{\theta}| \leq \frac{1}{2}\pi, \qquad (3.51)$$

for fixed l, l being given by (3.44).

The energy difference per unit area between the total energies of the monotonic distortion and the uniform orientation is given by

$$\Delta E(\bar{\theta}) = \frac{1}{2} \operatorname{sgn} \bar{\theta} (vH^2)^{-1/2} \int_0^{\bar{\theta}} (\bar{h} + 2\sin^2\psi) \left(\frac{f(\psi)}{\bar{h} + \sin^2\psi} \right)^{1/2} d\psi + w(\sin^2\bar{\theta}) - w(0).$$
(3.52)

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For energy functions which satisfy the inequalities (3.23) and (3.42), the energy of the homogeneous configuration always exceeds that of the distortion (see appendix 3). Hence, if these inequalities apply in a neighbourhood of $\bar{\theta} = 0$ and, in addition, the appropriate inequality and monotonicity condition obtain, we expect the distortion to appear as the layer thickness increases beyond its critical value for fixed H, or as the magnetic field decreases below its critical value for fixed l.

3.2. Perpendicular director orientation at the solid boundary

We now examine, very briefly, situations where the solid surface has been treated so that the director orientation there is normal to the boundary. Since the possibilities that are of interest are essentially the same as those examined in § 3.1, only the basic equations and the various critical values are given here. For either orientation of the magnetic field, it seems reasonable to consider director fields of the form

$$n_x = \sin \phi(z), \qquad n_y = 0, \qquad n_z = \cos \phi(z),$$
 (3.53)

with

$$\phi(0) = 0, \tag{3.54}$$

and we assume

$$-\pi < \phi < \pi. \tag{3.55}$$

We note that other solutions of the form (3.53), not subject to the restriction (3.55), do exist but are not investigated here. After manipulation involving (2.4), (2.13) and (3.53), the condition for balance of couple at the interface (see Jenkins and Barratt 1973) becomes

$$\overline{g}(\phi)\phi' - \overline{w}\sin 2\phi = 0 \qquad \text{on } z = l, \tag{3.56}$$

where

$$g(\phi) \equiv \alpha_3 \cos^2 \phi + \alpha_1 \sin^2 \phi \tag{3.57}$$

and, because with the director field (3.53) the surface energy is a function of $\cos^2 \overline{\phi}$, a dot denotes differentiation with respect to this argument.

If the magnetic field is parallel to the bounding surfaces and has component form (3.37), the equation governing the angle ϕ is

$$g(\phi)\phi'' + \frac{1}{2}(\phi')^2 \frac{dg}{d\phi} + \nu H^2 \sin \phi \cos \phi = 0.$$
 (3.58)

The uniform perpendicular orientation is an obvious solution of (3.58) subject to (3.54) and (3.56). Whenever $\overline{w} > 0$ in a neighbourhood of $\overline{\phi} = 0$, a smooth transition to a monotone distortion is possible at a value of the layer thickness l_4^c or field strength H_c given by

$$I_{4}^{c} = \left(\frac{\alpha_{3}}{\nu H^{2}}\right)^{1/2} \tan^{-1}\left(\frac{(\alpha_{3}\nu H^{2})^{1/2}}{2\dot{w}(1)}\right)$$
(3.59)

$$\left(\frac{vl^2}{\alpha_3}\right)^{1/2} H_c = \tan^{-1}\left(\frac{(\alpha_3 v)^{1/2} H_c}{2\dot{w}(1)}\right)$$
(3.60)

respectively. One may show that the distortion is stable, when it exists, provided that

$$\frac{w(1) - w(\cos^2\bar{\phi})}{\bar{w}\sin 2\bar{\phi}} > \frac{1}{2} \frac{E(\bar{\phi}|n)}{(1 + n\sin^2\bar{\phi})^{1/2}},$$
(3.61)

where

$$n \equiv \left(\frac{\alpha_1}{\alpha_3} - 1\right), \qquad -1 < n < \infty.$$
(3.62)

If on the other hand $\overline{w} < 0$ in a neighbourhood of $\overline{\phi} = 0$, a smooth transition to a distortion similar to (3.27) is possible at a layer thickness l_5^c or a field strength H_c , where

$$l_{5}^{c} = \left(\frac{\alpha_{3}}{\nu H^{2}}\right)^{1/2} \left\{ \pi - \tan^{-1} \left(-\frac{(\alpha_{3}\nu H^{2})^{1/2}}{2\dot{w}(1)}\right) \right\}$$
(3.63)

and

$$\left(\frac{\nu l^2}{\alpha_3}\right)^{1/2} H_{\rm c} = \pi - \tan^{-1} \left(-\frac{(\alpha_3 \nu)^{1/2} H_{\rm c}}{2\dot{w}(1)} \right). \tag{3.64}$$

It may be shown that the distortion is stable, when it exists, for those values of $\overline{\phi}$ for which

$$w(1) - w(\cos^2 \overline{\phi}) \ge \frac{\overline{w} \sin 2\overline{\phi} E(\overline{\phi}| - 1)}{2 \cos \overline{\phi}} = \overline{w} \sin^2 \overline{\phi}.$$
(3.65)

If the applied magnetic field is normal to the bounding planes and has component form (3.1), the equation for ϕ is

$$g(\phi)\phi'' + \frac{1}{2}(\phi')^2 \frac{dg}{d\phi} - vH^2 \sin\phi \cos\phi = 0.$$
 (3.66)

One observes immediately that the uniform perpendicular orientation is a possible solution of (3.66) subject to (3.54) and (3.56). A smooth transition to a monotone distortion is again possible at a layer thickness l_6^c or field strength H_c given by

$$l_{6}^{c} = \left(\frac{\alpha_{3}}{\nu H^{2}}\right)^{1/2} \sinh^{-1} \left(\frac{4\dot{w}^{2}(1)}{\alpha_{3}\nu H^{2}} - 1\right)^{-1/2}$$
(3.67)

and

$$\left(\frac{\nu l^2}{\alpha_3}\right)^{1/2} H_{\rm c} = \sinh^{-1} \left(\frac{4\dot{w}^2(1)}{\alpha_3 \nu H_{\rm c}^2} - 1\right)^{-1/2}, \qquad 0 < \nu H_{\rm c}^2 < \frac{4\overline{w}^2}{\overline{g}} \cos^2 \overline{\phi}, (3.68)$$

respectively, provided $\overline{w} < 0$ in an interval about $\overline{\phi} = 0$. The monotone distortion is stable, when it exists, whenever the inequality (3.65) obtains.

From the above analysis, it is clear that observations of director configurations in such a simple geometry can provide information about the form of the surface energy function for a given material. The existence of smooth transitions between either homogeneous orientation and a distorted configuration determines the sign and relative magnitude of the derivative of the surface energy at orientations parallel to or perpendicular to the interface. Further, the persistence of a distortion provides qualitative information about this derivative away from the parallel or perpendicular orientations, and the expression relating the layer thickness and the interfacial angle helps to characterize the surface energy function.

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Appendix 1

We show that if

$$\overline{\psi}\sin 2|\overline{\theta}| < 0 \tag{A.1}$$

and

$$w\left(\sin^2\bar{\theta}\right) - w(0) < \frac{\bar{w}\sin 2\bar{\theta}E(\bar{\theta}|m)}{2(1+m\sin^2\bar{\theta})^{1/2}},\tag{A.2}$$

then the energy difference (3.22) is always negative.

From (3.6) and (3.8), one obtains

$$\overline{w}\sin 2\overline{\theta} = -\operatorname{sgn}\overline{\theta}(\alpha_1 v H^2)^{1/2} (1 + m \sin^2\overline{\theta})^{1/2} (\overline{k}^2 - \sin^2\overline{\theta})^{1/2}.$$
(A.3)

Upon using (A.2) with (A.3) in (3.22), the energy difference is found to satisfy the inequality

$$\Delta E(\bar{\theta}) < \frac{1}{2} \operatorname{sgn} \bar{\theta} (\alpha_1 \nu H^2)^{1/2} \int_0^{\bar{\theta}} (1 + m \sin^2 \psi)^{1/2} \left(\frac{\bar{k}^2 - 2 \sin^2 \psi}{(\bar{k}^2 - \sin^2 \psi)^{1/2}} - (\bar{k}^2 - \sin^2 \bar{\theta})^{1/2} \right) d\psi.$$
(A.4)

With the change of variable (3.15), (A.4) becomes

$$\Delta E < \frac{1}{2} \operatorname{sgn} \lambda_0 (\alpha_1 \nu H^2)^{1/2} \bar{k}^2 \int_0^{\lambda_0} F(\lambda; \bar{k}, m) (\cos 2\lambda - \cos \lambda_0 \cos \lambda) \, \mathrm{d}\lambda, \tag{A.5}$$

where

$$F(\lambda; \bar{k}, m) \equiv \left(\frac{1 + m\bar{k}^2 \sin^2 \lambda}{1 - \bar{k}^2 \sin^2 \lambda}\right)^{1/2}.$$
 (A.6)

For sake of brevity, we restrict λ_0 so that

$$0 \le \lambda \le \lambda_0 \le \frac{1}{2}\pi. \tag{A.7}$$

Integrating the right-hand side of (A.5) by parts, one obtains

$$\Delta E < \frac{1}{2} (\alpha_1 \nu H^2)^{1/2} \bar{k}^2 \int_0^{\lambda_0} \sin \lambda (\cos \lambda_0 - \cos \lambda) \frac{\partial F}{\partial \lambda} d\lambda.$$
 (A.8)

Now

$$\sin\lambda(\cos\lambda_0 - \cos\lambda) \leqslant 0, \tag{A.9}$$

and

$$\frac{\partial F}{\partial \lambda} = \frac{1+m}{2} \frac{\bar{k}^2 \sin 2\lambda}{(1-\bar{k}^2 \sin^2 \lambda)^{3/2} (1+m\bar{k}^2 \sin^2 \lambda)^{1/2}} \ge 0$$
(A.10)

whenever m > -1. Hence the right-hand side of (A.8) is always negative. For

$$-\frac{1}{2}\pi \leqslant \lambda_0 \leqslant \lambda \leqslant 0, \tag{A.11}$$

one may repeat the argument with trivial modifications to reach the same conclusion.

Appendix 2

In the event that

$$\overline{w}\sin 2|\overline{\theta}| > 0 \tag{A.12}$$

and

$$w(\sin^2\bar{\theta}) - w(0) \leqslant \frac{\bar{w}\sin 2\bar{\theta}E(\bar{\theta}|-1)}{2\cos\bar{\theta}} = \bar{w}\sin^2\bar{\theta},\tag{A.13}$$

it is possible to prove that the energy difference (3.35) is always less than zero.

In this case it follows from (3.6) and (3.8) that

$$\bar{w}\sin 2\bar{\theta} = \operatorname{sgn}\bar{\theta}(\alpha_1 v H^2)^{1/2} (1 + m \sin^2\bar{\theta})^{1/2} (\sin^2\theta_m - \sin^2\bar{\theta})^{1/2}.$$
(A.14)

Utilizing (A.13) in (3.35) and (A.14) in the resulting expression one finds, after making the change of variable (3.30), that

$$\Delta E \leqslant \frac{1}{2} (\alpha_1 \nu H^2)^{1/2} \sin^2 \theta_m \left(\int_0^{\pi/2} F(\lambda; \sin^2 \theta_m, m) \cos 2\lambda \, d\lambda + \int_{\lambda_1}^{\pi/2} F(\lambda; \sin^2 \theta_m, m) \cos 2\lambda \, d\lambda + \frac{1}{2} F(\lambda_1; \sin^2 \theta_m, m) \sin 2\lambda_1 \right),$$
(A.15)

where the function F is defined by (A.6). After integrating the second integral in (A.15) by parts, one may rewrite (A.15) as

$$\Delta E \leqslant \frac{1}{2} (\alpha_1 \nu H^2)^{1/2} \sin^2 \theta_m \left(\int_0^{\pi/2} F \cos 2\lambda \, d\lambda - \frac{1}{2} \int_{\lambda_1}^{\pi/2} \frac{\partial F}{\partial \lambda} \sin 2\lambda \, d\lambda \right).$$
(A.16)

It follows from (A.6) and (A.10) that

$$F > 0$$
 and $\frac{\partial F}{\partial \lambda} \ge 0$, (A.17)

provided m > -1. Hence the right-hand side of (A.16) is always less than zero.

Appendix 3

Finally we show, here, that if

$$\overline{w}\sin 2|\overline{\theta}| < 0 \tag{A.18}$$

and

$$w(\sin^2\bar{\theta}) - w(0) \leqslant \frac{\bar{w}\sin 2\bar{\theta}E(\bar{\theta}|-1)}{2\cos\bar{\theta}} = \bar{w}\sin^2\bar{\theta},\tag{A.19}$$

then the energy difference (3.52) is always negative.

Here it follows from (3.6) and (3.39) that

$$\bar{w}\sin 2\bar{\theta} = -\operatorname{sgn}\bar{\theta}(\alpha_1 v H^2)^{1/2} (1 + m \sin^2\bar{\theta})^{1/2} (\bar{h} + \sin^2\bar{\theta})^{1/2}.$$
(A.20)

Utilizing (A.19) in (3.52) and (A.20) in the resulting expression, one obtains, with the change of variable (3.45), the energy difference as

$$\Delta E \leq \frac{1}{2} \operatorname{sgn} \lambda_2 (\alpha_1 \nu H^2)^{1/2} \bar{h} \left(\int_0^{\lambda_2} F(\lambda; \bar{h}, m) \cosh 2\lambda \, d\lambda - F(\lambda_2; \bar{h}, m) \sinh \lambda_2 \cosh \lambda_2 \right), \text{ (A.21)}$$

where the function F is given by (A.6).

For

$$0 \leqslant \lambda \leqslant \lambda_2 \leqslant \frac{1}{2}\pi,\tag{A.22}$$

integration by parts in (A.21) gives the inequality

$$\Delta E < -\frac{1}{2} (\alpha_1 \nu H^2)^{1/2} \hbar \int_0^{\lambda_2} \frac{\partial F}{\partial \lambda} \sinh 2\lambda \, d\lambda.$$
 (A.23)

Thus the inequalities (3.41) and (A.10) insure that the right-hand side of (A.23) is always negative. If

$$-\frac{1}{2}\pi \leqslant \lambda_2 \leqslant \lambda \leqslant 0, \tag{A.24}$$

one may use a similar argument to obtain the same result.

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