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Application of Continuum Smectic C Theory to Alignment Inversion Walls

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In this article we derive solutions to continuum equations for smectic C liquid crystals which exhibit alignment inversion walls under the application of an externally applied magnetic field. Plots of solutions obtained numerically are presented and the behaviour of the resulting inversion walls is discussed.

1. INTRODUCTION

The influence of an externally applied magnetic field on the average orientation of the long molecular axes in nematic liquid crystals has been theoretically studied by Helfrich.¹ This response is due to the anisotropy of the molecular diamagnetic susceptibility and gives the molecules a preferred alignment direction with respect to the applied field. Helfrich starts with the assumption that there is a reversal through 180° in the orientation of the long molecular axes in a plane between two uniform regions aligned parallel to the applied field. This reversal in alignment takes place gradually within a thin layer between the uniformly orientated regions, and Helfrich has termed this layer an alignment inversion wall. As was pointed out by Helfrich, these inversion walls resemble Bloch walls separating adjacent domains in ordered magnetic materials such as ferromagnets. In this paper we present an application of the non-chiral smectic C continuum theory recently introduced by Leslie *et al.*² to the case of alignment inversion walls.

The smectic liquid crystal phase is anisotropic and has a layered structure de-

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scribed by a density wave vector normal to the layers. It is common to introduce the director \mathbf{n} (de Gennes,³ Chapter 7) in smectic theory; however, in this work we follow Leslie *et al.*² and use the vectors \mathbf{a} and \mathbf{b} where \mathbf{a} is a unit vector normal to the layers and \mathbf{b} is a unit vector perpendicular to \mathbf{a} . In some applications the vector \mathbf{b} is related to the direction of the spontaneous polarisation. In Figure 1 we show our coordinate system for a constant layer thickness non-chiral smectic C. Also shown is the vector \mathbf{a} and the direction of the applied field. We wish to study the effects of the magnetic field on the vector \mathbf{b} by imposing a change in orientation through 180° in \mathbf{b} between $z = \pm \infty$. As with nematics, we find it useful to introduce the concept of an alignment inversion wall, or domain wall. We shall obtain equations which describe the behaviour of such domain walls. These equations in general have to be solved numerically.

The remainder of this paper is as follows: in section 2 we briefly describe the continuum theory for non-chiral smectic C liquid crystals as introduced by Leslie *et al.*² The bulk free energy and associated Euler-Lagrange equations are given. In section 3, these equations are solved for \mathbf{a} , \mathbf{b} and all associated Lagrange multipliers by means of a suitable substitution which enables the equations to be reduced to a single second order ordinary differential equation. Various solutions are derived for relative values of elastic constants and the energies related to these solutions are given. Further, we examine domain walls which arise from our boundary conditions. A solution for a domain wall is solved numerically and we provide an analytic solution in a special case when all elastic moduli are set equal. A "bounding" explicit analytic solution is also derived which places bounding criteria on the actual solution. Finally, in this section, we give plots related to the behaviour of the domain walls. In section 4 we give a brief discussion of the results presented in this work.

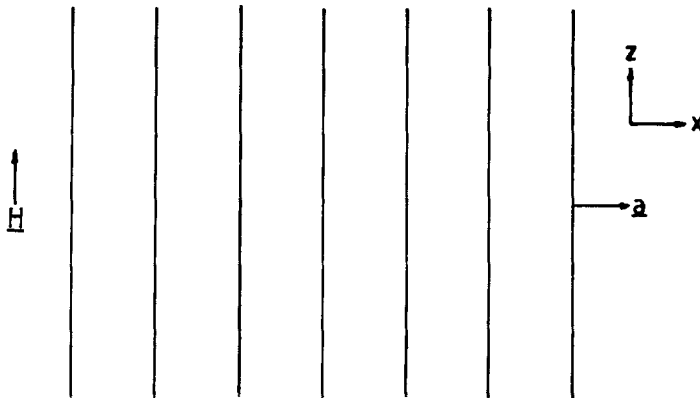


FIGURE 1 Coordinate system for constant layer thickness non-chiral smectic C. The magnetic field \mathbf{H} is applied along the layers and \mathbf{a} is the unit layer normal. The direction of \mathbf{b} is always in the plane of the layers.

2. NON-CHIRAL SMECTIC C THEORY

Following Leslie *et al.*,² we introduce the unit layer normal \mathbf{a} and a unit vector \mathbf{b} which is perpendicular to \mathbf{a} and thus

$$\mathbf{a} \cdot \mathbf{a} = \mathbf{b} \cdot \mathbf{b} = 1 \quad \mathbf{a} \cdot \mathbf{b} = 0. \quad (2.1)$$

Further, we suppose \mathbf{b} is axial and, as we do not consider disclinations, we require

$$\nabla \times \mathbf{a} = 0. \quad (2.2)$$

The bulk energy integrand W satisfies

$$W = W(-\mathbf{a}, \mathbf{b}, -\nabla \mathbf{a}, \nabla \mathbf{b}) = W(\mathbf{a}, \mathbf{b}, \nabla \mathbf{a}, \nabla \mathbf{b}) \quad (2.3)$$

and because chiral terms in W are not introduced, we assume W is even in alternators. The resulting energy integrand is found to be

$$\begin{aligned} 2W = & A_1 (\nabla \cdot \mathbf{a})^2 + A_2 (\mathbf{c} \cdot \nabla \times \mathbf{b})^2 + 2A_{12} (\nabla \cdot \mathbf{a}) (\mathbf{c} \cdot \nabla \times \mathbf{b}) \\ & + B_1 (\nabla \cdot \mathbf{b})^2 + B_2 (\mathbf{a} \cdot \nabla \times \mathbf{b})^2 + B_3 (\mathbf{b} \cdot \nabla \times \mathbf{b})^2 + 2B_{13} (\nabla \cdot \mathbf{b}) (\mathbf{b} \cdot \nabla \times \mathbf{b}) \\ & + 2C_1 (\nabla \cdot \mathbf{a}) (\mathbf{a} \cdot \nabla \times \mathbf{b}) + 2C_2 (\mathbf{c} \cdot \nabla \times \mathbf{b}) (\mathbf{a} \cdot \nabla \times \mathbf{b}) \end{aligned} \quad (2.4)$$

where $\mathbf{c} = \mathbf{a} \times \mathbf{b}$. Ignoring surface terms, and using various vector identities, (2.4) can be rewritten in cartesian component form as (see Leslie *et al.*)²

$$\begin{aligned} 2W = & K_1 (b_{i,i})^2 + K_2 b_{i,j} b_{i,j} + K_3 b_{i,j} b_j b_{i,k} b_k + K_4 (a_{i,i})^2 \\ & + K_5 (b_i a_{i,j} b_j)^2 + 2K_6 b_i a_{j,i} b_k a_{j,k} + 2K_7 b_{i,i} b_p e_{pjk} b_{k,j} \\ & + 2K_8 a_{i,i} a_p e_{pjk} b_{k,j} + 2K_9 b_i a_{i,j} b_j a_k e_{kpq} b_{q,p} \end{aligned} \quad (2.5)$$

where, for example, $a_{i,j}$ denotes partial differentiation with respect to j of the i th component of \mathbf{a} . e represents the usual alternator and repeated indices follow the Einstein summation convention and are summed from 1 to 3. Also, we have the relationships (in the bulk)

$$\begin{aligned} K_1 &= B_1 - B_3 & K_4 &= A_1 & K_7 &= B_{13} \\ K_2 &= B_3 & K_5 &= A_2 - B_2 & K_8 &= C_1 \\ K_3 &= B_2 - B_3 & K_6 &= A_{12} & K_9 &= C_2. \end{aligned} \quad (2.6)$$

The associated Euler-Lagrange equations are found to be

$$\left(\frac{\partial W}{\partial (a_{i,j})} \right)_{,j} - \frac{\partial W}{\partial a_i} + \gamma a_i + K b_i + e_{ijk} \beta_{k,j} + G_i = 0 \quad (2.7)$$

$$\left(\frac{\partial W}{\partial (b_{i,j})} \right)_{,j} - \frac{\partial W}{\partial b_i} + K a_i + \tau b_i + L_i = 0 \quad (2.8)$$

for $i = 1$ to 3 where γ , K , τ , β are Lagrange multipliers arising from the four constraints (2.1) and (2.2) and \mathbf{G} , \mathbf{L} are the general body forces associated with \mathbf{a} and \mathbf{b} respectively. From (2.5) we can write (2.7) and (2.8) as, respectively, for $i = 1, 2, 3$

$$\begin{aligned} & K_4 a_{k,ki} + K_5 (b_p a_{p,k} b_k b_i b_j)_{,j} + 2K_6 (b_j b_k a_{i,k})_{,j} + K_8 (a_p e_{pjk} b_{k,j})_{,i} \\ & + K_9 (b_i b_j a_k e_{kpq} b_{q,p})_{,j} - K_8 a_{p,p} e_{ijk} b_{k,j} - K_9 b_p a_{p,q} b_q e_{ijk} b_{k,j} \\ & + \gamma a_i + K b_i + e_{ijk} \beta_{k,j} + G_i = 0 \end{aligned} \quad (2.9)$$

and

$$\begin{aligned} & K_1 b_{k,ki} + K_2 b_{i,kk} + K_3 (b_{i,k} b_k b_j)_{,i} - K_3 b_{k,j} b_j b_{k,i} - 2K_5 b_p a_{p,q} b_q a_{i,j} b_j \\ & - 2K_6 a_{k,i} b_j a_{k,j} + K_7 (b_p e_{pjk} b_{k,j})_{,i} + K_7 (b_{p,p} b_k)_{,i} e_{kji} \\ & - K_7 b_{p,p} e_{ijk} b_{k,j} + K_8 a_{k,kj} a_p e_{pji} + K_9 a_k e_{kji} (b_p a_{p,q} b_q)_{,j} \\ & - 2K_9 a_k e_{kpq} b_{q,p} a_{i,j} b_j + K a_i + \tau b_i + L_i = 0. \end{aligned} \quad (2.10)$$

Further information and details of the above theory can be found in Leslie *et al.*²

3. DESCRIPTION OF THE PROBLEM AND SOLUTIONS

We consider the following problem as shown in Figure 1 above. Set

$$\mathbf{a} = (1, 0, 0) \quad \mathbf{b} = (0, b_2(z), b_3(z)) \quad \mathbf{H} = (0, 0, H). \quad (3.1)$$

From uniaxial considerations (see Appendix) we seek solutions to (2.9) and (2.10) when

$$\mathbf{G} = (0, 0, \Delta \chi^a b_2 H^2) \quad \text{and} \quad \mathbf{L} = (0, -\Delta \chi^b b_2 b_3^2 H^2, \Delta \chi^b b_2^2 b_3 H^2) \quad (3.2)$$

where $\Delta \chi^a = \Delta \chi^n S_1$ and $\Delta \chi^b = -\Delta \chi^n S_2$, $\Delta \chi^n$ being the usual magnetic anisotropic susceptibility associated with uniaxial liquid crystals and S_1 and S_2 are suitable

positive scaling constants. To simplify notation we now denote $\Delta\chi^b$ by $\Delta\chi$ and assume this quantity to be positive (that is, $\Delta\chi^n$ is negative). (Possible solutions for $\Delta\chi$ negative will be discussed in a future paper). Substituting (3.1) and (3.2) into (2.9) and (2.10) shows that we have to solve for $i = 1, 2, 3$

$$-K_8 b_{2,3i} - K_9 (b_i b_3 b_{2,3})_{,3} + \gamma a_i + K b_i + e_{ijk} \beta_{k,j} + G_i = 0 \quad (3.3)$$

and

$$\begin{aligned} K_1 b_{3,3i} + K_2 b_{i,33} + K_3 (b_{i,3} b_3^2)_{,3} - K_3 b_{k,3} b_3 b_{k,i} + K_7 e_{k3i} (b_{3,3} b_k)_{,3} \\ - K_7 b_{3,3} e_{i3k} b_{k,3} + K a_i + \tau b_i + L_i = 0. \end{aligned} \quad (3.4)$$

Taking the scalar product of (3.4) with \mathbf{a} we obtain

$$K = -K_7 \left((b_2 b_{3,3})_{,3} + b_{2,3} b_{3,3} \right). \quad (3.5)$$

By noticing that for any $\mathbf{A} \in C^2(\mathbb{R}^3)$

$$\operatorname{div} \mathbf{A} = 0 \text{ if and only if } \mathbf{A} = \nabla \times \mathbf{B} \quad (3.6)$$

for some $\mathbf{B} \in C^2(\mathbb{R}^3)$ we see that to solve (3.3) we may find suitable γ and β by taking the divergence of (3.3) and solving for a possible γ . The resulting equation, with K given by (3.5), is

$$\gamma_{,1} + (K b_3)_{,3} - \left(K_8 b_{2,333} + K_9 (b_3^2 b_{2,3})_{,33} \right) + \Delta\chi^a b_{2,3} H^2 = 0. \quad (3.7)$$

Thus we can find a suitable β using (3.6) when we set

$$\gamma = -x \left((K b_3)_{,3} - \left(K_8 b_{2,333} + K_9 (b_3^2 b_{2,3})_{,33} \right) + \Delta\chi^a b_{2,3} H^2 \right). \quad (3.8)$$

It now follows that solving (3.4) for \mathbf{b} subject to (3.5) allows us to find suitable γ and β (which need not be explicitly derived) which solve (3.3). We proceed to eliminate τ from (3.4). Clearly (3.4) is satisfied for $i = 1$ with the above γ , K , and β . For $i = 2$ we obtain

$$K_2 b_{2,33} + K_3 (b_{2,3} b_3^2)_{,3} + \tau b_2 - \Delta\chi b_2 b_3^2 H^2 = 0 \quad (3.9)$$

and for $i = 3$ we have

$$\begin{aligned} K_1 b_{3,33} + K_2 b_{3,33} + K_3 (b_{3,3} b_3^2)_{,3} - K_3 b_{k,3} b_3 b_{k,3} \\ + \tau b_3 + \Delta\chi b_2^2 b_3 H^2 = 0. \end{aligned} \quad (3.10)$$

Multiplying (3.9) by b_3 and (3.10) by b_2 we can eliminate τ from the equations to yield

$$K_1 b_2 b_{3,33} + K_2 b_2 b_{3,33} - K_2 b_3 b_{2,33} + K_3 b_2 (b_{3,3} b_3^2)_{,3} - K_3 b_3 (b_{2,3} b_3^2)_{,3} \\ - K_3 b_2 b_3 b_{k,3} b_{k,3} + \Delta \chi b_2 b_3 H^2 = 0. \quad (3.11)$$

Using the substitution

$$b_2(z) = \sin \phi(z) \quad b_3(z) = \cos \phi(z) \quad (3.12)$$

in (3.11) results in the following equation for ϕ :

$$\phi''(z) [K_1 \sin^2 \phi(z) + K_2 + K_3 \cos^2 \phi(z)] \\ + (\phi'(z))^2 \sin \phi(z) \cos \phi(z) [K_1 - K_3] = \Delta \chi H^2 \sin \phi(z) \cos \phi(z). \quad (3.13)$$

We now impose the following boundary conditions:

$$\lim_{z \rightarrow -\infty} \phi(z) = 0 \quad \lim_{z \rightarrow +\infty} \phi(z) = \pi \\ \lim_{z \rightarrow -\infty} \phi'(z) = \lim_{z \rightarrow +\infty} \phi'(z) = 0 \quad (3.14)$$

and we further assume that K_1 , K_2 and K_3 are positive (and hence B_1 , B_2 and B_3 are positive). Multiplying (3.13) with ϕ' and using (3.14) we have as a first integral

$$(\phi')^2 [K_1 \sin^2 \phi + K_2 + K_3 \cos^2 \phi] = \Delta \chi H^2 \sin^2 \phi. \quad (3.15)$$

We rewrite (3.15) in the form

$$(\Delta \chi / (K_2 + K_3))^{1/2} H \frac{dz}{d\phi} = \left[1 + [(K_1 - K_3) / (K_2 + K_3)] \sin^2 \phi \right]^{1/2} / \sin \phi \quad (3.16)$$

and solve (3.16). As we are looking for solutions ϕ which are continuous, (3.14) shows that $\phi(\alpha) = \pi/2$ for some $-\infty < \alpha < +\infty$. Without loss of generality we suppose $\alpha = 0$.

Case 1 $K_3 - K_1 > 0$ (or, equivalently, $B_2 - B_1 > 0$).

Set $k^2 = (K_3 - K_1) / (K_2 + K_3) = 1 - B_1/B_2$. By (3.15), solutions exist for the given boundary conditions since $k^2 \leq 1$. From tables of integrals in Gradshteyn and Ryzhik⁴ (p. 160 number 32) we have, on integrating from 0 to z

$$(\Delta \chi / (K_2 + K_3))^{1/2} H z \\ = -\frac{1}{2} \ln \left[\frac{u + \cos \phi}{u - \cos \phi} \right] + k \ln(k \cos \phi + u) - (k/2) \ln(1 - k^2) \quad (3.17)$$

where $u = [1 - k^2 \sin^2 \phi]^{1/2}$.

Case 2 $K_1 = K_3$ ($B_1 = B_2$).

The solution in this case can be easily verified as

$$\phi(z) = 2 \tan^{-1} [\exp [Hz (\Delta\chi/(K_1 + K_2))^{1/2}]] \quad (3.18)$$

which is similar in form to Helfrich's nematic solution (Reference 1, Equation 5).

Case 3 $K_3 - K_1 < 0$ ($B_2 - B_1 < 0$).

Set $k^2 = (K_1 - K_3)/(K_2 + K_3) = B_1/B_2 - 1$. From tables (Reference 4, p. 173 section 2.598 and p. 160 number 32) we have

$$\begin{aligned} & (\Delta\chi/(K_2 + K_3))^{1/2} Hz \\ &= -\frac{1}{2} \ln \left[\frac{v + \cos\phi}{v - \cos\phi} \right] + k \ln(k \cos\phi + v) - (k/2) \ln(1 + k^2) \end{aligned} \quad (3.19)$$

where $v = [1 + k^2 \sin^2\phi]^{1/2}$.

We remark that taking the limit as $K_3 \rightarrow K_1$ in either of (3.17) or (3.19) easily gives the explicit solution in (3.18). For example, in (3.19) we see that on taking limits

$$(\Delta\chi/(K_1 + K_2))^{1/2} Hz = -\frac{1}{2} \ln \left[\frac{1 + \cos\phi}{1 - \cos\phi} \right] = \ln[\tan(\phi/2)]. \quad (3.20)$$

From the three solutions derived above, it is now possible to compute all the Lagrange multipliers for \mathbf{b} given by (3.12) in each case using (3.5), (3.6), (3.8) and (for τ) (3.9) or (3.10).

The energy per unit area cross section associated with (3.12) is (compare de Gennes³, p 81, p. 144–148 and Helfrich¹)

$$\begin{aligned} E &= \int_{-\infty}^{\infty} W(\mathbf{a}, \mathbf{b}, \nabla \mathbf{a}, \nabla \mathbf{b}) dz + \frac{1}{2} \int_{-\infty}^{\infty} \Delta\chi H^2 \sin^2\phi dz \\ &= \frac{1}{2} \int_{-\infty}^{\infty} (\phi')^2 [K_1 \sin^2\phi + K_2 + K_3 \cos^2\phi] dz + \frac{1}{2} \int_{-\infty}^{\infty} \Delta\chi H^2 \sin^2\phi dz \\ &= \int_{-\infty}^{\infty} \Delta\chi H^2 \sin^2\phi dz \end{aligned} \quad (3.21)$$

where we have used (3.15). An application of (3.16) to (3.21) and the substitution $w = \cos\phi$ gives

$$\begin{aligned} E &= \int_{-\infty}^{\infty} (\Delta\chi)^{1/2} H \sin\phi [K_1 \sin^2\phi + K_2 + K_3 \cos^2\phi]^{1/2} \frac{d\phi}{dz} dz \\ &= \int_0^{\pi} (\Delta\chi)^{1/2} H \sin\phi [K_1 \sin^2\phi + K_2 + K_3 \cos^2\phi]^{1/2} d\phi \\ &= 2 \int_0^1 (\Delta\chi)^{1/2} H [K_1 + K_2 + (K_3 - K_1)w^2]^{1/2} dw. \end{aligned} \quad (3.22)$$

From (3.22) we obtain for $K_3 - K_1 > 0$

$$(\Delta\chi)^{-1/2}H^{-1}E = (K_2 + K_3)^{1/2} + (K_1 + K_2)(K_3 - K_1)^{-1/2}\ln\left[\frac{(K_3 - K_1)^{1/2} + (K_2 + K_3)^{1/2}}{(K_1 + K_2)^{1/2}}\right] \quad (3.23)$$

while for $K_1 = K_3$

$$(\Delta\chi)^{-1/2}H^{-1}E = 2(K_1 + K_2)^{1/2} \quad (3.24)$$

and for $K_3 - K_1 < 0$

$$(\Delta\chi)^{-1/2}H^{-1}E = (K_2 + K_3)^{1/2} + (K_1 + K_2)(K_1 - K_3)^{-1/2}\sin^{-1}\left[\frac{(K_1 - K_3)^{1/2}}{(K_1 + K_2)^{1/2}}\right]. \quad (3.25)$$

Notice that taking limits as $K_3 \rightarrow K_1$ in either of (3.23) or (3.25) and applying L'Hôpital's rule results in (3.24).

From (3.16) we also have for $z \geq 0$ and $\phi(0) = \pi/2$

$$\begin{aligned} (\Delta\chi)^{1/2}Hz &= \int_{\phi(0)}^{\phi(z)} (\sin\lambda)^{-1} [K_1\sin^2\lambda + K_2 + K_3\cos^2\lambda]^{1/2} d\lambda \\ &\leq \int_{\pi/2}^{\phi(z)} (\sin\lambda)^{-1} (K_1 + K_2 + K_3)^{1/2} d\lambda \\ &= (K_1 + K_2 + K_3)^{1/2}\ln [\tan(\phi(z)/2)]. \end{aligned} \quad (3.26)$$

It thus follows that for $z \geq 0$

$$\bar{\phi}(z) \leq \phi(z) \quad (3.27)$$

where

$$\bar{\phi}(z) = 2\tan^{-1} [\exp [Hz(\Delta\chi/(K_1 + K_2 + K_3))^{1/2}]]. \quad (3.28)$$

Similarly, for $z \leq 0$ we can show

$$\bar{\phi}(z) \geq \phi(z). \quad (3.29)$$

Following Helfrich¹ we now define the wall width L_ϕ to be the half value width over which ϕ changes from 45° to 135° . From (3.17) and (3.19) the wall widths are found to be in cases 1 and 3

$$L_\phi = ((K_2 + K_3)/(\Delta\chi))^{1/2}H^{-1} \left[\ln \left[\frac{m+1}{m-1} \right] + k \ln \left[\frac{m-k}{m+k} \right] \right] \quad (3.30)$$

where $m = (2 \pm k^2)^{1/2}$, the minus sign being taken in case 1 ($K_3 - K_1 > 0$) and the plus sign in case 3 ($K_3 - K_1 < 0$) with the corresponding k values as defined above. In case 2, ($K_3 = K_1$) the wall width is

$$L_\phi = ((K_1 + K_2)/(\Delta\chi))^{1/2} H^{-1} \ln \left[\frac{\tan(3\pi/8)}{\tan(\pi/8)} \right]. \quad (3.31)$$

Taking the limit as $K_3 \rightarrow K_1$ in (3.30) (i.e. as $k \rightarrow 0$) readily yields (3.31).

It is clear from (3.27) and (3.29) that solutions ϕ must satisfy the inequality

$$L_\phi \leq L\bar{\phi} = [\Delta\chi/(K_1 + K_2 + K_3)]^{1/2} H^{-1} \ln \left[\frac{\tan(3\pi/8)}{\tan(\pi/8)} \right]. \quad (3.32)$$

Further, from (3.30) and (3.31), it is seen that for any solution ϕ , $L_\phi \rightarrow 0$ as $H \rightarrow \infty$ and $L_\phi \rightarrow \infty$ as $H \rightarrow 0^+$.

It can also be easily shown that the expression $(K_1 + K_2 + K_3)$ may be replaced by $\max(B_1, B_2)$ in equations (3.26) to (3.32).

We have integrated equation (3.15) numerically when $K_3 > K_1$ (case 1 above) by using fourth-order Runge-Kutta. The numerical routine is taken from Press *et al.*⁵ and uses variable step-length designed to keep the estimated integration error below a level set by the user.

Since the solution of (3.15) is an initial value problem, we start the integration with the boundary condition that $\phi = \pi/2$ at $z = 0$. Two separation integrations are then performed; one with z advancing in the positive z -direction and the other with z advancing in the negative z -direction. In Figure 2, we present $\phi(z)$ (dashed line) in the region $-0.05 \leq z \leq 0.05$ in cgs units. The other parameters we use are: $K_1 = 0.7 \times 10^{-6}$ dyn, $K_2 = 0.43 \times 10^{-6}$ dyn, $K_3 = 1.7 \times 10^{-6}$ dyn and $\Delta\chi = 1.3 \times 10^{-7}$ cgs units. We use these values for the elastic moduli, since the dominant terms in our resulting equations are similar to those considered by Helfrich for nematics. In the case of the magnetic anisotropy $\Delta\chi$, it is pointed out by de Gennes³ (page 286) that the values for nematics and smectics will be comparable. In Figure 2 we also present $\bar{\phi}(z)$ (solid line) as given by the analytic equation (3.28). This solution provides an upper bound limit for the solution ϕ of (3.15) when $z \leq 0$ and a lower bound limit for ϕ for $z \geq 0$. To obtain the curve for $\bar{\phi}(z)$ we have used the same parameter values as for $\phi(z)$. It is seen that, as expected, $\phi(z)$ lies "inside" $\bar{\phi}(z)$ and by interpolating $\bar{\phi}(z)$ at 45° and 135° we obtain the maximum possible domain wall width for a given set of elastic moduli, magnetic anisotropy and applied magnetic field.

We now present the behaviour of the vector $\mathbf{b}(z)$ along a given smectic layer in the presence of an externally applied magnetic field. From (3.12) we see that this essentially requires knowledge of $\phi(z)$. We have chosen to use (3.18) and set all elastic moduli equal. In this case, the behaviour of $\phi(z)$ is qualitatively the same as when the moduli are unequal, and since the former is given by an explicit analytic solution, we do not recourse to numerical integration. In Figure 3 we plot $b_2(z)$ and $b_3(z)$, shown by continuous and dashed lines respectively. Here $K_1 = K_2 = K_3 = 0.7 \times 10^{-6}$ dyn, $\Delta\chi = 1.3 \times 10^{-7}$ cgs and $H = 500$ Oe. It is seen that

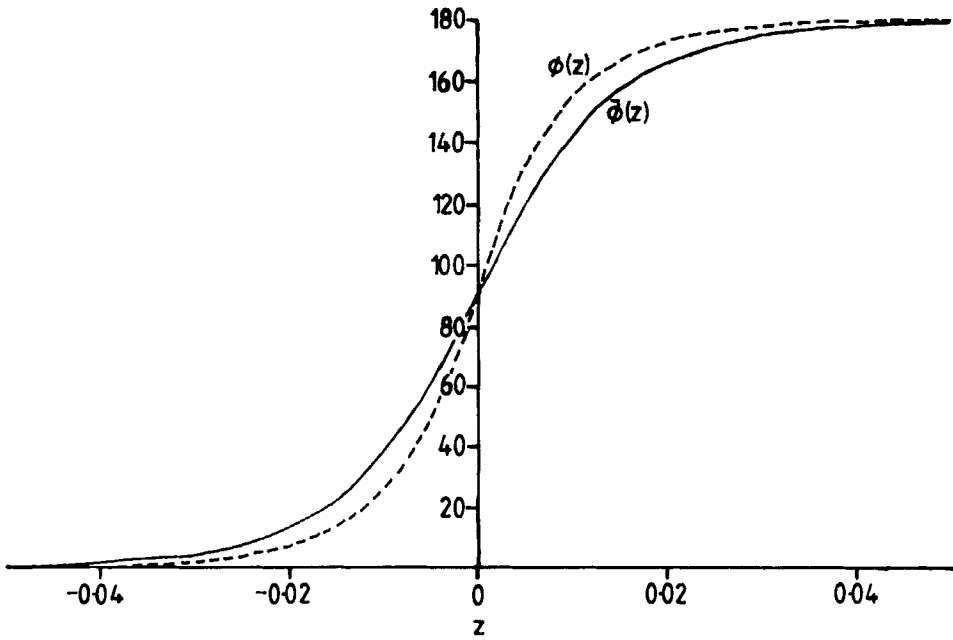


FIGURE 2 The numerical solution for $\phi(z)$, (dashed line), in the case when $K_3 > K_1$. Also shown is the "bounding" solution $\bar{\phi}(z)$, (continuous line). In both cases the applied magnetic field is 500 Oe and we use the elastic moduli and magnetic anisotropy given in the text.

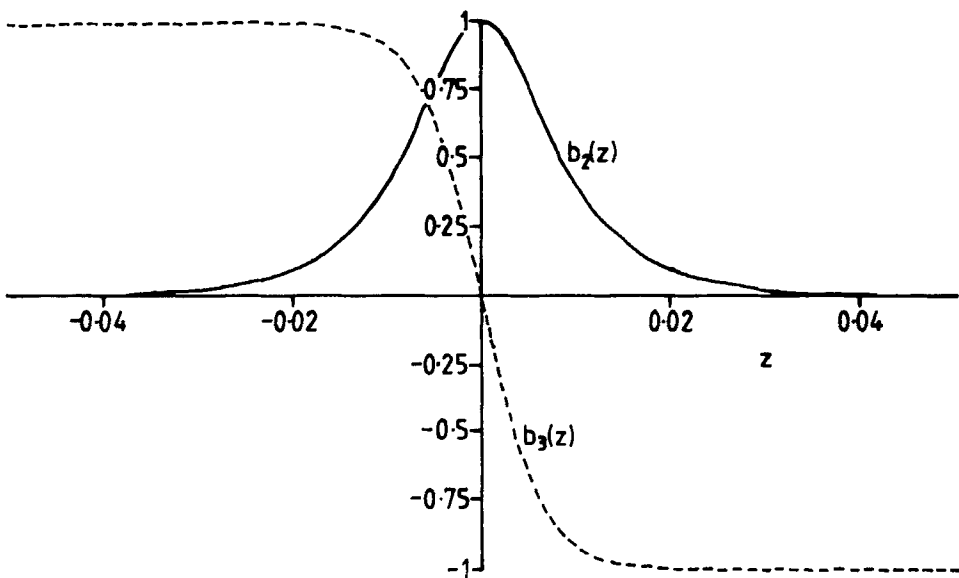


FIGURE 3 The continuous line is $b_2(z)$ and the dashed line is $b_3(z)$. All elastic moduli are set to 0.7×10^{-6} dyn, $\Delta\chi = 1.3 \times 10^{-7}$ cgs and $H = 500$ Oe.

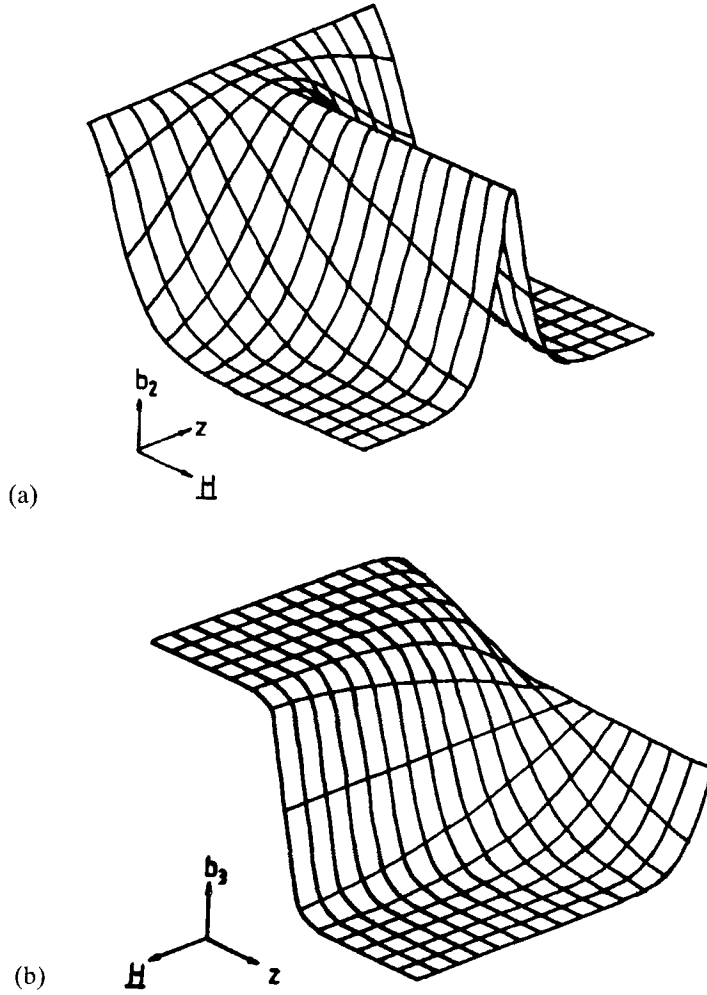


FIGURE 4 Surface plots for: (a) $b_2(z, H)$ and (b) $b_3(z, H)$. In both cases $-0.05 \leq z \leq 0.05$ cm and $0.0 \leq H \leq 1000$ Oe. Also, the elastic moduli are set to 0.7×10^{-6} dyn and $\Delta\chi = 1.3 \times 10^{-7}$ cgs.

increasing the magnetic field diminishes the domain wall and we can observe this effect from the surface plots presented below in Figure 4(a) and 4(b). The elastic moduli and magnetic anisotropy chosen for these plots are the same as those used in Figure 3. With these values fixed, we let z and H be the independent variables and $b_2(z)$ (Figure 4(a)) and $b_3(z)$ (Figure 4(b)) be the dependent variables. In both Figure 4(a) and 4(b), we have $-0.05 \leq z \leq 0.05$ cm and $0.0 \leq H \leq 1000$ Oe. It is seen that with no externally applied field, $b_2 = 1$ throughout a layer and $b_3 = 0$. As the strength of the applied field increases, the region occupied by zero field solutions diminishes around $z = 0$ and consequently the domain wall diminishes.

4. DISCUSSION

The main results of this work are the provision of solutions $\phi(z)$ to equation (3.16) and the derivation of an explicit “bounding” solution $\bar{\phi}(z)$ for each particular ϕ . Equation (3.16) is general and can be solved numerically when all the elastic constants differ (or analytically in some special cases) whenever $\Delta\chi > 0$. Solving for ϕ provides, by (3.12), a complete description of the orientation of \mathbf{b} within a smectic layer.

Equation (3.28) is useful because it describes, by means of a simple analytic expression, the bounds on the behaviour of ϕ and consequently the behaviour of the vector \mathbf{b} . This result leads to (3.32) which, for a given set of elastic constants, magnetic anisotropy and applied magnetic field, gives the maximum possible domain wall width.

The cases we have considered here are restricted to non-chiral smectic C liquid crystals. It is hoped to extend these results to include chirality.

It should be remarked that the bulk free energy expression (2.4) can be shown to be related to the free energy discussed by the Orsay Group.⁶

Appendix

Motivated by considerations of the torque in uniaxial liquid crystals we assume the resultant body couple takes the form

$$\mathbf{K} = \Delta\chi''(\mathbf{n} \cdot \mathbf{H})\mathbf{n} \times \mathbf{H} \quad (\text{i})$$

where \mathbf{H} is the magnetic field and \mathbf{n} is the usual director. Using the above \mathbf{a} , \mathbf{b} , and \mathbf{c} notation \mathbf{n} can be written as $\mathbf{n} = C\mathbf{a} + S\mathbf{c}$ where $C = \cos\vartheta$ and $S = \sin\vartheta$, ϑ being the tilt angle of the director in the smectic layers. Then

$$\mathbf{K} = \Delta\chi''(C(\mathbf{a} \cdot \mathbf{H}) + S(\mathbf{c} \cdot \mathbf{H}))(C\mathbf{a} \times \mathbf{H} + S\mathbf{c} \times \mathbf{H}). \quad (\text{ii})$$

Since $\mathbf{c} \times \mathbf{H} = -(\mathbf{a} \cdot \mathbf{H})\mathbf{a} \times \mathbf{c} - (\mathbf{b} \cdot \mathbf{H})\mathbf{b} \times \mathbf{c}$ it follows that (ii) can be written as

$$\mathbf{K} = \mathbf{a} \times \mathbf{G} + \mathbf{b} \times \mathbf{L} \quad (\text{iii})$$

where

$$\mathbf{G} = \Delta\chi''(C(\mathbf{a} \cdot \mathbf{H}) + S(\mathbf{c} \cdot \mathbf{H}))(C\mathbf{H} - S(\mathbf{a} \cdot \mathbf{H})\mathbf{c}) \quad (\text{iv})$$

and

$$\mathbf{L} = -\Delta\chi''(C(\mathbf{a} \cdot \mathbf{H}) + S(\mathbf{c} \cdot \mathbf{H}))(S(\mathbf{b} \cdot \mathbf{H})\mathbf{c}). \quad (\text{v})$$

Equation (3.2) follows from (iv) and (v) by noticing that $\mathbf{a} \cdot \mathbf{H} = 0$ for the particular geometry imposed.

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References

1. W. Helfrich, *Phys. Rev. Lett*, **21**, 1518 (1968).
2. F. M. Leslie, M. Nakagawa and I. W. Stewart, to appear.
3. P. G. de Gennes, *The Physics of Liquid Crystals*, Oxford University Press, Oxford, 1974.
4. I. S. Gradshteyn and I. W. Ryzhik, *Tables of Integrals, Series and Products*, Academic Press, New York, 1965.
5. W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical Recipes: the Art of Scientific Computing*, Cambridge University Press, Cambridge, 1986.
6. Orsay Group on Liquid Crystals, *Solid State Comm.*, **9**, 653 (1971).