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Static periodic distortion above bend Freedericksz transition in nematics

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The linearized mathematical model developed by Allender, Hornreich and Johnson [1987, *Phys. Rev. Lett.*, **59**, 2654], for explaining the appearance of the magnetic field induced stripe phase (**SP**) above the bend Freedericksz threshold in a nematic close to the smectic transition, is generalized to the case of uniform tilt θ_1 of the nematic director $\mathbf{n}_0$ away from the homeotropic with the field **H** acting normal to $\mathbf{n}_0$. Calculations of SP threshold and domain wave vector Q are presented for different elastic ratios and tilts θ_1 by exact computation of the ground state homogeneous deformation (**HD**) under the rigid anchoring hypothesis. Approximate estimates based on energetics, explicitly taking into account the modal symmetry of perturbations, agree well with the results of exact calculations based on the solution of torque equations. For homeotropic alignment ($\theta_1 = 0$) calculations predict that the SP domain width should decrease when the sample is heated away from the smectic transition point; at a given temperature when **H** is rotated through a small angle with respect to the sample planes the domains should grow wider. These points can be verified experimentally. It is also shown that for sufficiently high initial tilt θ_1 away from the homeotropic director alignment, SP may be quenched. Materials, such as nematic polymers, which exhibit static periodic domains (**PD**) in splay geometry (of the kind discovered by Lonberg and Meyer, 1985, *Phys. Rev. Lett.*, **55**, 718) may also show SP for director tilts θ_1 close to the homeotropic. It appears possible to make tentative predictions regarding the effects of weak anchoring and oblique magnetic fields on the SP threshold and domain wave vector.

1. Introduction

The Oseen–Frank continuum theory of curvature elasticity [1–4] has successfully accounted for the elastic behaviour of nematic liquid crystals acted upon by external influences such as a magnetic field **H**. This theory describes the elastic response of nematics in terms of the splay, twist and bend elastic constants, K_1, K_2, K_3, respectively. The elastic constants can be conveniently determined by studying magnetic field induced Freedericksz transitions for different symmetric initial orientations of the nematic director $\mathbf{n}_0$ in a flat sample. When **H** is increased above the Freedericksz threshold the director field suffers a homogeneous distortion (HD) whose optical detection leads to the determination of the effective elastic constant of the geometry.

The elastic constants, which are functions of temperature, are of the same order of magnitude in most nematics. In certain nematics, however, one or more of the elastic constants may attain anomalous values. For instance, in certain compounds near the nematic–smectic A transition temperature T_{NA}, K_3 (and even K_2) may become very large [1–4]. In certain nematic polymers, K_1 and K_3 are large compared with K_2 [5]. It is natural to expect interesting deviations from normal behaviour when such systems are subjected to external fields.

It was demonstrated by Cladis and Torza [6] that a deformed nematic layer undergoes a transition to a periodically distorted stripe phase (SP) when the sample is cooled to near T_{NA}; they also presented theoretical analysis to account for SP. While studying the bend Freedericksz transition in similar nematic systems, Gooden *et al.* [7] observed SP at temperatures close to T_{NA} for sufficiently strong H.

In a recent paper, Allender *et al.* [8] offered a plausible explanation for the onset of SP by assuming that close to T_{NA}, in the bend geometry, a splay-bend HD first occurs for $H \gtrsim H_B$, the bend Freedericksz threshold. When H is further increased, HD gets further deformed and subsequently becomes energetically unfavourable as K_3 is very large. The total free energy can be reduced if the director field relaxes out of the ($\mathbf{H}$, $\mathbf{n}_0$) plane via a deformation having periodicity normal to the ($\mathbf{H}$, $\mathbf{n}_0$) plane; this is SP. Using the rigid anchoring hypothesis and an approximate mathematical model, Allender *et al.* [8] have obtained good qualitative agreement with the results of [7].

Mention may now be made of a related field effect—the static periodic distortion (PD) discovered by Lonberg and Meyer [9] in the splay geometry of a polymer nematic having $K_1 \gg K_2$ [5]; instead of the usual splay—bend HD which is expected for $H \gtrsim H_S$, the splay Freedericksz threshold, Lonberg and Meyer observed a distortion having periodicity normal to the ($\mathbf{n}_0$, $\mathbf{H}$) plane. Using the continuum theory they showed that PD, which is associated with both splay and twist distortions close to the PD threshold, has a lower threshold than HD as long as K_1 is sufficiently higher than K_2. Linear threshold analysis [10–14], which has been reported on the possible effects of anchoring energy [15, 16], oblique magnetic field [17, 18] and initial director tilt on PD threshold, does suggest that in many cases PD develops out of perturbation modes having a particular symmetry.

Interestingly, the values of elastic ratios definining the range of SP in the calculation of [8] do, to a certain extent, overlap the elastic ratios of polymer nematics [5]. The questions, therefore, arise (i) whether SP can occur in the bend geometry of polymer nematics (ii) whether SP can be regarded as growing out of perturbation modes having a particular symmetry (iii) how SP threshold and domain width are affected by initial director tilt, weakening of the anchoring energy, tilt of $\mathbf{H}$ relative to the sample planes and effect of applying $\mathbf{H}$ obliquely normal to $\mathbf{n}_0$.

In this communication, which essentially complements [8], an attempt is made to answer some of the above questions. In §2 the mathematical model is described, the governing equations set up and the boundary conditions discussed. Section 3 describes the approximate and exact methods of solution. In §4 the results are presented, compared with experiment and interpreted where possible. Section 5 gives a brief account of PD in tilted nematics and helps build a phase diagram for the different deformations occurring in different ranges of director tilt. In the last section, tentative predictions are made of the possible effects of weak anchoring and oblique field on the SP threshold and domain wave vector.

2. Governing equations

Consider a nematic uniformly aligned between plates $z = \pm h$ making angle θ_1 with the z axis such that

$$\mathbf{n}_0 = (S, O, C); \quad S = \sin\theta_1; \quad C = \cos\theta_1. \tag{2.1}$$

A magnetic field $\mathbf{H} = (HC, O, -HS)$ is applied normal to $\mathbf{n}_0$ in the xz plane. It is known from the continuum theory that above the Freedericksz threshold

$$H_c(\theta_1) = (\pi/2h)[(K_1 S^2 + K_3 C^2)/\chi_a]^{1/2} \tag{2.2}$$

the director field suffers a homogeneous deformation such that

$$\left.\begin{aligned} \mathbf{n} &= (S_\theta, O, C_\theta); \quad S_\theta = \sin\theta(\xi), \quad C_\theta = \cos\theta(\xi); \\ & a(\theta)d^2\theta/d\xi^2 + b(\theta)(d\theta/d\xi)^2 + d(\theta) = 0; \\ & \xi = z/h; \quad a(\theta) = K_1 S_\theta^2 + K_3 C_\theta^2; \\ b(\theta) &= (K_1 - K_3)S_\theta C_\theta; \quad d(\theta) = \chi_a h^2 H^2\{\sin(2\theta - 2\theta_1)\}/2 \end{aligned}\right\} \tag{2.3}$$

where $\chi_a(>0)$ is the diamagnetic susceptibility anisotropy. As done earlier [8], the nematic is assumed to be rigidly anchored at the sample planes so that to obtain the ground state HD, we solve (2.3) along with the boundary condition

$$\theta(z = \pm h) = \theta_1 \quad \text{or} \quad \theta(\xi = \pm 1) = \theta_1. \tag{2.4}$$

It is obvious that the HD is even with respect to the sample centre. This fact has a bearing on the symmetry of the perturbations as shall be seen presently.

Considering perturbations $\theta'(x, y, z)$ and $\phi'(x, y, z)$ imposed on HD(2.3) such that

$$\mathbf{n}' = [\sin(\theta + \theta')\cos\phi', \sin\phi', \cos(\theta + \theta')\cos\phi']. \tag{2.5}$$

By retaining terms to second order in the perturbations and perturbation gradients, the excess free energy corresponding to the perturbations, $F_B^{(2)}$, is written down. The torque equations are obtained by minimizing $F_B^{(2)}$ with respect to the perturbations:

$$\left.\begin{aligned} \Gamma_\theta &= K_2\theta'_{,yy} + a(\theta)\theta'_{,zz} + 2b(\theta)\theta_{,z}\theta'_{,z} + e(\theta)\phi'_{,yz} + f(\theta)\theta_{,z}\phi'_{,y} \\ &\quad + \theta'\{g(\theta)\theta_{,z}^2 + 2b(\theta)\theta_{,zz} + \chi_a H^2\cos(2\theta - 2\theta_1)\} \\ &\quad + [h(\theta)\theta'_{,xx} - 2b(\theta)\theta'_{,xz} - g(\theta)\theta_{,z}\theta'_{,x} + i(\theta)\phi'_{,xy}] = 0; \\ \Gamma_\phi &= K_1\phi'_{,yy} + j(\theta)\phi'_{,zz} + k(\theta)\theta_{,z}\phi'_{,z} + e(\theta)\theta'_{,yz} + l(\theta)\theta_{,z}\theta'_{,y} \\ &\quad + \phi'\{m(\theta)\theta_{,zz} + n(\theta)\theta_{,z}^2 - \chi_a H^2\sin^2(\theta - \theta_1)\} \\ &\quad + [p(\theta)\phi'_{,xx} - k(\theta)\phi'_{,xz} + \theta_{,z}q(\theta)\phi'_{,x} + i(\theta)\theta'_{,xy}] = 0; \\ e(\theta) &= (K_2 - K_1)S_\theta; \quad f(\theta) = (K_3 - K_2)C_\theta; \\ g(\theta) &= (K_1 - K_3)(C_\theta^2 - S_\theta^2); \quad h(\theta) = K_1 C_\theta^2 + K_3 S_\theta^2; \\ i(\theta) &= (K_1 - K_2)C_\theta; \quad j(\theta) = K_2 S_\theta^2 + K_3 C_\theta^2; \\ k(\theta) &= 2(K_2 - K_3)S_\theta C_\theta; \quad l(\theta) = C_\theta(2K_2 - K_3 - K_1); \\ m(\theta) &= (K_1 - K_2)S_\theta C_\theta; \quad n(\theta) = 2(K_3 - K_2)C_\theta^2 + K_1 C_\theta^2 + K_2 S_\theta^2; \\ p(\theta) &= K_2 C_\theta^2 + K_3 S_\theta^2; \quad q(\theta) = (K_3 - K_2)(C_\theta^2 - S_\theta^2) \end{aligned}\right\} \tag{2.6}$$

where a prime denotes partial differentiation with respect to the subscript(s). These torque equations are solved with boundary conditions

$$\theta'(z = \pm h) = 0; \quad \phi'(z = \pm h) = 0; \tag{2.7}$$

for rigid anchoring. Following [8], we shall consider only the y, z dependence of the perturbations; this means we ignore, for the moment, the terms enclosed by [ ] in (2.6). Taking into account the symmetry of the ground state deformation θ, it is seen that (2.6) supports two uncoupled modes:

$$\left.\begin{array}{l}\text{Mode 1: } \theta' \text{ even, } \phi' \text{ odd with respect to } z = 0 \text{ or } \xi = 0;\\ \text{Mode 2: } \theta' \text{ odd, } \phi' \text{ even with respect to } z = 0 \text{ or } \xi = 0.\end{array}\right\} \tag{2.8}$$

As θ is even and as Mode 1 conforms to the same symmetry, it is natural to expect that Mode 1 will have a lower threshold than Mode 2 for a given set of parameters. It may be noted that Mode 1 has the same spatial symmetry as the mode studied in connection with PD [9–14]. This fact is helpful in comparing SP and PD in §5.

3. Methods of solution

The SP threshold has been determined from two different view points which are briefly described below.

The approximate solution is obtained almost exactly as suggested by [8] but with slight differences. For a given set of material constants K_1, K_3, χ_a, and director tilt θ_1, (2.3) and (2.4) are numerically solved by employing the orthogonal collocation method [19, 20]; the zeros of the Legendre polynomial of order 24 are used as collocation points [21]. With the field H slightly higher than $H_c(\theta_1)$ of (2.2) the ground state HD is determined from (2.3), (2.4). From (2.6), it is seen that θ' and ϕ' are out of phase along y. Taking note of the symmetry of Mode 1 and also the boundary conditions (2.7), it is assumed that

$$\theta' = \alpha \cos(\pi\xi/2)\cos(Qy'); \quad \phi' = \beta \sin(\pi\xi)\sin(Qy'); \quad y' = y/h, \tag{3.1}$$

where α and β are constants of first order magnitude. The remaining steps follow as in [8]. The excess free energy due to the perturbations, $F_B^{(2)}$, is written to second order in α and β. The demand that $F_B^{(2)}$ should vanish leads to a quadratic in Q^2. As Q^2 is real, one finds the condition

$$D = 0, \tag{3.2}$$

(equation (10) of [8]). H is increased in small steps; for each value of H, the HD is computed. This is done till (3.2) is satisfied for $H = H_{SP}$; simultaneously, Q, the wave vector at SP threshold is calculated from equation (13) of [8] (please see note 22 in the references).

In the exact method of solution, $\theta(\xi)$ is calculated as before from (2.3), (2.4). To solve the torque equations (2.6), the following ansatz is used:

$$\theta' = u(\xi)\cos Q_y y'; \quad \phi' = v(\xi)\sin Q_y y'. \tag{3.3}$$

This results in a pair of coupled linear ordinary differential equations in u and v with (variable) coefficients which are functions of the ground state HD, the material constants (including K_i) and the scaled wave vector of periodicity along y, Q_y. Using the collocation method, a compatibility condition results if the boundary values (2.7) are to be satisfied. For a given, sufficiently high value of Q_y, the compatibility condition is satisfied for a field $H = H(Q_y)$ (as pointed out by Allender *et al.* [8], as Q_y is decreased, $H(Q_y)$ increases; when Q_y diminishes beyond a certain lower limit, no solution can be found for $H(Q_y)$). When Q_y is increased, $H(Q_y)$ decreases until it reaches a minimum $H(Q)$ when $Q_y = Q$; it must be remembered that $H(Q)$ is still higher than $H_c(\theta_1)$. We regard $H_{SP} = H(Q)$ to be the SP threshold and Q to be the SP wave vector at threshold. $Q = 2\pi h/\lambda$ where $\lambda/2$ can be said to be the 'width' of the dark (or bright) bands which result as SP threshold. As made clear [22], H_{SP} found from the approximate and exact methods agrees well; Q from the exact calculation is found to be slightly lower than Q found from the approximate one.

It is seen from (2.3) and (2.6) that H always occurs in combinations of the form $\chi_a h^2 H^2$. It is thus possible to scale out both χ_a and h by choosing some convenient values for them. In this work, it is throughout assumed that $\chi_a = 10^{-7}$ cgs (which is valid for many nematics [1–4]) and that $h = 0{\cdot}01$ cm. SP can now be described by the scaled wave vector Q and by the scaled field

$$h_s = h_s(\theta_1) = H_{SP}/H_c(\theta_1) = H(Q)/H_c(\theta_1). \quad (3.4)$$

The value $h_s = 1$ would correspond to the HD threshold (2.2). The tilt angle θ_1 is measured in radian. The values of the elastic constants are also taken in the range 10^{-6}–10^{-7} cgs [1–4]. Ultimately, the results are all presented in terms of the elastic ratios or reduced elastic constants.

4. Results

In this section, SP threshold and wave vector are described for different elastic ratios and initial director tilt. As already mentioned, the approximate and exact calculations agree well with each other as also with figure 2 of [8] so far as threshold is concerned. Hence, only the results of the exact method are presented. To the extent that the variation of Q with different parameter is also presented here, the present work can be said to complement the effort of [8]; we have some knowledge of the way the domain size is expected to vary according to the continuum theory.

It may be noted that in the calculations of [8], the authors have considered the elastic ratio K_3/K_1 varying from about 7 to 50 and K_2/K_1 in the range 0·25 to 0·75. Interestingly, there appears to be a polymer nematic **TMV** (tobacco mosaic virus) whose elastic ratios fall in this range [23]; $K_3/K_1 = 8{\cdot}8$; $K_2/K_1 = 0{\cdot}22$. Thus it appears that a rigidly anchored homeotropic layer of such a nematic may exhibit SP when subjected to **H** in the bend geometry. In addition, an elastic ratio $K_2/K_1 = 0{\cdot}22$ would correspond to a nematic which should exhibit PD under rigid anchoring in the splay geometry ($\theta_1 = \pi/2$) and also for certain tilts away from the homogeneous [9–14]. This motivates a study of the different regions of existence of PD, the Freedericksz HD and SP in the case of a system like TMV taking molecular tilt as a parameter. Keeping this in mind, the material parameters are so chosen as to include the elastic ratios $K_3/K_1 = 10$, $K_2/K_1 = 0{\cdot}25$ as subsets. Initially, the results are presented for the homeotropic configuration ($\theta_1 = 0$) for different elastic ratios. As these ranges of the material parameters roughly correspond to those expected close to T_{NA}, it seems possible to compare these results with those of [7, 8].

Figure 1 contains plots of h_s and Q as functions of $k_3 = K_3/K_1$ for different values of $k_2 = K_2/K_1$. At a given k_2, as k_3 is decreased, h_s and Q increase. When $k_3 \to$ a lower limit $k_{3L}(k_2)$, h_s and Q diverge showing that for $k_3 < k_{3L}$, SP cannot occur. Predictably, k_{3L} increases with k_2; the k_3 range of occurrence of SP increases when k_2 is diminished. Figure 1 is in good agreement with figure 2 of [8] as far as the variation of h_s is concerned. As k_3 decreases when the sample is heated away from T_{NA}, one has the qualitative conclusion [7, 8] that when the temperature of the sample is raised sufficiently away from T_{NA}, SP is suppressed.

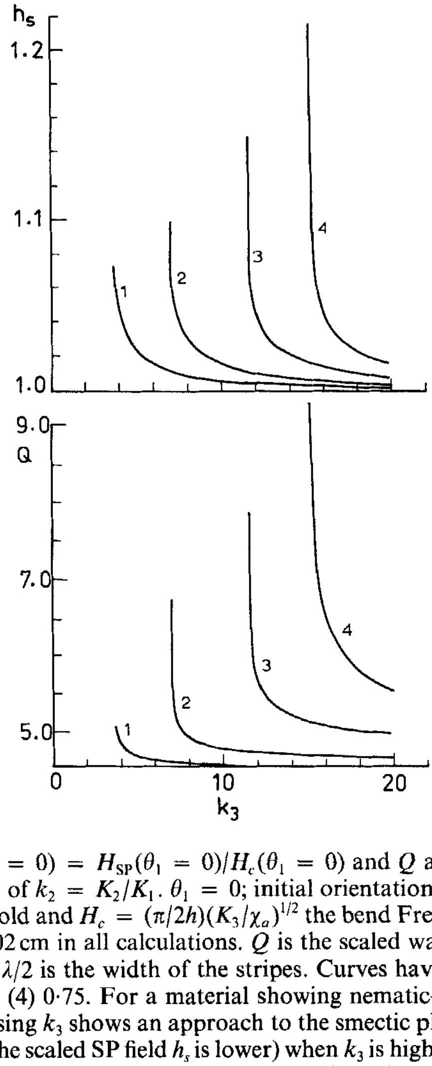

Figure 1. Plots of $h_s(\theta_1 = 0) = H_{SP}(\theta_1 = 0)/H_c(\theta_1 = 0)$ and Q as functions of $k_3 = K_3/K_1$ for different values of $k_2 = K_2/K_1$. $\theta_1 = 0$; initial orientation is homeotropic. H_{SP} is the stripe phase threshold and $H_c = (\pi/2h)(K_3/\chi_a)^{1/2}$ the bend Freedericksz field. The sample thickness $2h = 0{\cdot}02$ cm in all calculations. Q is the scaled wave vector at SP threshold; $Q = 2\pi h/\lambda$ where $\lambda/2$ is the width of the stripes. Curves have been drawn for $k_2 =$ (1) 0·1 (2) 0·25 (3) 0·5 (4) 0·75. For a material showing nematic–smectic A transitions, the direction of increasing k_3 shows an approach to the smectic phase. The occurrence of SP is favourable (i.e. the scaled SP field h_s is lower) when k_3 is high and k_2 small. The h_s curves are in good agreement with those of [8], figure 2. The polymer nematic TMV has elastic ratios roughly corresponding to $k_2 = 0{\cdot}25$, $k_3 = 10$ [23]. For a given k_2 both h_s and Q diverge when k_3 is sufficiently diminished. This indicates that when the sample is heated sufficiently away from the smectic point, SP is quenched and the SP domain width becomes narrower before SP disappears; the latter point can be checked experimentally.

These conclusions are reflected in figures 2 and 3. Figure 2 depicts the variations of h_s and Q as functions of k_2 for different k_3. For a given k_3, h_s and Q increase with k_2; both h_s and Q diverge when $k_2 \rightarrow$ an upper limit $k_{2L}(k_3)$; higher the value of k_3, greater the corresponding k_{2L}.

Figure 3 is included mainly for completeness and shows the dependence of h_s and Q on K_1 for a given K_2 and different K_3. For fixed (K_2, K_3), h_s initially increases with K_1 and then diverges when $K_1 \rightarrow$ an upper limit $K_{1L}(K_2, K_3)$; K_{1L} increases with K_3. The domain wave vector Q shows a more interesting behaviour in that it diverges both in the limit $K_1 \rightarrow K_2$ and when $K_1 \rightarrow K_{1L}$; at an intermediate K_1, Q shows a minimum.

One of the conclusions of experiment [7] is that for initial homeotropic orientation $(\theta_1 = 0)$ when $\mathbf{H}$ is tilted in the xz plane away from the x axis by a small angle θ_H,

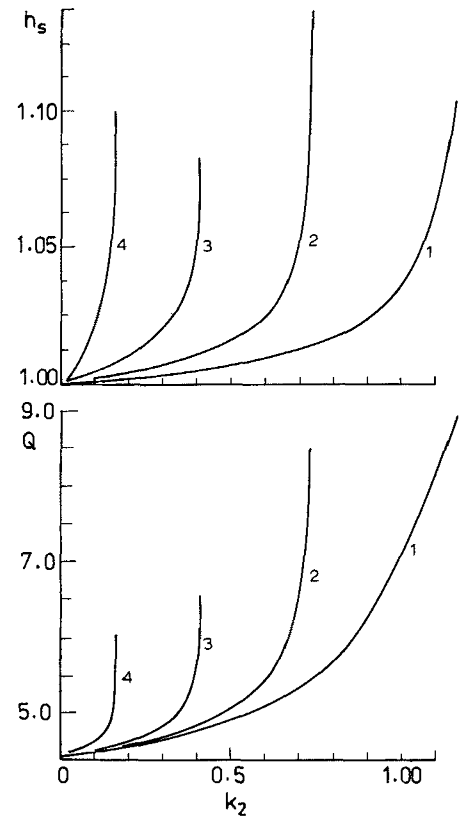

Figure 2. Variations of $h_s(\theta_I = 0)$ and Q with $k_2 = K_2/K_1$ for different k_3. Curves are drawn for k_3 = (1) 20 (2) 15 (3) 10 (4) 5. Initial homeotropic orientation. The results of figure 2 essentially complement those of figure 1. As k_2 may also diverge when the nematic is cooled towards the smectic A point, the direction of increasing k_2 indicates approach to the smectic phase. It is seen that high k_3 and small k_2 encourage formation of SP.

SP is suppressed. It has been mentioned by Allender *et al.* [8] that they have obtained results in qualitative agreement with the above fact. Figure 4, which gives plots of h_s and Q with θ_H, essentially shows agreement with the findings of [7, 8]. It must be borne in mind that now the initial director tilt is $\mathbf{n}_0 = (0, 0, 1)$ but the field $\mathbf{H} = (H\cos\theta_H, 0, -H\sin\theta_H)$; in such a configuration, one no longer has a Freedericksz threshold; HD can develop at any nonzero field amplitude [24]. Thus, in this case, H_{SP} is divided by $H_c(\theta_I = 0)$, the bend Freedericksz threshold, purely for the purpose of scaling. The change over to a tilted field is achieved by simply changing θ_I to θ_H in (2.3) and (2.6); (2.4) is left unchanged. It is found from figure 4 that as θ_H is increased h_s increases but Q diminishes. Beyond a certain limit $\theta_H = \theta_L$, solutions are no longer found for the SP threshold; in the same limit, Q decreases to a lower limiting value. Figure 4 shows that θ_L increases when k_2 is enhanced but decreases when k_3 is increased. As both k_2 and k_3 are expected to increase when a nematic is cooled toward T_{NA}, it is not straightforward to predict how θ_L will vary as the smectic point is approached.

At this stage it may be advisable to explicitly compare the theoretical results obtained here and in [8] with the experimental observations of [7]. The nonoccurrence

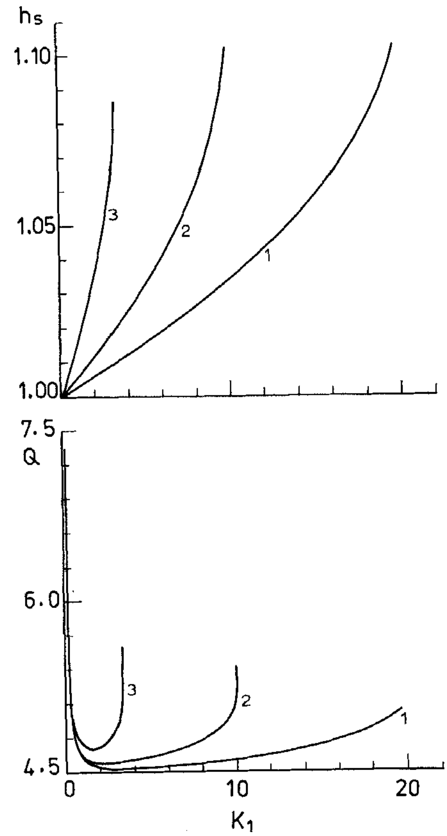

Figure 3. Plots of $h_s(\theta_1 = 0)$ and Q versus K_1 for different values of K_2 and K_3. Initial orientation is homeotropic. The elastic constants are measured in dynes. The sample thickness $2h = 0{\cdot}02\,\mathrm{cm}$. The diamagnetic susceptibility anisotropy $\chi_a = 10^{-7}$ cgs. $K_2 = 0{\cdot}25 \times 10^{-7}$ dyne. Curves have been drawn for $K_3 = (1)\,2 \times 10^{-6}\,(2)\,1{\cdot}5 \times 10^{-6}$ (3) 10^{-6} dyne. These plots have been presented mainly for the sake of completeness and illustrate a rather different kind of variation of Q. For fixed K_2, K_3, h_s and Q diverge showing that an increase of K_1 is unfavourable for SP to occur. When K_1 decreases to about K_2 at a given K_3, Q again diverges but $h_s \to 1$. Thus the indication that SP may not exist when K_1 and K_2 are of comparable magnitude. The reason why h_s does not diverge in the region of small K_1 could be that though $k_2 = K_2/K_1$ increases, $k_3 = K_3/K_1$ also become appreciable.

of SP for small k_3 and the suppression of SP by tilting **H** in the xz plane are points in qualitative agreement with [7]. But the conclusions regarding variation of SP domain width are still open to investigation. Does the SP domain width decrease with k_3; ie, do the SP domains become narrower as the sample is heated away from T_{NA}? Similarly at a given temperature, when **H** is tilted away from the x axis by a small angle, does the SP domain width increase? These points appear to merit a more detailed experimental survey.

Another fact that must be clearly stated is that Gooden *et al.* [7] have found SP to occur above the bend Freedericksz transition only over a small temperature range; close to T_{NA}, the undistorted homeotropic orientation appears to go over directly to SP, apparently without the intervening HD. Thus, at this point of time, one can only

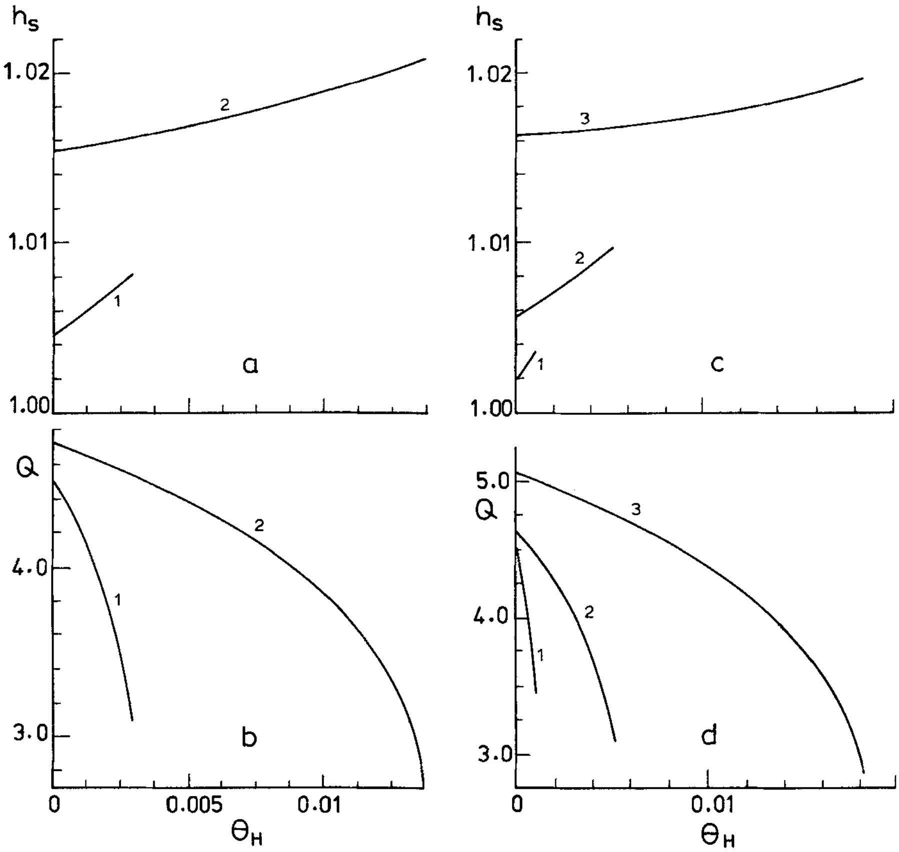

Figure 4. Plots of $h_s(\theta_H)$ and Q as functions of θ_H, the tilt angle of **H** with the x axis. Undistorted orientation is homeotropic; $\mathbf{n}_0 = (0, 0, 1)$; $\theta_1 = 0$. The field $\mathbf{H} = (H\cos\theta_H, 0, -H\sin\theta_H)$ is in the xz plane. In figures *a*, *b*, $k_3 = 10$; $k_2 =$ (1) 0·1 (2) 0·25. In figures *c*, *d*, $k_3 = 15$; $k_2 =$ (1) 0·1 (2) 0·25 (3) 0·5. For $\theta_H \neq 0$, homogeneous deformation develops without a threshold. $h_s(\theta_H) = H_{SP}(\theta_H)/H_c(\theta_1 = 0)$; division by the bend Freedericksz field is only to ensure scaling. Beyond the limit $\theta_H = \theta_L$, SP threshold does not seem to exist. In the limit $\theta_H \to \theta_L$, $Q \to$ a lower limit showing that SP domains should widen as **H** is rotated away from the x axis; this can be verified experimentally.

say that the theoretical results only account for roughly half the observations of [7]. One cannot rule out the possibility, as suggested earlier by Chu and McMillan [25], that very close to T_{NA}, perhaps SP occurs as a first order transition directly from the undistorted ground state.

We now consider the case of initial uniform tilt at the sample boundaries ($\theta_1 \neq 0$). Figure 5 contains plots of h_s and Q as functions of θ_1 for different elastic ratios. It must be remembered that **H** is applied in the xz plane normal to the initial director orientation so that once more we consider SP occurring above the HD threshold. Both h_s and Q are found to decrease when θ_1 is increased (ie the initial director tilt moves away from the homeotropic). When $\theta_1 \to \theta_S$, $h_s \to 1$ (i.e. the SP threshold approaches the HD threshold) and Q tends to a lower limiting value. For a given k_3, θ_S is found to increase with k_2. Calculations have been presented for two different values of k_3. For a material such as TMV, $\theta_S \approx 0{\cdot}03$ radian. Thus, when the initial

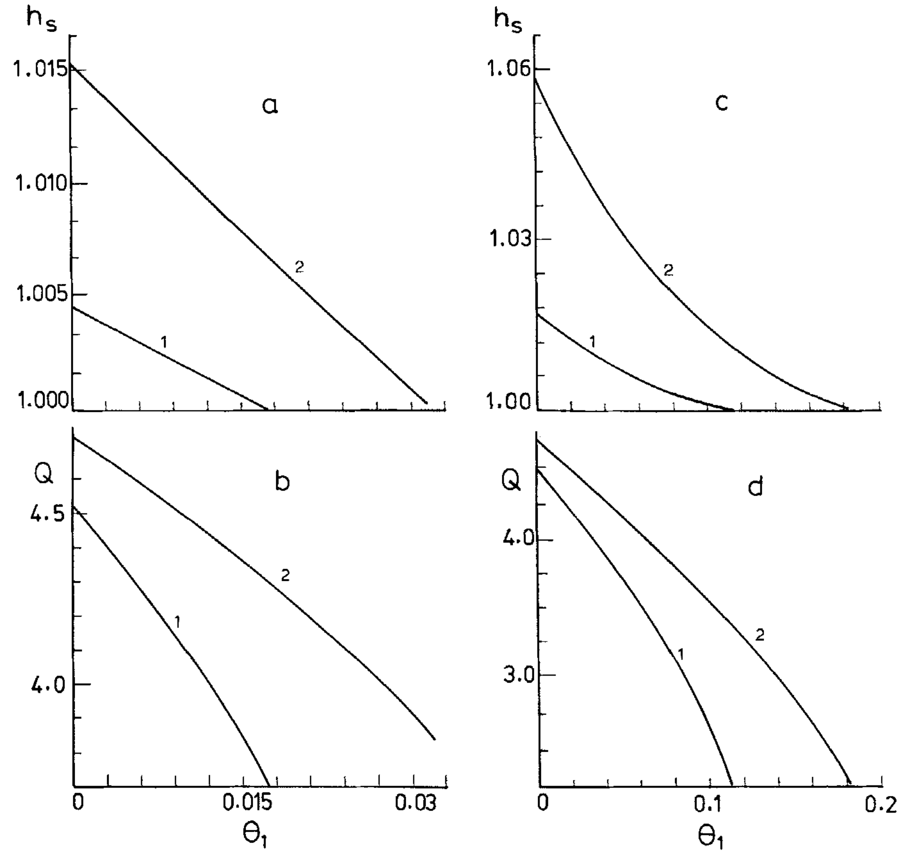

Figure 5. Variation of $h_s(\theta_1)$ and Q with θ_1, the initial director tilt away from the homeotropic. Initial director orientation $\mathbf{n}_0 = (S, O, C)$; $\mathbf{H} = (HC, O, -HS)$ as in equation (2.1). When H exceeds $H_c(\theta_1)$ of equation (2.2), a homogeneous distortion first sets in. When H is increased further, SP occurs at a threshold $H_{SP}(\theta_1)$; $h_s(\theta_1) = H_{SP}(\theta_1/H_c(\theta_1)$. Curves are drawn for k_2 = (1) 0·1 (2) 0·25. In figures (*a*), (*b*) $k_3 = 10$. In (*c*) and (*d*), $k_3 = 1{\cdot}33$. As $\theta_1 \to \theta_S$, $h_s \to 1$ and $Q \to$ a lower limit. When the SP threshold diminishes too close to the HD threshold the ground state distortion necessary to generate SP is not available so that SP is quenched. It is seen that an increase of k_2 or a diminution of k_3 widens the θ_1 range of occurrence of SP. The table shows that this is directly related to an increase in $h_s(\theta_1 = 0)$.

director tilt is sufficiently away from the homeotropic it should be possible to suppress SP which occurs above the HD threshold.

In the related, though mathematically simpler, case of PD it is shown [27] that the language of torques [26] developed for understanding the instability mechanism of convective flows can be utilized to obtain a qualitative understanding of the PD instability. This task is not very simple in the present case as all expressions contain functions of the HD tilt θ which is itself a nontrivial function of z (or ξ). Still, certain qualitative statements can be made. Stating that the director field minimizes its total free energy by relaxing out of the xz plane via a twist is equivalent to asserting that the ground state is unstable against a twist fluctuation owing to a positive feedback mechanism; after all, the torque equations have been dervied by minimizing the excess free energy $F_B^{(2)}$ associated with the perturbations. As in the case of PD [27], this minimization can be traced to the occurrence of cross terms in $F_B^{(2)}$ which are proportional to terms $\theta'_{,y}\phi'_{,z}$, $\theta'_{,z}\phi'_{,y}$ etc.

While applying the torque language, the total torque is split up into different terms out of which those torques, which have a destabilizing influence, are singled out. In the present case it can be tentatively suggested that there are, perhaps, two destabilizing mechanisms at work: torques $\sim e(\theta)\phi'_{,yz}$, $e(\theta)\theta'_{,yz}$ may be expected to act near the sample centre while terms $\sim f(\theta)\theta_{,z}\phi'_{,y}$, $l(\theta)\theta_{,z}\theta'_{,y}$ may be important near the sample boundaries; the latter torques owe their existence explicitly to the distortion of the ground state.

In order to bring out another facet of the phenomenon it should be noted that SP occurs through the growth of the perturbations θ', ϕ'. Naively, any factor that helps (or deters) the growth of the perturbations can be said to help (or deter) the formation of SP. In this light, it is worth understanding the role of **H**. To the extent that an increase of H enhances the amount of HD making the ground state unstable against the twist, **H** can be said to aid the formation of SP. But the torque equations (2.6) show that **H** stabilizes both perturbations via torques $\chi_a H^2\theta'$, $\chi_a H^2\phi'$. Thus an increase of H to large values above SP threshold may be able to quench SP; this can be put to test.

The above remarks also help understand the behaviour of h_s when k_2 increases or k_3 decreases. Such variations of elastic anisotropy increase H_{SP} (and hence h_s) as a higher HD is needed to bring about SP. But a higher H implies a greater magnetic stabilization of both θ' and ϕ'; this would cause the SP threshold to increase further. Thus it is clear that when the elastic ratios reach their respective limits, h_s should diverge. In the next section we shall briefly examine the case of PD to show how differently **H** acts on the perturbations leading to a qualitatively different behaviour of the PD threshold.

The nonoccurrence of SP when **H** is rotated by a sufficiently large angle θ_H in the xz plane (figure 4) can also be tentatively understood from the above consideration. Let H_F be the Freedericksz threshold in a given configuration ($\theta_H = 0$). For $\theta_H \neq 0$, **H** is no longer normal to the initial director field $\mathbf{n}_0$ so that a Freedericksz threshold no longer exists; in addition, the effective distortion at any given field ($> H_F$) will be less than the deformation at the same field in the Freedericksz geometry [24]. Hence, as the angle θ_H increases, the effective ground state distortion decreases so that for SP to occur, higher fields H are necessary to produce the requisite level of HD. The possibility, therefore, cannot be ruled out that a limiting value of the field tilt may be reached beyond which the stabilizing effects of an enhanced H on the perturbations far out weigh the destabilizing influence caused by the increased HD; SP may get quenched.

A physical explanation of the diminution of h_s to 1 as the initial director tilt θ_1 exceeds a limiting angle (figure 5) does not appear to be straightforward. It is easy to appreciate that for small tilts θ_1 away from the homeotropic, the decrease in the Freedericksz threshold is roughly represented by $(dH_c/d\theta_1)/H_G \sim (1 - k_3)\theta_1/k_3$. But for h_s to decrease with increasing θ_1, H_{SP} has to diminish faster than H_c does; this would only indicate a strengthening of the destabilizing torques with increasing θ_1 and a consequent decrease in the HD necessary to give rise to SP. In the limit $\theta_1 \to \theta_S$, as $H_{SP} \to H_c(\theta_1)$, the very mechanism (of HD) required for generating SP ceases to exist so that SP may be suppressed for initial director tilt sufficiently away from the homeotropic.

For TMV, θ_S being only 0·03 radian may look very small; but we must note that in this case the homeotropic value h_s ($\theta_1 = 0$) is itself slightly above 1 ($\approx$ 1·015). In

$k_2 = K_2/K_1$ and $k_3 = K_3/K_1$ are elastic ratios. The stripe phase occurs above the homogeneous distortion when $0 \leqslant \theta_1 < \theta_S$ where θ_1 is the initial director tilt (radian). ($\theta_1 = 0$ is homeotropic orientation). θ_S is determined from the exact calculation described in §4. In the range $\theta_S < \theta_1 < \theta_P$ the stripe phase will not set in above the Freedericksz transition. In the interval $\theta_P < \theta_1 \leqslant \pi/2$, a static periodic deformation should occur; a homogeneous distortion is no longer favourable ($\theta_1 = \pi/2$ is homogeneous alignment). θ_P is found from (5.2). The polymeric nematic TMV [23] has $k_2 = 0{\cdot}25$, $k_3 = 10$. $h_s(\theta_1 = 0) = H_{SP}(\theta_1 = 0)/H_c(\theta_1 = 0)$ is the ratio of the stripe phase threshold to the bend Freedericksz field. Note that θ_S, the θ_1 range of occurrence of SP, is wider larger the value of $h_s(\theta_1 = 0)$.

k_2	k_3	θ_S	θ_P	$h_s(\theta_1 = 0)$
0·010	1·0	0·211	0·228	1·0604
0·010	1·5	0·115	0·277	1·0210
0·025	2·0	0·116	0·486	1·0342
0·010	2·0	0·070	0·317	1·0111
0·100	5·0	0·057	1·079	1·0235
0·250	10·0	0·032	1·439	1·0153
0·100	10·0	0·018	1·209	1·0046
0·250	15·0	0·016	1·463	1·0056

addition, figure 5 shows that greater $h_s(\theta_1 = 0)$, higher the corresponding θ_S. Thus, the θ_1 range of existence of SP broadens when k_3 is decreased and k_2 enhanced. This is borne out by the above table which lists θ_S and $h_s(\theta_1 = 0)$ for different elastic ratios. Lastly, the variation of h_s or Q with θ_1 is not linear; the nonlinearity is more pronounced when k_2 is sufficiently small (figures 5 (*c*), (*d*)).

5. Static periodic distortion (PD) in tilted nematic

Consider the nematic aligned as in (2.1) at an angle θ_1 with z axis. Let $\mathbf{H}$ be impressed normal to $\mathbf{n}_0$ in the xz plane. If k_2 is sufficiently small, a periodic distortion (PD) having the symmetry of Mode 1 (2.8) and periodicity along y should occur at a threshold $H_P(\theta_1)$ lower than the homogeneous Freedericksz threshold $H_c(\theta_1)$ of (2.2). For given k_2, k_3 the ratio $R_P(\theta_1) = H_P(\theta_1)/H_c(\theta_1)$ will be lowest for $\theta_1 = \pi/2$ (homogeneous $\mathbf{n}_0$). As θ_1 is diminished, $R_P(\theta_1)$ increases until, when $\theta_1 \to \theta_P(k_2, k_3)$, $R_P(\theta_1) \to 1$; thus, for $\theta_1 < \theta_P$, PD is no longer possible; only HD should occur. It must be remembered that in the limit $R_P(\theta_1) \to 1$, the domain wave vector of PD, $Q_P \to 0$. Thus, PD and HD have a meeting point; this is an important qualitative difference between SP and PD [8].

It seems instructive to deduce θ_P for different elastic ratios and compare these values with the corresponding values of θ_S. The method followed in [13] is most suited for this purpose. With θ = constant and θ', ϕ' depending only on y, z, (2.6) becomes

$$\left.\begin{aligned} \Gamma_\theta &= K_2\theta'_{,yy} + a(\theta_1)\theta'_{,zz} + e(\theta_1)\phi'_{,yz} + \chi_a H^2\theta' = 0; \\ \Gamma_\phi &= K_1\phi'_{,yy} + j(\theta_1)\phi'_{,zz} + e(\theta_1)\theta'_{,yz} = 0 \end{aligned}\right\} \tag{5.1}$$

The boundary conditions are still (2.7). Seeking solutions of the form (3.3), q_y is used as the order parameter of PD. The threshold condition obtained from (5.1) and (2.7) is expanded in powers of q_y^2 and the limit $q_y \to 0$ yields the following expression for the critical angle θ_P:

$$\sin^2\theta_P = k_2k_3/[(1 - 8/\pi^2)(1 - k_2)^2 + k_2(k_3 - k_2)]. \tag{5.2}$$

PD is more favourable than HD only when $\sin^2\theta_1 > \sin^2\theta_P$.

Before taking up particular cases for study the following points must be noted. To linear order, as is clear from (5.1), the out of plane ϕ' perturbation is not coupled to **H**; the twist occurs essentially in a plane normal to **H**. This appears to be the main reason why PD and HD have a meeting point. When $\theta_1 \to \theta_P$, $H_P(\theta_1) \to H_c(\theta_1)$ and in the same limit the dimensionless PD domain wave vector $Q_P \to 0$. This behaviour of PD should be contrasted with the behaviour of SP; when $\theta_1 \to \theta_S$, through $h_s \to 1$, Q does not approach zero but approaches a lower limiting value.

A list of θ_P values for different k_2, k_3 are presented in the table alongside the θ_S values. Take, for instance, TMV with $k_2 = 0.25$, $k_3 = 10$; for this material, $\theta_S = 0{\cdot}03$ and $\theta_P = 1{\cdot}44$. This means that for this material one should be able to detect a Freedericksz transition in the interval $0{\cdot}03 < \theta_1 < 1{\cdot}44$; above the Freedericksz threshold, SP will not occur. In the range $1{\cdot}44 < \theta_1 \leqslant \pi/2$, PD should set in; HD is not energetically favourable in this range of initial director tilt. When $0 \leqslant \theta_1 < 0{\cdot}03$, first HD appears above the Freedericksz threshold and then, at a higher field, SP will set in. Thus, in a way, table represents a phase diagram which gives the different intervals of existence of the distortions with respect to the initial director tilt. It is seen that the θ_1 range of existence of SP increases when k_3 decreases or k_2 increases. On the other hand, the θ_1 range of occurrence of PD widens when k_2 and k_3 are diminished.

The behaviour of PD may be qualitatively understood as follows [10, 27]. When the director tilt is close to homogeneous, k_2 is the principal elastic ratio which decides the occurrence of PD; a smaller k_3 naturally widens the range of existence of PD. As the bend couples to only splay in HD but couples to both splay and twist in PD, it is natural that an increase in k_3 will result in an enhancement of the PD threshold relative to the HD threshold; thus an increase in k_3 should curtail the θ_1 range of occurrence of PD.

6. Related geometries and concluding remarks

As the unstable modes in SP and PD have the same symmetry, it appears possible to make tentative predictions on the SP threshold in two cases which have not been considered so far in the present work.

6.1. *Oblique director tilt; rigid anchoring; oblique magnetic field*

Consider the initial director field (2.1) subjected to the oblique magnetic field

$$\mathbf{H}' = (H'C\cos\psi,\ H'\sin\psi,\ -H'S\cos\psi) \tag{6.1}$$

applied normal to $\mathbf{n}_0$. If the nematic possesses moderate elastic anistropy then above the HD threshold

$$H'_F(\psi, \theta_1) = (\pi/2h)[a(\theta_1)j(\theta_1)/\chi_a\{a(\theta_1)\sin^2\psi + j(\theta_1)\cos^2\psi\}]^{1/2} \tag{6.2}$$

the homogeneous distortion will be

$$\mathbf{n} = (\sin\theta\cos\phi,\ \sin\phi,\ \cos\theta\cos\phi);\quad \theta = \theta(z);\quad \phi = \phi(z);$$
$$\theta(\pm h) = \theta_1;\quad \phi(\pm h) = 0. \tag{6.3}$$

Both θ and ϕ, which are even with respect to the sample centre, are governed by two nonlinear coupled equations.

If k_2, k_3 are sufficiently small and $\psi \approx 0$, then instead of HD(6.3), PD sets in with the perturbations θ', ϕ' having the symmetry of Mode 1 as the PD threshold $H'_P(\psi, \theta_1)$

is lower than H'_F (6.2). When ψ is enhanced (i.e. when $\mathbf{H}'$ becomes more oblique) θ', ϕ' do not retain their modal purity. The modes get mixed so that each perturbation results from a superposition of odd and even parts. As Mode 2 is energetically less favourable than Mode 1, the mode mixing effectively enhances H'_P with respect to H'_F. When $\psi \to$ a higher limit ψ_P, H'_P exceeds H'_F so that for $\psi > \psi_P$, PD is suppressed and HD should occur [10].

If the nematic possesses suitable k_2, k_3 then first HD(6.3) sets in at H'_F. When H' is incremented further, Mode 1 SP can be expected to occur, at $H'_{SP}(\psi, \theta_1)$ if $\psi \approx 0$ as the ground state twist ϕ will not be appreciable. The similarities of the modal symmetry between PD and SP indicate that when ψ is increased, the scaled threshold $h_s(\psi, \theta_1) = H'_{SP}(\psi, \theta_1)/H'_F(\psi, \theta_1)$ should also increase. When $\psi \to$ a limit ψ_S, $h_s(\psi, \theta_1)$ may diverge so that for $\psi > \psi_S$, SP may not occur. This may be true particularly for materials with sufficiently high θ_S (i.e. nematics with low k_2, k_3; see the table). The above possibility may not be realized for materials having very low θ_S (i.e. k_2 small and k_3 large) as the effects of $\mathbf{H}'$ may not change appreciably with ψ.

6.2. *Effects of weak anchoring; $\boldsymbol{H}$, $\boldsymbol{n}_0$ in xz plane*

We now go back to the initial configuration (2.1) and $\mathbf{H}$ applied normal to $\mathbf{n}_0$ in the xz plane. Using the Rapini–Papoular picture and the assumption of equal anchoring energy at the two sample planes, the ground state is found to be described by the surface free energy density W_σ

$$W_\sigma = (B_\theta/2)\sin^2(\theta - \theta_1) \quad \text{at} \quad z = +h, -h \tag{6.4}$$

corresponding to the boundary conditions.

$$a(\theta)\theta_{,z} \pm (B_\theta/2)\sin(2\theta - 2\theta_1) = 0 \quad \text{at} \quad z = \pm h \tag{6.5}$$

where B_θ is the splay anchoring strength. The ground state HD is calculated by solving (2.3) with (6.5). In the limit $B_\theta h \gg a(\theta_1)$, (6.5) reduces to (2.4) corresponding to rigid anchoring. When B_θ is reduced, not only does the HD threshold diminish, the effective HD in the sample also decreases; this is mainly because θ at $z = \pm h$ does not remain at θ_1 but relaxes away from that value in order to accommodate the distortion in the bulk as H is increased. This yielding of the director orientation at the boundaries brings down the effective HD in the sample.

The perturbations θ', ϕ' are associated with the additional surface free energy density

$$W'_\sigma = (B_\theta/2)(\theta')^2\cos(2\theta - 2\theta_1) + (B_\phi/2)(\phi')^2 \quad \text{at} \quad z = +h, -h, \tag{6.6}$$

which yields the boundary conditions

$$\left.\begin{aligned} a(\theta)\theta'_{,z} - K_1 S_\theta \phi'_{,y} + 2b(\theta)\theta_{,z}\theta' \pm B_\theta\theta'\cos(2\theta - 2\theta_1) - [b(\theta)\theta'_{,x}] &= 0 \\ \text{at} \quad z = \pm h&, \\ j(\theta)\phi'_{,z} + K_2 S_\theta \theta'_{,y} + m(\theta)\theta_{,z}\phi' \pm B_\phi\phi' - [\{k(\theta)/2\}\phi'_{,x}] &= 0 \\ \text{at} \quad z = \pm h&, \end{aligned}\right\} \tag{6.7}$$

where B_ϕ is the twist anchoring strength; in (6.7), we again ignore the terms [ ] as we consider θ', ϕ' to depend on y and z. It may be noted that while HD is determined by B_θ, SP will depend upon both B_θ and B_ϕ.

At this stage it may be recalled [11–14] that if the nematic has suitable elastic anisotropy (k_2, k_3 small) then instead of HD, PD will set in. It has been rigourously shown [11–14] that the formation of PD is encouraged by a diminution of B_ϕ; on the other hand, a decrease in B_θ may suppress PD altogether. Within reasonable limits, a slackening of either anchoring leads to a widening of the domains.

The above results appear to be valid for SP also. The following statements can be tentatively made: (1) A lowering of B_ϕ should bring down the SP threshold as a slackening of the twist anchoring should encourage the generation of the additional (twist) degree of freedom ϕ'. (2) As mentioned earlier, a decrease in B_θ is associated with diminution of total distortion of HD as the boundary orientation yields when H is enhanced. Thus, the scaled SP threshold h_s may increase when B_θ is diminished; there may even exist a cutoff limit for B_θ such that SP cannot exist when B_θ is decreased below this limit. (3) The SP domain width can be expected to increase when either anchoring strength is diminished; this is due to the nonrigid boundary conditions (6.7) which no longer ensure that the two perturbations vanish at the boundaries.

6.3. *Concluding remarks*

The threshold and domain wave vector of SP have been studied as functions of elastic ratios and initial director tilt under the assumption that SP occurs when H is raised above the HD threshold. Approximate and exact calculations yield results in good agreement with previous theoretical work [8] and in partial agreement with experiment [7]. While some of the results (notably those connected with SP threshold) can be qualitatively understood on the basis of energetics, the variation of SP domain which is not very clear. The realization that SP and PD (which occurs in certain polymer nematics) may set in due to the growth of perturbation modes of the same spatial symmetry encourages a comparison of these distortions and leads to tentative predictions for SP in configurations involving oblique magnetic field or weak anchoring. The rather wide range of elastic ratios over which SP is shown to exist [8] indicates that SP, which has been primarily observed in low molecular weight nematics close to T_{NA} [7] may also occur in polymer nematics such as TMV [23].

The main results may be summarized as follows: (1) SP should be favourable when k_2 is small and k_3 large. Heating the sample away from T_{NA} should cause SP domains to become narrower before SP is quenched. While the divergence of SP threshold is known [7, 8], it appears necessary to gather more detailed data on SP domain width; (2) At a given temperature SP should be quenched when a small angle of rotation of the field makes the field nonorthogonal to the initial undistorted director orientation. Here again the present work is in qualitative agreement with [7, 8] but the result that SP domains should widen when the field is rotated is subject to an experimental check; (3) When the initial director tilt is sufficiently removed from the homeotropic SP may not occur above the HD threshold; as the SP wave vector shows a sharp decline with variation of director tilt, it is concluded that SP may get quenched. These calculations, which may be of only academic interest at present, have been presented mainly to compare SP with PD. SP has no meeting point with HD, but PD does merge into HD when elastic ratios and initial director tilt approach their respective limits. It becomes clear from the present work that nematics with sufficient elastic anisotropy may undergo PD, HD and also SP above HD threshold for different ranges of director tilt.

All the above results have been derived by assuming that perturbations are small. The linear threshold calculations are only valid at threshold and are not of much use to predict the absolute magnitudes of perturbations above SP threshold. Thus the possibility suggested by the torque equations (2.6), that SP may be quenched when H is increased sufficiently above SP threshold, must be checked experimentally; it should be interesting to find out how the SP domain width varies in this case. The results have been obtained using the rigid anchoring hypothesis. A systematic study of SP with different substrates would make it worth while to perform more realistic calculations including the effect of finite anchoring energy.

Lastly, the possibility cannot be ruled out that an electric field substituted for **H** in the bend Freedericksz geometry may generate SP above the HD threshold. In this case, however, it may be necessary to take into account flexoelectricity as well as the distortion of the electric field caused by director gradients to obtain accurate theoretical estimates of SP threshold and width.

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