



HAL
open science

Magnetic field induced generalized Freedericksz transition in a rigidly anchored simple twisted nematic

U.D. Kini

► **To cite this version:**

U.D. Kini. Magnetic field induced generalized Freedericksz transition in a rigidly anchored simple twisted nematic. *Journal de Physique*, 1987, 48 (7), pp.1187-1196. 10.1051/jphys:019870048070118700 . jpa-00210543

HAL Id: jpa-00210543

<https://hal.science/jpa-00210543>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Classification

Physics Abstracts

02.60 — 36.20 — 61.30 — 62.20

Magnetic field induced generalized Fredericksz transition in a rigidly anchored simple twisted nematic

U. D. Kini

Raman Research Institute, Bangalore 560 080, India

(Reçu le 30 septembre 1986, révisé le 31 décembre, accepté le 27 mars 1987)

Résumé. — On considère un film nématique dans une situation de torsion simple et d'ancrage rigide aux parois. Un champ magnétique appliqué normalement aux parois peut induire soit des domaines statiques et périodiques, soit une déformation homogène. On étudie ce théorème dans le cadre de la théorie du continuum pour l'élasticité de courbure des nématiques, dans l'approximation des perturbations faibles. Dans le cas d'un polymère nématique qui a été étudié récemment, on trouve que seul l'un des deux modes périodiques est favorable. Cependant le calcul montre que l'autre mode périodique peut survenir dans des matériaux d'élasticité extrêmement anisotrope soumis à des torsions fortes. Il semble qu'on ne puisse pas éliminer le mode périodique par une torsion de la configuration initiale des directeurs.

Abstract. — Using the continuum theory of curvature elasticity of nematics in the small perturbation approximation, the occurrence of magnetic field — induced static periodic domains (PD) relative to that of the homogeneous deformation (HD) is studied for a rigidly anchored simple twisted nematic film as a function of material constants and twist angle, the field being applied normal to the plates. One of two distinct modes of PD is found to be favourable in the case of a polymer nematic studied recently. A model calculation shows, however, that the other PD mode may occur for large twists in materials exhibiting extreme elastic anisotropy. There seems to be no way by which PD can be eliminated by twisting the original director configuration.

1. Introduction.

The Oseen-Frank continuum theory of curvature elasticity [1-2] has met with a good measure of success in accounting for the elastic properties of nematic liquid crystals (for reviews on the subject see, for example, [3-7]). In this theory, the bulk elastic free energy density W is written as a quadratic in the spatial gradients of the unit director vector field \mathbf{n} which describes the average molecular orientation at any given point in the sample. W depends on three curvature elastic constants K_1 , K_2 and K_3 pertaining, respectively, to splay, twist and bend deformations of \mathbf{n} .

Perfectly aligned nematic samples (with $\mathbf{n} = \mathbf{n}_0 = \text{constant}$) corresponding to minimum elastic free energy can be prepared between flat plates by suitable treatment of the bounding surfaces. Owing to the diamagnetic susceptibility anisotropy χ_a of a nematic a magnetic field \mathbf{H} can exert a disrupting torque on \mathbf{n} ; this destabilizing influence is countered by stabilizing elastic torques.

When \mathbf{H} is applied normal to the plates of a

nematic film with $\chi_a > 0$ and \mathbf{n}_0 parallel to the sample boundaries (splay geometry) and $|\mathbf{H}|$ is increased from a low value, \mathbf{n} remains unperturbed for $|\mathbf{H}| < a$ critical value H_c called the splay Fredericksz threshold. For $|\mathbf{H}| \geq H_c$, a splay distortion occurs which is uniform in the sample plane. Such a deformation is known as a homogeneous deformation (HD) whose optical detection leads to the evaluation of K_1 in the splay geometry if \mathbf{n} is assumed to be rigidly anchored at the sample boundaries. In the same (rigid anchoring) hypothesis K_2 and K_3 can be evaluated separately by applying \mathbf{H} along other directions normal to \mathbf{n}_0 in the same geometry and in the bend geometry, respectively.

Recently, Lonberg and Meyer found that when a certain polymer nematic is subjected to \mathbf{H} in the splay geometry the deformation above a well defined threshold is spatially periodic in the sample plane, the direction of periodicity being roughly normal to \mathbf{n}_0 [8]. They showed that such a periodic distortion (PD) involving splay and twist close to the threshold is more favourable than HD for $K_1 > 3.3 K_2$ when \mathbf{n}

is rigidly anchored at the sample walls ; this inequality is certainly valid for the material studied [8, 9]. Apart from being a new effect the occurrence of PD imposes a serious restriction on using the conventional method of determining K_1 .

Employing the rigid anchoring hypothesis and the small perturbation approximation it is found [10] that HD may become more favourable than PD when \mathbf{n}_0 is oblique relative to the sample boundaries or when \mathbf{H} is applied obliquely in a plane normal to \mathbf{n}_0 (as studied earlier by Deuling *et al.* [11]) ; these configurations may enable a determination of K_1 through a suppression of PD. PD appears to be favourable when \mathbf{H} is applied normal to \mathbf{n}_0 but parallel to the sample plane if the material is such that $K_2 > K_1$ (as, for instance, in nematics close to a smectic transition [12]). A one-one correspondence exists between the PD thresholds and wave vectors for the two opposite cases $K_1 > K_2$ and $K_1 < K_2$ owing to a symmetry transformation.

The above conclusions on PD have been arrived at by Oldano [13] and independently by Zimmermann and Kramer [14]. These authors have also concluded, by using different forms of a simple expression for the surface free energy density [15a, b] that weak director anchoring may considerably affect the relative occurrences of PD and HD. The results of [13, 14] have been generalized and presented in some detail in [16].

A configuration of much practical importance is the simple twisted nematic cell in which \mathbf{n} is initially aligned parallel to the sample walls. A uniform twist is subsequently imposed on \mathbf{n} by turning one of the plates in its own plane about an axis normal to the sample through an angle $2\phi_0 < \pi/2$. Leslie [17] derived the HD threshold for such a configuration when \mathbf{H} is applied normal to the plates. The subsequent work of Schadt and Helfrich [18], who replaced the disrupting influence of \mathbf{H} by that of an electric field \mathbf{E} (which exerts a torque on \mathbf{n} via the dielectric susceptibility anisotropy ε_a), paved the way for the development of the twisted nematic display.

In this communication, the occurrence of PD in a simple twisted nematic cell is studied by considering the effects of \mathbf{H} . In section 2 the differential equations and boundary conditions are enumerated. In sections 3 and 4 results are presented for the threshold and domain wave vectors of two distinct PD modes which are generally found to exist. Section 5 concludes the discussion by pointing out some of the limitations of the mathematical model used in the present work.

2. Governing equations, sample geometry, boundary conditions and modal analysis.

The Oseen-Frank elastic free energy density of a nematic is given by [3-7]

$$W = [K_1(\text{div } \mathbf{n})^2 + K_2(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 + K_3(\mathbf{n} \cdot \text{grad } \mathbf{n})^2]/2. \quad (1)$$

At equilibrium \mathbf{n} satisfies the differential equations

$$- (n_{k,i} \partial W / \partial n_{k,j})_{,j} + [\chi_{\perp} H_k + \chi_a n_k (n_m H_m)] H_{k,i} = (p + G)_{,i} \quad (2)$$

$$(\partial W / \partial n_{i,j})_{,j} - (\partial W / \partial n_i) + \chi_a (H_k n_k) H_i + \gamma n_i = 0 \quad (3)$$

where p is the hydrostatic pressure, G the gravitational potential, χ_{\perp} the diamagnetic susceptibility normal to \mathbf{n} and γ a Lagrangian multiplier ; a comma denotes partial differentiation and repeated indices are summed over. Equations (2) and (3) correspond, respectively, to translational and rotational equilibrium of \mathbf{n} . As shown by Leslie [17, 19], (2) is satisfied provided that (3) holds and p is restricted by the condition

$$p = [\chi_a (H_k n_k) (H_j n_j) + \chi_{\perp} H_m H_m] - W - G + p_0 \quad (4)$$

p_0 being an arbitrary constant. In what follows, (4) is assumed to hold and solutions of (3) alone are considered in the light of suitable boundary conditions.

The nematic is assumed to be confined between plates $z = \pm h$ such that at equilibrium,

$$\mathbf{n}_0 = (C, S, 0); \quad C = \cos(q_0 z); \quad S = \sin(q_0 z); \quad q_0 = \phi_0/h \quad (5)$$

in Cartesian coordinates. Thus, with half-twist angle ϕ_0 such that $0 \leq \phi_0 < \pi/4$, $\mathbf{n}_0(z = \pm h) = (\cos \phi_0, \pm \sin \phi_0, 0)$. The upper limit on ϕ_0 is imposed so that the sample may be regarded as monodomain. The coordinates are so chosen that at the sample centre $z = 0$, $\mathbf{n}_0 = (1, 0, 0)$ regardless of the twist. This helps in a separation of the independent modes of solutions of (3). Under the action of $\mathbf{H} = (0, 0, H_z)$, \mathbf{n} is assumed to be perturbed into the form

$$\mathbf{n} = [\cos(q_0 z + \phi) \cos \theta, \sin(q_0 z + \phi) \cos \theta, \sin \theta] \quad (6)$$

where $\theta \equiv \theta(x, y, z)$ and $\phi \equiv \phi(x, y, z)$ are assumed to be small. By using (1), (3) and linearizing wrt θ and ϕ the following equations result :

$$\begin{aligned} \phi_{,xx} (K_1 S^2 + K_3 C^2) + \phi_{,yy} (K_1 C^2 + K_3 S^2) + K_2 \phi_{,zz} + 2SC (K_3 - K_1) \phi_{,xy} + (K_2 - K_1) S \theta_{,xz} + \\ + (K_1 - K_2) C \theta_{,yz} + [\phi_0 (K_3 - K_2) C/h] \theta_{,x} + [\phi_0 (K_3 - K_2) S/h] \theta_{,y} = 0; \end{aligned}$$

$$\theta_{,xx}(K_2 S^2 + K_3 C^2) + \theta_{,yy}(K_2 C^2 + K_3 S^2) + K_1 \theta_{,zz} + 2 SC (K_3 - K_2) \theta_{,xy} + [\chi_a H_z^2 + \phi_0^2(2 K_2 - K_3)/h^2] \times \theta + S(K_2 - K_1) \phi_{,xz} + C (K_1 - K_2) \phi_{,yz} + [(2 K_2 - K_1 - K_3) \phi_0/h] (C \phi_{,x} + S \phi_{,y}) = 0. \quad (7)$$

As a first step, the rigid anchoring hypothesis is invoked ; the director is assumed to be rigidly fixed at the boundaries. Then, the vanishing of the perturbations at the boundaries

$$\theta(z = \pm h) = 0; \quad \phi(z = \pm h) = 0 \quad (8)$$

provides the boundary conditions for solving (7).

For a homogeneous deformation (HD), with θ and ϕ depending on z alone, (7), (8) reduce to the HD threshold [4, 17]

$$H_{zH} = [\{ K_1 \pi^2 + 4 \phi_0^2 (K_3 - 2 K_2) \} / 4 h^2 \chi_a]^{1/2}; \quad \chi_a > 0. \quad (9)$$

This corresponds to Mode H_1 in which θ is even wrt the sample centre. (Mode H_2 , with θ odd, has twice the threshold of Mode H_1 and is consequently of no interest. For both modes, however, $\phi = 0$ to first order near the threshold.) For H_{zH} to exist [17]

$$K_1 \pi^2 + 4 \phi_0^2 (K_3 - 2 K_2) > 0. \quad (10)$$

This condition is satisfied for all values of material parameters chosen in this work. In nematics which exhibit a low temperature smectic phase, (10) may be violated ; in such a case the equilibrium configuration may be rather different [20] from (5).

Using energetics it can be shown [17] that the deformed state for $H_z \geq H_{zH}$ has lower total free energy than the ground state (5) only if

$$\phi_0^2 < \phi_M^2; \quad \phi_M^2 = K_2 K_3 \pi^2 / 4 (K_2^2 - K_2 K_3 + K_3^2). \quad (11)$$

Interestingly enough, ϕ_M depends only on K_3 and K_2 but not on K_1 . This condition will be seen to have an important bearing on results discussed in later sections as, even if (10) holds, the value of H_{zH} obtained from (9) may be of only academic interest if (11) is not satisfied.

While seeking more general solutions of (7), (8) the following observations may be made :

(i) If θ, ϕ are assumed to depend on y, z but not on x , (7)-(8) support two independent Modes,

$$\begin{aligned} \text{Mode } Y_1: & \quad \theta \text{ even}, \quad \phi \text{ odd} \\ & \quad \text{and} \\ \text{Mode } Y_2: & \quad \theta \text{ odd}, \quad \phi \text{ even}. \end{aligned}$$

Modes Y_1, Y_2 can be regarded as generalizations of Modes H_1, H_2 , respectively. It is also seen, by comparison, that Mode Y_1 has the same structure as the mode studied in [8] for a planar untwisted sample (PUS). In a way, this is not surprising as a

PUS can be regarded as a simple twisted nematic having zero twist. In particular, it must also be noted that Mode Y_1 has the same symmetry as the non-linear solution studied in [17]. Lastly, the twist associated with Mode Y_1 is odd, similar to the twist of the ground state (5).

(ii) If θ, ϕ are assumed to depend on x, z but not on y , the independent Modes are

$$\begin{aligned} \text{Mode } X_1: & \quad \theta, \quad \phi \text{ even} \\ & \quad \text{and} \\ \text{Mode } X_2: & \quad \theta, \quad \phi \text{ odd}. \end{aligned}$$

Modes X_1, X_2 are again seen to be extensions, respectively, of Modes H_1, H_2 . There exists one important difference ; the even twist associated with Mode X_1 is not in conformity either with (5) or with the non-linear solution of [17].

(iii) In the case of θ, ϕ depending on x, y, z the perturbations are, in general, asymmetrical so that (7)-(8) do not support independent modes.

To solve for the Mode Y_1 threshold, for example, θ and ϕ are assumed to have variations of the form $f(z) \cos(q_y y)$ and $g(z) \sin(q_y y)$, respectively. Then, (7) reduces to a pair of coupled ordinary differential equations with variable coefficients in f and g . The solution of these equations with (8) leads to a threshold condition. Starting with q_y close to zero, the lowest possible $H_z = H_{zc}(q_y)$ satisfying the threshold condition is found ; H_{zc} is generally close to H_{zH} of (9). When q_y is increased, $H_{zc}(q_y)$ decreases. A variation of q_y leads to a neutral stability curve $H_{zc} = H_{zc}(q_y)$ from which the minimum $H_{zP} = H_{zc}(q_{yc})$ is found, occurring at $q_y = q_{yc}$. Then, H_{zP} is regarded as the Mode Y_1 PD threshold and q_{yc} is considered to be the domain wave vector at PD threshold. [At threshold the domain wavelength $\lambda_{yc} = 2 \pi / q_{yc}$. An increase (or decrease) in q_{yc} results in a decrease (or increase) of domain size.] The ratio

$$R_H = H_{zP} / H_{zH}$$

is now determined. If $R_H < 1$, PD is assumed to be more favourable than HD. If, on the other hand, $R_H \geq 1$, HD is assumed to occur provided that (11) holds. The study of R_H eliminates χ_a and h from the final results and facilitates the use of any convenient value for χ_a such as unity. The solution for the X Modes can be found similarly. In the case of the x, y, z variation one has to find the minimum $H_{zP} = H_{zc}(q_{xc}, q_{yc})$ of a neutral stability surface $H_{zc} = H_{zc}(q_x, q_y)$.

Equations (7) and (8) have been solved numerically by employing the orthogonal collocation method (for details see [21, 22]) with the zeroes of the Legendre polynomial of order twelve [23] as collocation points. Results have been randomly checked by a Fourier series method adapted from [24] and also by using the twenty four point collocation. It is found that Modes Y_1 , X_1 have lower thresholds than Modes Y_2 , X_2 , respectively.

A comparison of (7) with the differential equations for PUS [8] shows that the effect of uniform twist in n_0 is to bring in the bend elastic constant K_3 and the half-twist angle ϕ_0 as additional parameters. All physical quantities are measured in cgs units. As only the ratios of elastic constants are ultimately relevant in this work, it is found convenient to fix K_2 at unity. The angle ϕ_0 is measured in radian. By changing over to a dimensionless variable $\varepsilon = z/h$, h can be absorbed into the dimensionless wave vector

$Q_y = q_y h$ or $Q_x = q_x h$. The semi-sample thickness is fixed at $h = 0.01$ cm in all calculations. Results for Modes Y_1 and X_1 have been plotted together for the same set of parameters ; in all diagrams the primed curves correspond to the X_1 Mode. To avoid confusion results for the two modes are discussed separately.

3. Results for Mode Y_1 .

Figure 1 illustrates the plots of R_H and Q_{yc} (the dimensionless wave vector at Mode Y_1 threshold) as functions of K_1 for different values of K_3 and ϕ_0 . While for polymer nematics [8, 9] $K_1 \sim 11$ and $K_3 \sim 13$, a rather wide range of values have been considered purely for the sake of completeness. The following points may be noted :

(i) At given ϕ_0 and K_3 , when K_1 is sufficiently high (say 20), $R_H < 1$. As K_1 is decreased, R_H

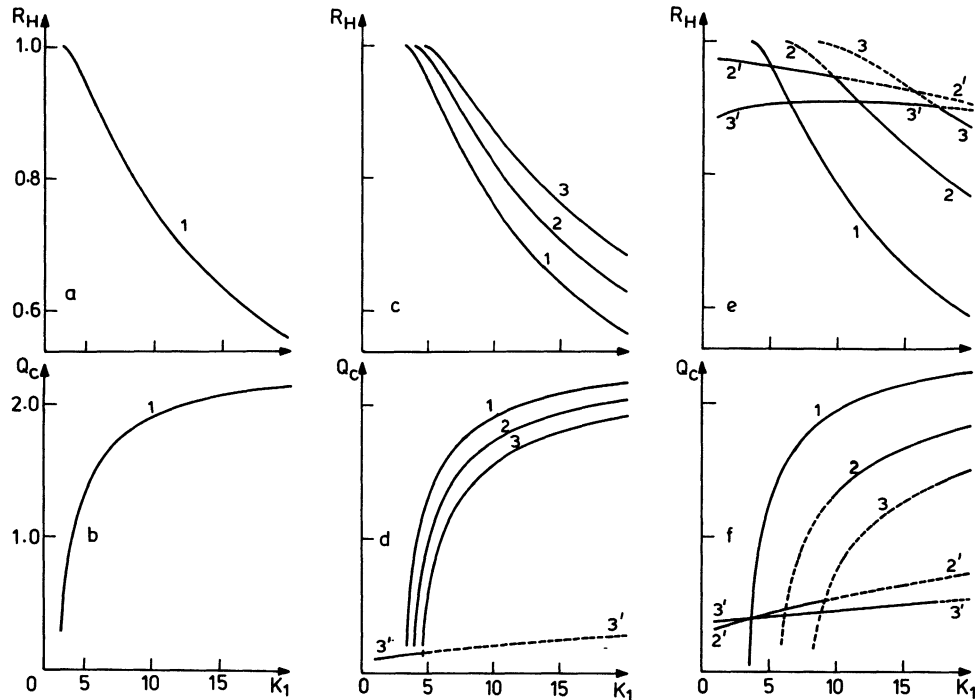


Fig. 1. — Plots of $R_H = H_{zp}/H_{zH}$, the ratio of PD and HD thresholds and Q_c , the dimensionless domain wave vector at PD threshold as functions of the splay elastic constant K_1 for different values of bend elastic constant K_3 and the half-twist angle ϕ_0 (radian). $K_2 = 1$ in all cases. Curves 1, 2, 3 correspond to Mode Y_1 while the primed curves represent Mode X_1 for the same set of parameters. Curves for Mode X_1 have been drawn only for those set of parameters where Mode X_1 becomes more favourable than Mode Y_1 at least over part of the range. Dashed parts of curves show regions of no real interest. Curves are drawn for $K_3 = (1) 1, (2) 10$ and $(3) 20$ in all diagrams. Three values of $\phi_0 = (a, b) 0.05$; $(c, d) 0.4$; $(e, f) 0.775$ have been chosen. As the curves for Mode Y_1 are almost coincident in (a, b) for all three K_3 values only one curve has been shown in figures a, b. In (c, d) Mode X_1 becomes more favourable than Mode Y_1 only at small K_1 ($\phi_0 = 0.4, K_3 = 20$). The R_H curve for Mode X_1 has not been included in (c) for the sake of clarity as R_H is very close to unity and decreases slowly with K_1 . This proximity to HD is reflected in the very low value of Q_{xc} . When $\phi_0 = 0.775$, Mode Y_1 remains favourable for $K_3 = 1$ though Mode X_1 dominates for higher K_3 , especially in regions of smaller K_1 . Thus when ϕ_0 is high and K_3 sufficiently larger than K_1 Mode X_1 dominates ; when ϕ_0 and K_3 are smaller Mode Y_1 is favourable. The K_1 range of existence of Mode Y_1 is curtailed when K_3 or ϕ_0 is enhanced. As per equation (11) (Fig. 4) $\phi_M(10) = 0.52$ and $\phi_M(20) = 0.36$. The results of curves 3 (Figs. c, d, e, f) and curves 2 (Figs. e, f) merely indicate that where PD exists, the PD threshold $<$ the HD threshold ; for these values of parameters HD is itself not energetically more favourable than the ground state (5).

increases and Q_{yc} diminishes. When $K_1 \rightarrow$ a lower limit K_{10} , $R_H \rightarrow 1$ and $Q_{yc} \rightarrow 0$. Thus, for $K_1 < K_{10}$, HD is more favourable than PD. It must be noted that K_{10} is, in general, a function of K_3 and ϕ_0 . The variations of R_H and Q_{yc} with K_1 for different values of ϕ_0 and K_3 are qualitatively similar to those for a PUS.

(ii) When ϕ_0 is small ($= 0.05$; Figs. 1a, 1b) the curves for different K_3 very nearly coincide. K_{10} is practically independent of K_3 and has almost the same value (≈ 3.3) as for a PUS [8]. This is natural as the results for Mode Y_1 must go over to those of [8] in the limit $\phi_0 \rightarrow 0$ and also because in a PUS K_3 does not determine the PD threshold.

(iii) When ϕ_0 is higher (Figs. 1c-1f) K_3 does have a marked effect on R_H , Q_{yc} and K_{10} . For fixed

K_1 and ϕ_0 , when K_3 is enhanced R_H increases and Q_{yc} diminishes (Figs. 2c-2f). This has the predictable effect that for a fixed ϕ_0 , K_{10} increases with K_3 ; as K_3 is enhanced, the K_1 range of existence of Mode Y_1 shrinks.

(iv) For given K_1 and K_3 , R_H increases with ϕ_0 (Figs. 3a-3h). If K_3 is small enough (curves 1, Figs. 1d, 1f) Q_{yc} increases with ϕ_0 ; for higher values of K_3 (curves 2, 3; Figs. 1d, 1f) Q_{yc} decreases when ϕ_0 is enhanced. Thus an increase in the domain size with the twist angle may be generally expected in polymer nematics [8, 9].

Owing to the variable coefficients in the differential equations the task of physical interpretation of the above results is rather formidable. To facilitate a tentative discussion it is necessary to write down W_Y , the elastic free energy density for the Y modes,

$$2 W_Y = K_1(C\phi_{,y} + \theta_{,z})^2 + K_2[(C\theta_{,y} - \phi_{,z})^2 - 2(C\theta_{,y} - \phi_{,z})\phi_0/h - 2(\phi_0/h) \times (\phi_0\theta^2/h - S\theta_{,y}\phi + S\theta\phi_{,y})] + K_3[S^2\phi_{,y}^2 + S^2\theta_{,y}^2 + \phi_0^2\theta^2/h^2 + 2S\phi_0\phi_{,y}\theta/h]. \quad (12)$$

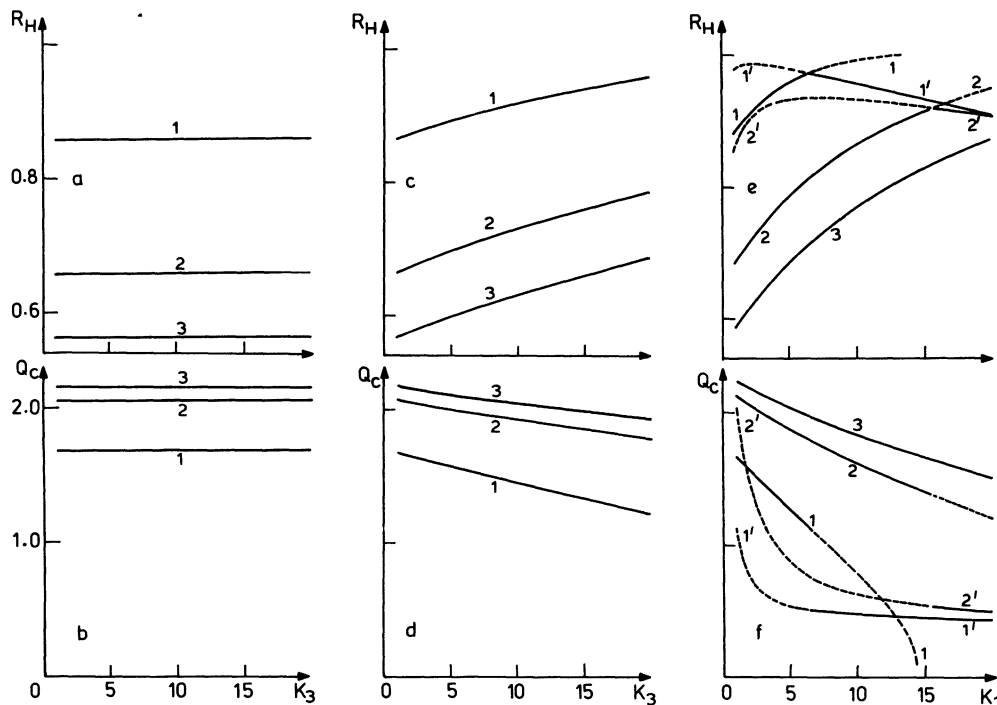


Fig. 2. — Plots of R_H and Q_c as functions of K_3 for different K_1 and ϕ_0 . Modes Y_1 and X_1 are represented; curves for Mode X_1 are identified by primes and are presented only where Mode X_1 exhibits a crossover with Mode Y_1 . $K_2 = 1$ for all calculations. In all diagrams, $K_1 = (1) 7, (2) 14$ and $(3) 20$. The different diagrams correspond to $\phi_0 = (a, b) 0.05; (c, d) 0.4; (e, f) 0.775$ radian. Dashed parts of curves indicate regions of no interest. For low twists K_3 has little or no effect on the Mode Y_1 threshold or domain size. When ϕ_0 is large enough and K_1 sufficiently smaller than K_3 , Mode Y_1 PD can be suppressed. But in this region Mode X_1 is more favourable than HD though its domain size is somewhat large. The conclusions of figure 1 are essentially reinforced. Here again equation (11) (Fig. 4) demands that part of the result be treated with caution. It must be noted that $\phi_M(16) = 0.4$ radian and $\phi_M(5) = 0.77$ radian. Hence, results for $K_3 > 16$ in figures c, d and results for $K_3 > 5$ in figures e, f have to be understood in the light of the fact that in these regions HD is not less energetic than the original director configuration (5).

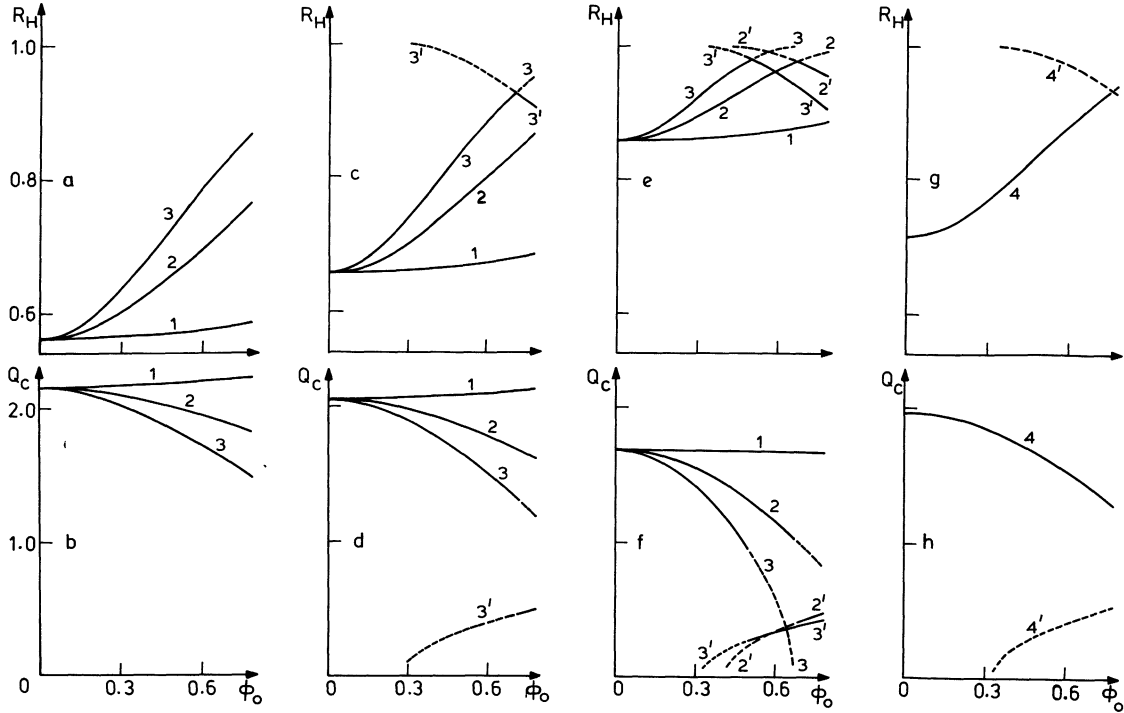


Fig. 3. — Plots of R_H and Q_c vs. ϕ_0 the half-twist angle for different materials. $K_2 = 1$ in all cases. the bend elastic constant $K_3 = (1) 1, (2) 10$ and $(3) 20$ in all diagrams. The splay elastic constant $K_1 = (a, b) 20$; $(c, d) 14$; $(e, f) 7$. Results for both Y_1 and X_1 PD Modes are presented. Curves for Mode X_1 are identified by primes and are included in only those situations where Mode X_1 shows crossover with Mode Y_1 . Dashed parts of curves depict regions of no interest. When ϕ_0 is high enough and K_1 sufficiently smaller than K_3 , Mode Y_1 can be suppressed. In these regions Mode X_1 prevails, though with a much larger domain size. In figures (g, h) the polymer nematic studied in [8, 9] having $K_1 = 11.4$ and $K_3 = 13$ is considered. For this material Mode Y_1 appears to prevail over most of the ϕ_0 range. Mode X_1 may be favourable close to the upper permissible limit of $\phi_0 = \pi/4$. Equation (11) (Fig. 4) imposes the following limits: $\phi_M(10) = 0.52$; $\phi_M(13) = 0.46$; $\phi_M(20) = 0.36$. It must be kept in mind that in a given curve HD may not be less energetic than the ground state (5) when $\phi_0 > \phi_M$.

To understand (iii) and (iv) qualitatively it must be noted that close to HD threshold, $\phi \approx 0$ so that the elastic free energy density for HD is

$$W_H = [K_1 \theta_{,z}^2 + \phi_0^2 (K_3 - 2K_2) \theta^2 / h^2] / 2$$

which is determined by θ and $\theta_{,z}$. On the other hand, W_Y depends on θ , ϕ and their gradients. If now one separates the part of W_Y depending on K_3 and ϕ_0 it is found that the term

$$W_1 = \phi_0^2 \theta^2 (K_3 - 2K_2) / h^2 \quad (13)$$

is common to both HD and PD. Hence, when K_3 is large enough W_1 , which increases with K_3 or with ϕ_0 , contributes the same increase to both W_H and W_Y . However, an enhancement of K_3 or ϕ_0 can cause additional increase in W_Y as W_Y depends on other terms such as

$$W_2 \equiv K_3 S^2 (\phi_{,y}^2 + \theta_{,y}^2) + (2S\phi_0/h) [K_2 \phi \theta_{,y} + (K_3 - K_2) \theta \phi_{,y}]. \quad (14)$$

It must also be noted that $S = \sin(\phi_0 z/h)$ increases with ϕ_0 when $0 \leq |\phi_0 z/h| \leq \pi/2$. Thus when

K_3 or ϕ_0 is augmented the increase in W_Y can be greater than that in W_H . This may cause H_{zP} to increase more steeply than H_{zH} causing an increase in $R_H = H_{zP}/H_{zH}$. An enhancement of R_H effectively brings PD closer to HD at a given K_1 . As HD corresponds to the limit $Q_{yc} \rightarrow 0$ it is intuitively clear that Q_{yc} must decrease, in general, when K_3 or ϕ_0 is augmented. Another fact to be kept in mind is that when K_3 or ϕ_0 is enhanced, a further increase in Q_{yc} would cause an inordinate increase in W_Y and the lowering of Q_{yc} may also be demanded by energetics for equilibrium to exist. The increased proximity of HD to PD with an enhancement of K_3 or ϕ_0 may naturally be expected to shift the limit K_{10} (at which $R_H \rightarrow 1$ and $Q_{yc} \rightarrow 0$) to a higher value.

The one exception to the above discussion occurs when K_3 is very small and ϕ_0 is increased; Q_{yc} increases with ϕ_0 . Qualitatively this may be attributed to the term

$$W_1 \sim \phi_0^2 (K_3 - 2K_2) \theta^2 / h^2$$

in W_Y becoming more negative as ϕ_0 is augmented. It seems possible, therefore, that for the terms such as (14) to balance W_1 , Q_{yc} may have to be higher.

In all the discussion above though it has been suggested that Mode Y_1 may be energetically more favourable than HD, no attempt has been made to establish that Mode Y_1 is energetically more favourable than the ground state (5) : nor has the existence of the HD threshold been examined in the light of (11). The importance of this will be seen later in the same section.

Figure 2 contains plots of R_H and Q_{yc} as functions of K_3 for different K_1 and ϕ_0 . The results are essentially those of figure 1. When ϕ_0 is small (Figs. 2a, 2b) R_H and Q_{yc} depend only on K_1 and hardly change with K_3 . At a given K_1 , when ϕ_0 is fixed at a higher value, R_H increases and Q_{yc} diminishes when K_3 is enhanced (Figs. 2c-2f). At given K_3 and ϕ_0 , when K_1 is diminished R_H increases and Q_{yc} decreases.

Figures 2e, 2f show that when K_1 is low enough and ϕ_0 sufficiently large, the variations of R_H and Q_{yc} with K_3 are rather pronounced (curves 1). When K_3 is enhanced from a low value R_H increases and Q_{yc} decreases until, when $K_3 \rightarrow K'_3$, $R_H \rightarrow 1$ and $Q_{yc} \rightarrow 0$. Thus for $K_3 > K'_3$, Mode Y_1 PD gets suppressed. At this point it therefore seems possible that if other PD modes are not more favoured than HD for $K_3 > K'_3$, then in such materials it may be possible to excite HD and thus determine K_1 from H_{zH} (9) provided that the other quantities are known. It seems appropriate to return to this point at the end of this section and pass over to the next diagram by remarking that K'_3 is a function of K_1 and ϕ_0 ; also K'_3 may exist for the other K_1 values but may be much higher.

Figure 3 illustrates the variations of R_H and Q_{yc} as functions of the half-twist angle ϕ_0 for different materials. For the sake of relevance, the polymer nematic studied in [8, 9] has also been considered (Figs. 3g, 3h). Some of the results are similar to those depicted in the two earlier diagrams. For a given material, R_H increases and Q_{yc} decreases when ϕ_0 is enhanced. (As noted earlier, an exception to this occurs for small K_3 where Q_{yc} increases with ϕ_0 .) When K_1 is sufficiently smaller than K_3 , $R_H \rightarrow 1$ and $Q_{yc} \rightarrow 0$ as $\phi_0 \rightarrow \phi'_0$. Thus, in such a material, for $\phi_0 > \phi'_0$ it seems reasonable to expect that HD may be generated and K_1 determined. It must be borne in mind that ϕ'_0 is a function of the material (i.e. of K_1 and K_3).

At this stage it seems necessary to view the results presented above more critically. Mode Y_1 threshold H_{zP} is calculated for a given set of parameters; the HD threshold H_{zH} is also calculated for the same set of parameters; now the two thresholds are compared. Only a tentative argument has been put forward to indicate that PD may be energetically more favourable than HD. However, owing to the complexity of the calculation involved, Mode Y_1 has not been proved to be energetically more favourable

than the ground state (5). Again, no thought has been expended to find out whether HD is itself a state of lower energy than (5).

The last mentioned point assumes significance when we interpret conclusions of figures 2e, 2f and 3e, 3f. For sufficiently high K_3 or ϕ_0 Mode Y_1 can be suppressed. This ought to solve the problem of estimating K_1 by a study of HD which is more favourable than Mode Y_1 . A study of (11) shows that this may not happen; in regions where Mode Y_1 is suppressed HD is found to be energetically less favourable than the ground state (5) though the HD threshold (9) exists.

Figure 4 shows a plot of $\phi_M(K_3)$ as a function of K_3 . It may be recalled from section 2 that HD has less energy than (5) only if $\phi_0 < \phi_M(K_3) \leq \pi/4$ [17]. It is clear from figure 4 that $\phi_M(K_3) < \pi/4$ for $K_3 > 5$ (since only the range $K_3 \geq 1$ is physically meaningful; also, $\phi_M(10) = 0.52$, $\phi_M(13) = 0.46$ and $\phi_M(20) = 0.36$). All results presented in figures 1, 2, 3 must be appreciated in the light of figure 4. Thus, for instance, in figures 3e, 3f we can no longer say that for $K_1 = 7$, $K_3 = 20$, HD can exist for $\phi_0 > 0.67$. This is because $\phi_M(20) = 0.36 < 0.67$. A similar argument will suffice to show that in figures 2e, 2f one cannot assert that for $K_1 = 7$, $\phi_0 = 0.775$, HD can exist when $K_3 > 15$. This is because, $\phi_M(15) = 0.42 < 0.775$. Figure 4 (or Eq. (11)) can be similarly used to demarcate ranges of parameters over which Mode Y_1 PD threshold $<$ the HD threshold but HD is not energetically more favourable than (5). These have been indicated fully in the figure legends.

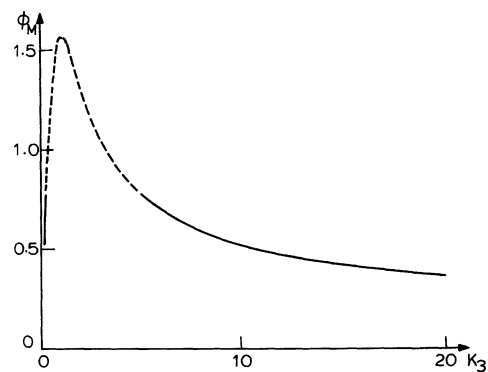


Fig. 4. — Plot of ϕ_M (radian) vs. K_3 . $K_2 = 1$. ϕ_M is a limiting value of the half-twist angle (Eq. (11)) such that for $\phi_0 > \phi_M$, the ground state (5) has less total free energy than HD even though the HD threshold (9) may exist [17]. For $K_3 = 1, 10, 13$ and 20 , $\phi_M = \pi/2, 0.52, 0.46$ and 0.36 respectively. Results of figures 1, 2 and 3 have to be viewed in the light of this diagram. For $\phi_M > \pi/4$, the curve is drawn with dashed lines.

As HD cannot exist in regions where Mode Y_1 is suppressed it seems reasonable to look for other solutions which are more favourable than HD

at least in terms of their threshold. This task is done in the next section.

4. Results for Mode X_1 .

We now turn to the variations of $R_H = H_{zP}/H_{zH}$ and Q_{xc} with different parameters. Here, H_{zP} is the Mode X_1 PD threshold and Q_{xc} the dimensionless wave vector. To facilitate comparison with Mode Y_1 , results for Mode X_1 have been included in the same figures. However, to avoid confusion, the results for Mode X_1 have not been shown in places where Mode Y_1 alone is favourable over the whole range of a particular parameter. All curves for Mode X_1 are identified by adding an apostrophe to the corresponding number for the Y_1 Mode.

Figure 1 shows plots of R_H and Q_{xc} as functions of K_1 for different K_3 and ϕ_0 . It is seen that for small ϕ_0 ($= 0.05$; Figs. 1a, 1b) the X_1 Mode is not favourable. This is natural as it is known that in the limit $\phi_0 \rightarrow 0$, for a PUS, this mode does not exist [10]. When ϕ_0 takes on a higher value ($= 0.4$; Figs. 1c, 1d) Mode X_1 becomes more favourable than Mode Y_1 only at high K_3 ($= 20$) and low K_1 (< 5). Interestingly, Mode X_1 can exist down to $K_1 \sim 1$ though Q_{xc} is very small; the domain size is very large and R_H is only slightly less than unity. When ϕ_0 attains values close to its higher limit ($\approx \pi/4$; Figs. 1e, 1f) Mode X_1 becomes more favourable than Mode Y_1 even at lower K_3 ($= 10$). However, the K_1 range of existence of Mode X_1 increases considerably only when K_3 increases from 10 to 20. In general, at fixed ϕ_0 and K_1 , R_H and Q_{xc} decrease when K_3 is augmented.

In figure 2, R_H and Q_{xc} are shown as functions of K_3 for different K_1 and ϕ_0 . At small ϕ_0 ($= 0.05$; 0.4; Figs. 2a, 2b, 2c, 2d) Mode X_1 does not exist. When ϕ_0 is high ($\approx \pi/4$; Figs. 2e, 2f) Mode X_1 is found to exist when K_3 is sufficiently higher than K_1 . As can be seen, the K_3 range of existence of Mode X_1 , for fixed ϕ_0 , broadens when K_1 decreases. At fixed ϕ_0 and K_1 , R_H and Q_{xc} decrease when K_3 increases, especially in the higher ranges. At given K_3 and ϕ_0 , R_H increases and Q_{xc} diminishes when K_1 is decreased.

Figure 3 contains plots of R_H and Q_{xc} vs. ϕ_0 for different materials (K_1 and K_3). When K_1 is very high ($= 20$; Figs. 3a, 3b) Mode X_1 is found to be unfavourable over the entire permissible range of ϕ_0 even when $K_3 \sim K_1$. When K_1 decreases to 14 (Figs. 3c, 3d) Mode X_1 is found to be favourable at high ϕ_0 ($\approx \pi/4$) and K_3 ($= 20$). When K_1 is much smaller ($= 7$; Figs. 3e, 3f) Mode X_1 can exist even for $K_3 = 10$ though it must be stressed that the ϕ_0 range of occurrence of Mode X_1 does broaden considerably only when K_3 increases to 20. At given K_1 and K_3 , R_H diminishes and Q_{xc} increases when ϕ_0 is enhanced. When ϕ_0 and K_1 are fixed and

K_3 diminished, R_H and Q_{xc} increase in the K_3 range where Mode X_1 is favoured wrt Mode Y_1 .

In figures 3g, 3h, R_H and Q_{xc} are studied as functions of ϕ_0 for the polymer nematic studied in [8, 9] for which $K_1 = 11.4$, $K_3 = 13$. It is found that Mode X_1 may be more favourable than Mode Y_1 only in a small ϕ_0 range close to the upper limit of $\pi/4$. An experiment may be able to settle this point. It must also be noted that if, at a high ϕ_0 , a cross over does occur from Mode Y_1 to Mode X_1 this would involve the domains occurring with periodicity in an orthogonal direction; the domain size would also increase by a factor of two.

Keeping in mind the rather insignificant range of existence of Mode X_1 for realistic parameters an attempt will not be made to study qualitatively the occurrence of this Mode relative to that of Mode Y_1 or HD; such a task is also not very straightforward. It may, however, be pertinent to remark that though Mode X_1 (θ, ϕ even) can be regarded as an extension of Mode H_1 (θ even), the ϕ perturbation associated with it does not conform to the symmetry of the ground state (whose twist angle $= q_0 z$ varies as an antisymmetric function wrt the sample centre). When Mode Y_1 (with odd ϕ) develops in a given situation the director at the sample centre can be expected to be left undisturbed except for a splay and the total twist angle remains antisymmetric. On the other hand when Mode X_1 grows in a sample the director at the sample centre suffers not only a splay but also a twist; the total twist angle ($q_0 z + \phi$) becomes asymmetric. This might tentatively account for the generally high R_H and low Q_{xc} associated with Mode X_1 , even in the parameter ranges where this Mode is favourable. As was stressed in the previous section equation (11) shows that in regions of high ϕ_0 or K_3 , HD has higher free energy than (5). This fact has to be kept in mind as the Mode X_1 threshold has been compared with H_{zH} in regions of high ϕ_0 or K_3 where Mode X_1 is generally favourable. The ranges of parameters which are restricted by equation (11) are indicated in the figure legends.

Before passing over to the concluding section it must be mentioned that the general asymmetric case (iii of section 2) has also been studied. Preliminary calculations, in the range of parameters indicated in figures 1 to 3, shows that this case has higher threshold than the PD Mode which is generally favourable at a given point. A more complete calculation may indicate some range of parameters where the asymmetric case has lower threshold than the other two Modes studied in this work.

5. Conclusions; limitations of the mathematical model used in this work.

In conclusion, one can state that for a polymer nematic [8, 9] Mode Y_1 PD is favourable over almost

the entire range of twist angles. However, a model study, made by varying K_1 , K_3 and ϕ_0 , has shown that while Mode Y_1 is certainly favourable in the range of small ϕ_0 and K_3 , Mode X_1 may dominate when ϕ_0 is large and K_1 sufficiently smaller than K_3 . There seems to be no way by which an imposed twist can suppress PD in favour of HD and make possible a determination of K_1 .

Mode Y_1 has the same nature as PD in PUS and is associated with a twist fluctuation ϕ which is odd wrt the sample centre like the original antisymmetric twist in \mathbf{n}_0 . Mode X_1 PD which has a symmetric twist fluctuation occurs generally with a relatively high threshold and large domain size. Modes Y_2 and X_2 have been ignored as their thresholds are higher than those of Modes Y_1 and X_1 respectively.

The coordinates have been so chosen that as ϕ_0 is enhanced, \mathbf{n}_0 ($z = \pm h$) rotate in opposite directions leaving \mathbf{n}_0 ($z = 0$) fixed at $(1, 0, 0)$. In this frame Mode Y_1 (or Mode X_1) PD occurs with a periodicity along y (or x) i.e. in a direction parallel to the plates and normal to (or parallel to) x axis. If \mathbf{n}_0 at $z = -h$ were fixed along $(1, 0, 0)$ and \mathbf{n}_0 at $z = +h$ along $(\cos 2\phi_0, \sin 2\phi_0, 0)$ we would find Mode Y_1 (or Mode X_1) PD developing with periodicity along a direction making an angle $\phi_0 + \pi/2$ (or ϕ_0) with the x axis.

Results have been obtained by employing the linear perturbation approximation. The linear (Mode Y_1 or Mode X_1) PD threshold is compared with the HD threshold. It has not been possible to show that above the PD threshold, PD has lower free energy than the ground state (5). The present approach has, therefore, to be viewed in the light of (11) or figure 4. When ϕ_0 or K_3 is high one can no longer assert unequivocally that PD, which is more favourable than HD, will exist. This uncertainty appears to exist even for a realistic material [8, 9] for which $\phi_M(K_3) \equiv \phi_M(13) = 0.46$. The question is: will Mode Y_1 PD occur in this material for $\phi_0 > \phi_M$? An experiment may be able to answer this question. On the other hand, a feature worth remarking is that (11) depends on K_3 and K_2 but not on K_1 . It has been made clear that [17] this condition (11), derived by considering fields slightly above HD threshold, may not be a sufficient condition. It seems interesting to solve the non-linear equations [17], calculate the free energy of HD numerically and check that the validity of (11) does not depend on the value of K_1 chosen.

Another well known feature of studying linear thresholds is that the perturbations are assumed to be analytical functions of the coordinates. This results in an eigenvalue problem in which the eigenvectors (absolute amplitudes of perturbations at threshold) are indeterminate. Physically, the equality of free energy for the configurations (θ, ϕ) and $(-\theta, -\phi)$ can lead to the formation of

domains when the field is increased well above threshold. The present work cannot shed much light on the nature of such domains or on other non-linear effects such as change of effective pitch caused by perturbations.

The director has been assumed to be rigidly anchored at the boundaries. Recent studies [13, 14, 16] have shown the importance of weak anchoring in determining the relative occurrence of PD and HD in PUS. Undoubtedly, finiteness of anchoring energy will considerably influence the domain of existence of PD wrt HD. The rigid anchoring hypothesis has been used in the present work not only because it simplifies matters mathematically, but also because it is not very straightforward to study the effects of weak anchoring in a general way using the simple picture [15]. One can certainly follow Nehring *et al.* [25] and consider only the « splay » part,

$$B_\phi \sin^2 \theta \sim B_\phi \theta^2$$

of the surface free energy under the assumption that the undistorted state is still given by (5); this would mean that while the splay fluctuation is weakly anchored, the twist angle of the director is rigidly fixed at the boundaries. If, however, the « twist » part of the surface free energy is also included it is found that this may influence even the original director configuration. The uniform twist can relax to a lower value T and

$$\mathbf{n}_0 = (\cos Tz, \sin Tz, 0); \quad Th = \phi_L; \\ \phi_L + (B_\phi h/2 K_2) \sin(2\phi_L - 2\phi_0) = 0 \dots \quad (15)$$

where B_ϕ is the anchoring strength for twist. To study PD in the context of weak director anchoring, perturbations have to be imposed on \mathbf{n}_0 given in (15); this will be treated elsewhere.

From the point of view of an experiment the effect of an electric field \mathbf{E} is more important [18]. It is well known that the case of an electric field is complicated owing to the field inside the sample being modified by the induced dielectric polarization [5]. One can write down the differential equations for \mathbf{E} assuming that the sample is an insulator and that the director is rigidly anchored at the boundaries. The modal structures explored in section 2 are left undisturbed except for admitting electric field perturbations \mathbf{E}' as new infinitesimal variables. Thus the picture is not merely an extension of the case of \mathbf{H} by a replacement of χ_a by $\epsilon_a/4\pi$, for it is no longer possible to factor out ϵ_a ; as the individual dielectric susceptibilities ϵ_{\parallel} and ϵ_{\perp} enter the picture it is necessary to study the effect of varying an additional parameter such as the ratio $\epsilon_{\parallel}/\epsilon_{\perp}$. The Maxwell equations, which provide relations between director fluctuations and \mathbf{E}' , have also to be taken into account. It seems proper, therefore, to study this case separately.

Mention must also be made of an important (though obvious) difference between the present case and PUS with $\mathbf{n}_0 = (1, 0, 0)$. In PUS there exists a symmetry in the governing differential equations [10, 13, 14] owing to which results for PD with $K_1 > K_2$ and field H_z can be mapped in a one-one manner onto those for PD with $K_1 < K_2$ and field H_y . In the present case the twist in \mathbf{n}_0 destroys the symmetry transformation. A field H_y annihilates the uniformity of twist in \mathbf{n}_0 and this happens without a threshold ; the director field will then be given by

$\mathbf{n}_0 = (\cos \varphi, \sin \varphi, 0)$ where φ is a function of z which has to be calculated numerically. Thus, results obtained in the present work for $K_1 > K_2$ (relevant to polymer nematics) and field H_z cannot be used to predict results for $K_2 > K_1$ (relevant to nematics in the vicinity of a smectic phase) and field H_y .

Acknowledgments.

The author thanks the Referees for their helpful criticism of earlier versions of the manuscript.

References

- [1] OSEEN, C. W., *Trans. Faraday Soc.* **29** (1933) 883.
- [2] FRANK, F. C., *Disc. Faraday Soc.* **25** (1958) 19.
- [3] ERICKSEN, J. L., in *Advances in Liquid Crystals*, G. H. Brown, editor (Academic Press) 1976, p. 223.
- [4] DE GENNES, P. G., *The Physics of Liquid Crystals* (Clarendon Press, Oxford) 1974.
- [5] DEULING, H. J., *Solid State Phys. Suppl.* **14** (1978) 77.
- [6] CHANDRASEKHAR, S., *Liquid Crystals* (Cambridge University Press) 1977.
- [7] BLINOV, L. M., *Electro-optical and Magneto-optical Properties of Liquid Crystals* (John Wiley) 1983.
- [8] LONBERG, F. and MEYER, R. B., *Phys. Rev. Lett.* **55** (1985) 718.
- [9] TARATUTA, V. G., HURD, A. J. and MEYER, R. B., *Phys. Rev. Lett.* **55** (1985) 246.
- [10] KINI, U. D., *J. Physique* **47** (1986) 693.
- [11] DEULING, H. J., GABAY, M., GUYON, E. and PIERANSKI, P., *J. Physique* **36** (1975) 689.
- [12] CHEUNG, L., MEYER, R. B. and GRULER, H., *Phys. Rev. Lett.* **31** (1973) 349.
- [13] OLDANO, C., *Phys. Rev. Lett.* **56** (1986) 1098.
- [14] ZIMMERMAN, W. and KRAMER, L., *Phys. Rev. Lett.* **56** (1986) 2655.
- [15] a. RAPINI, A. and PAPOULAR, M., *J. Physique Colloq.* **30** (1969) C4-54.
b. GUYON, E. and URBACH, W., *Nonemissive Electrooptic Displays*, A. R. Kmetz and F. K. von Willisen, editors (Plenum Press) 1976, p. 121.
- [16] KINI, U. D., *J. Physique* **47** (1986) 1829.
- [17] LESLIE, F. M., *Mol. Cryst. Liquid Cryst.* **12** (1970) 57.
- [18] SCHADT, M. and HELFRICH, W., *Appl. Phys. Lett.* **18** (1971) 127.
- [19] LESLIE, F. M., *J. Phys. D : Appl. Phys.* **3** (1970) 889.
- [20] LESLIE, F. M., *Pramana Suppl.* **1** (1975) 41.
- [21] FINLAYSON, B. A., *The Method of Weighted Residuals and Variational Principles* (Academic Press) 1972.
- [22] TSENG, H. C., SILVER, D. L. and FINLAYSON, B. A., *Phys. Fluids* **15** (1972) 1213.
- [23] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, editors (Dover Publications) 1972.
- [24] MANNEVILLE, P. and DUBOIS-VIOLETTE, E., *J. Physique* **37** (1976) 1115.
- [25] NEHRING, J., KMETZ, A. R. and SCHEFFER, T. J., *J. Appl. Phys.* **47** (1976) 850.