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

U. D. Kini

Raman Research Institute, Bangalore 560 080, India

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Résumé. — On considère un film némantique 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 némantiques, dans l’approximation des perturbations faibles. Dans le cas d’un polymère némantique 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 \( \mathbf{n} = \mathbf{n}_0 = \) 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 \( \chi_s \) 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 \( \chi_s > 0 \) 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 Freedericksz 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 $n_0$ is oblique relative to the sample boundaries or when $H$ is applied obliquely in a plane normal to $n_0$ (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 $H$ is applied normal to $n_0$ 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 $n$ is initially aligned parallel to the sample walls. A uniform twist is subsequently imposed on $n$ by turning one of the plates in its own plane about an axis normal to the sample through an angle $\theta_0 \equiv \pi/2$. Leslie [17] derived the HD threshold for such a configuration when $H$ is applied normal to the plates. The subsequent work of Schadt and Helfrich [18], who replaced the disrupting influence of $H$ by that of an electric field $E$ (which exerts a torque on $n$ via the dielectric susceptibility anisotropy $\varepsilon_3$), 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 $H$. 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]

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

At equilibrium $n$ satisfies the differential equations

$$- (n_{k,i} \partial W/\partial n_{k,j})_j + \chi_k n_{k,m} (\partial W/\partial n_{m,j})_j H_{k,i} = (p + G)_j \quad (2)$$

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

where $p$ is the hydrostatic pressure, $G$ the gravitational potential, $\chi_k$ the diamagnetic susceptibility normal to $n$ and $\gamma$ 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 $n$. As shown by Leslie [17, 19], (2) is satisfied provided that (3) holds and $p$ is restricted by the condition

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

$p_0$ 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, $n_0 = (C, S, 0)$; $C = \cos (q_0 z)$; $S = \sin (q_0 z)$; $q_0 = \phi_0/h \quad (5)$

in Cartesian coordinates. Thus, with half-twist angle $\phi_0$ such that $0 = \phi_0 < \pi/4$, $n_0 (z = \pm h) = (\cos \phi_0, \pm \sin \phi_0, 0)$. The upper limit on $\phi_0$ is imposed so that the sample may be regarded as monodomain. The coordinates are so chosen that at the sample centre $z = 0$, $n_0 = (1, 0, 0)$ regardless of the twist. This helps in a separation of the independent modes of solutions of (3). Under the action of $H = (0, 0, H_z)$, $n$ is assumed to be perturbed into the form

$$n = [\cos (q_0 z + \phi_0) \cos \theta, \quad \sin (q_0 z + \phi_0) \cos \theta, \sin \theta] \quad (6)$$

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

$$\phi_{,xx} (K_1 S^2 + K_3 C^2) + \phi_{,yy} (K_1 C^2 + K_3 S^2) + K_2 \phi_{,xz} + 2 SC (K_3 - K_1) \phi_{,xy} + (K_2 - K_1) S \theta_{,xz} +$$

$$+ (K_1 - K_2) C \theta_{,yz} + [\phi_0 (K_3 - K_2) C/h] \theta_{,x} + [\phi_0 (K_3 - K_2) S/h] \theta_{,y} = 0 \quad ;$$
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

\[ \theta(z = \pm h) = 0; \quad \phi(z = \pm h) = 0 \]  

provides the boundary conditions for solving (7).

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

\[ H_{2H} = \left[ \{ K_1 \pi^2 + 4 \phi_0 (K_3 - 2 K_2) \} / 4 h^2 x_s \right]^{1/2}; \quad x_s > 0. \]  

This corresponds to Mode H1 in which \( \theta \) is even wrt the sample centre. (Mode H2, with \( \theta \) odd, has twice the threshold of Mode H1 and is consequently of no interest. For both modes, however, \( \phi = 0 \) to first order near the threshold.) For \( H_{2H} \) to exist [17]

\[ K_1 \pi^2 + 4 \phi_0 (K_3 - 2 K_2) > 0. \]  

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 \( H_t \geq H_{2H} \) has lower total free energy than the ground state (5) only if

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

Interestingly enough, \( \phi_M \) 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 \( H_{2H} \) 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 \( \theta, \phi \) are assumed to depend on \( x, z \) but not on \( y \), (7)-(8) support two independent Modes,

\[ \text{Mode Y}_1: \quad \theta \text{ even}, \quad \phi \text{ even}; \quad \text{Mode Y}_2: \quad \theta \text{ odd}, \quad \phi \text{ odd}. \]

Modes \( \text{Y}_1, \text{Y}_2 \) can be regarded as generalizations of Modes H1, H2, respectively. It is also seen, by comparison, that Mode \( \text{Y}_1 \) 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 \( \text{Y}_1 \) has the same symmetry as the non-linear solution studied in [17]. Lastly, the twist associated with Mode \( \text{Y}_1 \) is odd, similar to the twist of the ground state (5).

(ii) If \( \theta, \phi \) are assumed to depend on \( x, z \) but not on \( y \), the independent Modes are

\[ \text{Mode X}_1: \quad \theta, \quad \phi \text{ even}; \quad \text{Mode X}_2: \quad \theta, \quad \phi \text{ odd}. \]

Modes \( \text{X}_1, \text{X}_2 \) are again seen to be extensions, respectively, of Modes H1, H2. There exists one important difference; the even twist associated with Mode \( \text{X}_1 \) is not in conformity either with (5) or with the non-linear solution of [17].

(iii) In the case of \( \theta, \phi \) 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 \( \text{Y}_1 \) threshold, for example, \( \theta \) and \( \phi \) 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 \( H_t = H_{2H}(q_y) \) satisfying the threshold condition is found; \( H_{2H} \) is generally close to \( H_{2H} \) of (9). When \( q_y \) is increased, \( H_{2H}(q_y) \) decreases. A variation of \( q_y \) leads to a neutral stability curve \( H_{2H} = H_{2H}^c(q_y) \) from which the minimum \( H_{2H} = H_{2H}^c(q_y) \) satisfying the threshold condition is found; \( H_{2H}^c \) is generally close to \( H_{2H} \) of (9). When \( q_y \) is increased, \( H_{2H}^c(q_y) \) decreases. A variation of \( q_y \) leads to a neutral stability curve \( H_{2H}^c = H_{2H}^c(q_y) \) from which the minimum \( H_{2H} = H_{2H}^c(q_y) \) is found, occurring at \( q_y = q_{yc} \). Then, \( H_{2H}^c \) is regarded as the Mode \( \text{Y}_1 \) PD threshold and \( q_{yc} \) is considered to be the domain wavelength 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

\[ R_t = H_{2H}^c / H_{2H} \]

is now determined. If \( R_t < 1 \), PD is assumed to be more favourable than HD. If, on the other hand, \( R_t > 1 \), HD is assumed to occur provided that (11) holds. The study of \( R_t \) eliminates \( \chi_s \) and \( h \) from the final results and facilitates the use of any convenient value for \( x_s \) 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 \( H_{2H} = H_{2H}^c(q_x, q_{yc}) \) of a neutral stability surface \( H_{2H} = H_{2H}^c(q_x, q_{yc}) \).
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 Y₁, X₁ have lower thresholds than Modes Y₂, X₂, respectively.

A comparison of (7) with the differential equations for PUS [8] shows that the effect of uniform twist in n₀ is to bring in the bend elastic constant K₃ and the half-twist angle φₒ 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 K₂ at unity. The angle φₒ 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 \( h = 0.01 \text{ cm} \) in all calculations. Results for Modes Y₁ and X₁ have been plotted together for the same set of parameters; in all diagrams the primed curves correspond to the X₁ Mode. To avoid confusion results for the two modes are discussed separately.

3. Results for Mode Y₁.

Figure 1 illustrates the plots of \( R_H = H_{P} / H_{H} \), the ratio of PD and HD thresholds and \( Q_y \), 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 \( \phi_o \) (radian). \( K_2 = 1 \) in all cases. Curves 1, 2, 3 correspond to Mode Y₁ while the primed curves represent Mode X₁ for the same set of parameters. Curves for Mode X₁ have been drawn only for those set of parameters where Mode X₁ becomes more favourable than Mode Y₁ 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 \( \phi_o = (a, b) \ 0.05 \); (c,e) \ 0.4 ; (e, f) \ 0.775 \) have been chosen. As the curves for Mode Y₁ 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 X₁ becomes more favourable than Mode Y₁ only at small \( K_1 \) (\( \phi_o = 0.4, K_3 = 20 \)). The \( R_H \) curve for Mode X₁ 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 \( Q_{ac} \). When \( \phi_o = 0.775 \), Mode Y₁ remains favourable for \( K_3 = 1 \) though Mode X₁ dominates for higher \( K_3 \), especially in regions of smaller \( K_1 \). Thus when \( \phi_o \) is high and \( K_3 \) sufficiently larger than \( K_1 \) Mode X₁ dominates; when \( \phi_o \) and \( K_3 \) are smaller Mode Y₁ is favourable. The \( K_1 \) range of existence of Mode Y₁ is curtailed when \( K_3 \) or \( \phi_o \) 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).

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Fig. 1. — Plots of \( R_H = H_{P} / H_{H} \), the ratio of PD and HD thresholds and \( Q_y \), 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 \( \phi_o \) (radian). \( K_2 = 1 \) in all cases. Curves 1, 2, 3 correspond to Mode Y₁ while the primed curves represent Mode X₁ for the same set of parameters. Curves for Mode X₁ have been drawn only for those set of parameters where Mode X₁ becomes more favourable than Mode Y₁ 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 \( \phi_o = (a, b) \ 0.05 \); (c,d) \ 0.4 ; (e, f) \ 0.775 \) have been chosen. As the curves for Mode Y₁ 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 X₁ becomes more favourable than Mode Y₁ only at small \( K_1 \) (\( \phi_o = 0.4, K_3 = 20 \)). The \( R_H \) curve for Mode X₁ 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 \( Q_{ac} \). When \( \phi_o = 0.775 \), Mode Y₁ remains favourable for \( K_3 = 1 \) though Mode X₁ dominates for higher \( K_3 \), especially in regions of smaller \( K_1 \). Thus when \( \phi_o \) is high and \( K_3 \) sufficiently larger than \( K_1 \) Mode X₁ dominates; when \( \phi_o \) and \( K_3 \) are smaller Mode Y₁ is favourable. The \( K_1 \) range of existence of Mode Y₁ is curtailed when \( K_3 \) or \( \phi_o \) 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 $K_1 \to$ a lower limit $K_{10}$, $R_H \to 1$ and $Q_{yc} \to 0$. 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 $\phi_0$. The variations of $R_H$ and $Q_{yc}$ with $K_1$ for different values of $\phi_0$ and $K_3$ are qualitatively similar to those for a PUS.

(ii) When $\phi_0$ 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 a PUS [8] in the limit $\phi_0 \to 0$ and also because in a PUS $K_3$ does not determine the PD threshold.

(iii) When $\phi_0$ 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 $\phi_0$, when $K_3$ is enhanced $R_H$ increases and $Q_{yc}$ diminishes (Figs. 2c-2f). This has the predictable effect that for a fixed $\phi_0$, $K_{10}$ 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 $\phi_0$ (Figs. 3a-3h). If $K_3$ is small enough (curves 1, Figs. 1d, 1f) $Q_{yc}$ increases with $\phi_0$ ; for higher values of $K_3$ (curves 2, 3 ; Figs. 1d, 1f) $Q_{yc}$ decreases when $\phi_0$ 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,

$$2W_Y = K_1(C\phi_0 + \theta_0)^2 + K_2[(C\theta_0 - \phi_0)^2 - 2(C\theta_0 - \phi_0)\phi_0/h - 2(\phi_0/h) \times$$

$$\times (\phi_0 \theta_0^2/h - S\theta_0 \phi + S\theta \phi_0)] + K_3[S^2\phi_0^2 + S^2\theta_0^2 + \theta_0^2 + 2S\phi_0 \phi_0 \theta_0/h] .$$

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Fig. 2. — Plots of $R_H$ and $Q_a$ as functions of $K_3$ for different $K_1$ and $\phi_0$. 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 $Y_1$, $K_3 = 1$ for all calculations. In all diagrams, $K_3 = (1) 7$, (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 $K_1$ has little or no effect on the Mode $Y_1$ threshold or domain size. When $\phi_0$ 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 some what 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 $\phi_0(16) = 0.4$ radian and $\phi_0(5) = 0.77$ 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. $\phi_0$, 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 $\phi_0$ 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 $\phi_0$ 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: $\phi_0(10) = 0.52$; $\phi_0(13) = 0.46$; $\phi_0(20) = 0.36$. 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, $\phi = 0$ so that the elastic free energy density for HD is

$$W_H = [K_1 \theta_z^2 + \phi_0^2(K_3 - 2K_2) \theta_z^2/h^2]/2$$

which is determined by $\theta$ and $\theta_z$. On the other hand, $W_Y$ depends on $\theta$, $\phi$ and their gradients. If now one separates the part of $W_Y$ depending on $K_3$ and $\phi_0$ it is found that the term

$$W_1 = \phi_0^2 \theta_z^2(K_3 - 2K_2)/h^2$$

(13)

is common to both HD and PD. Hence, when $K_3$ is large enough $W_1$, which increases with $K_3$ or with $\phi_0$, contributes the same increase to both $W_H$ and $W_Y$. However, an enhancement of $K_3$ or $\phi_0$ can cause additional increase in $W_Y$ as $W_Y$ depends on other terms such as

$$W_2 = K_5 S^2(\phi_y^2 + \phi_z^2) + (2 S\phi_0/h)[K_2 \phi_{\theta_y} + (K_3 - K_2) \theta_\phi_{\theta_y}].$$

(14)

It must also be noted that $S = \sin(\phi_0 z/h)$ increases with $\phi_0$ when $0 \leq |\phi_0 z/h| \leq \pi/2$. Thus when $K_3$ or $\phi_0$ is augmented the increase in $W_Y$ can be greater than that in $W_H$. This may cause $H_{x\phi}$ to increase more steeply than $H_{z\phi}$ causing an increase in $R_H = H_{x\phi}/H_{z\phi}$. An enhancement of $R_H$ effectively brings PD closer to HD at a given $K_1$. As HD corresponds to the limit $Q_{\infty} \rightarrow 0$ it is intuitively clear that $Q_{\infty}$ must decrease, in general, when $K_3$ or $\phi_0$ is augmented. Another fact to be kept in mind is that when $K_3$ or $\phi_0$ is increased, a further increase in $Q_{\infty}$ would cause an inordinate increase in $W_Y$ and the lowering of $Q_{\infty}$ may also be demanded by energetics for equilibrium to exist. The increased proximity of HD to PD with an enhancement of $K_3$ or $\phi_0$ may naturally be expected to shift the limit $K_0$ (at which $R_H \rightarrow 1$ and $Q_{\infty} \rightarrow 0$) to a higher value.

The one exception to the above discussion occurs when $K_3$ is very small and $\phi_0$ is increased; $Q_{\infty}$ increases with $\phi_0$. Qualitatively this may be attributed to the term

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

in $W_Y$ becoming more negative as $\phi_0$ is augmented. It seems possible, therefore, that for the terms such as (14) to balance $W_1$, $Q_{\infty}$ 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 \( Q_{nc} \) as functions of \( K_1 \) for different \( K_1 \) and \( \phi_0 \). The results are essentially those of figure 1. When \( \phi_0 \) is small (Figs. 2a, 2b) \( R_H \) and \( Q_{nc} \) depend only on \( K_1 \) and hardly change with \( K_1 \). At a given \( K_1 \), when \( \phi_0 \) is fixed at a higher value, \( R_H \) increases and \( Q_{nc} \) diminishes when \( K_3 \) is enhanced (Figs. 2c-2f). At given \( K_3 \) and \( \phi_0 \), when \( K_1 \) is diminished \( R_H \) increases and \( Q_{nc} \) decreases.

Figures 2e, 2f show that when \( K_1 \) is low enough and \( \phi_0 \) sufficiently large, the variations of \( R_H \) and \( Q_{nc} \) with \( K_3 \) are rather pronounced (curves 1). When \( K_3 \) is enhanced from a low value \( R_H \) increases and \( Q_{nc} \) decreases until, when \( K_1 \rightarrow K_3 \), \( R_H \rightarrow 1 \) and \( Q_{nc} \rightarrow 0 \). Thus for \( K_1 > K_3 \), 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 \( K_3 > K_1 \), then in such materials it may be possible to excite HD and thus determine \( K_1 \) from \( H_{hh} \) (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 \( K'_1 \) is a function of \( K_1 \) and \( \phi_0 \); 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 \( Q_{nc} \) as functions of the half-twist angle \( \phi_0 \) 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 \( Q_{nc} \) decreases when \( \phi_0 \) is enhanced. (As noted earlier, an exception to this occurs for small \( K_3 \) where \( Q_{nc} \) increases with \( \phi_0 \).) When \( K_1 \) is sufficiently smaller than \( K_3 \), \( R_H \rightarrow 1 \) and \( Q_{nc} \rightarrow 0 \) 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 \( \phi_0^* \) 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 \( H_{pp} \) is calculated for a given set of parameters; the HD threshold \( H_{hh} \) 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 \( \phi_0 \) 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 \( \phi_0 < \phi_M(K_3) = \pi/4 \) [17]. It is clear from figure 4 that \( \phi_M(K_3) < \pi/4 \) for \( K_3 > 5 \) (since only the range \( K_3 \approx 1 \) 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.

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![Graph](image-url)
at least in terms of their threshold. This task is done in the next section.

4. Results for Mode X1.

We now turn to the variations of \( R_H = H_{22}/H_H \) and \( Q_{xc} \) with different parameters. Here, \( H_{22} \) is the Mode X1 PD threshold and \( Q_{xc} \) the dimensionless wave vector. To facilitate comparison with Mode Y1, results for Mode X1 have been included in the same figures. However, to avoid confusion, the results for Mode X1 have not been shown in places where Mode Y1 alone is favourable over the whole range of a particular parameter. All curves for Mode X1 are identified by adding an apostrophe to the corresponding number for the Y1 Mode.

Figure 1 shows plots of \( R_H \) and \( Q_{xc} \) as functions of \( K_1 \) for different \( K_3 \) and \( \phi_0 \). It is seen that for small \( \phi_0 \) (\( = 0.05 \); Figs. 1a, 1b) the X1 Mode is not favourable. This is natural as it is known that in the limit \( \phi_0 \to 0 \) for a PUS, this mode does not exist [10]. When \( \phi_0 \) takes on a higher value (\( = 0.4 \); Figs. 1c, 1d) Mode X1 becomes more favourable than Mode Y1 only at high \( K_3 \) (\( = 20 \)) and low \( K_1 \) (<5). Interestingly, Mode X1 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 \( \phi_0 \) attains values close to its higher limit (\( \approx \pi/4 \); Figs. 1e, 1f) Mode X1 becomes more favourable than Mode Y1 even at lower \( K_3 \) (\( = 10 \)). However, the \( K_1 \) range of existence of Mode X1 increases considerably only when \( K_3 \) increases from 10 to 20. In general, at fixed \( \phi_0 \) 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 \( \phi_0 \). At small \( \phi_0 \) (\( = 0.05 \); 0.4; Figs. 2a, 2b, 2c, 2d) Mode X1 does not exist. When \( \phi_0 \) is high (\( \approx \pi/4 \); Figs. 2e, 2f) Mode X1 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 X1, for fixed \( \phi_0 \), broadens when \( K_1 \) decreases. At fixed \( \phi_0 \) and \( K_1 \), \( R_H \) and \( Q_{xc} \) decrease when \( K_3 \) increases, especially in the higher ranges. At given \( K_1 \) and \( \phi_0 \), \( R_H \) increases and \( Q_{xc} \) diminishes at \( K_3 \) is decreased.

Figure 3 contains plots of \( R_H \) and \( Q_{xc} \) vs. \( \phi_0 \) for different materials (\( K_1 \) and \( K_3 \)). When \( K_3 \) is very high (\( \geq 20 \); Figs. 3a, 3b) Mode X1 is found to be unfavourable over the entire permissible range of \( \phi_0 \) even when \( K_3 \sim K_1 \). When \( K_1 \) decreases to 14 (Figs. 3c, 3d) Mode X1 is found to be favourable at high \( \phi_0 \) (\( \approx \pi/4 \)) and \( K_3 \) (\( = 20 \)). When \( K_1 \) is much smaller (\( \approx 7 \); Figs. 3e, 3f) Mode X1 can exist even for \( K_3 = 10 \) though it must be stressed that the \( \phi_0 \) range of occurrence of Mode X1 does broaden considerably only when \( K_1 \) increases to 20. At given \( K_1 \) and \( K_3 \), \( R_H \) diminishes and \( Q_{xc} \) increases when \( \phi_0 \) is enhanced. When \( \phi_0 \) and \( K_1 \) are fixed and \( K_3 \) diminished, \( R_H \) and \( Q_{xc} \) increase in the \( K_3 \) range where Mode X1 is favoured wrt Mode Y1.

In figures 3g, 3h, \( R_H \) and \( Q_{xc} \) are studied as functions of \( \phi_0 \) for the polymer nematic studied in [8, 9] for which \( K_1 = 11.4 \), \( K_3 = 13 \). It is found that Mode X1 may be more favourable than Mode Y1 only in a small \( \phi_0 \) 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 \( \phi_0 \), a cross over does occur from Mode Y1 to Mode X1, 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 X1 for realistic parameters an attempt will not be made to study qualitatively the occurrence of this Mode relative to that of Mode Y1 or HD; such a task is also not very straightforward. It may, however, be pertinent to remark that though Mode X1 (\( \theta, \phi \) even) can be regarded as an extension of Mode H1 (\( \theta \) even), the \( \phi \) 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 Y1 (with odd \( \phi \)) 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 X1 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 X1, 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 \( \phi_0 \) or \( K_3 \), HD has higher free energy than (5). This fact has to be kept in mind as the Mode X1 threshold has been compared with \( H_{22} \) in regions of high \( \phi_0 \) or \( K_3 \) where Mode X1 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 Y1 PD is favourable over almost
the entire range of twist angles. However, a model study, made by varying $K_1$, $K_3$ and $\phi_0$, has shown that while Mode $Y_1$ is certainly favourable in the range of small $\phi_0$ and $K_3$, Mode $X_1$ may dominate when $\phi_0$ is large and $K_3$ sufficiently smaller than $K_1$. 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 $\phi$ which is odd wrt the sample centre like the original antisymmetric twist in $n_0$. Mode $X_1$ PD which has a symmetric twist fluctuation occurs generally with a relatively high threshold and large domain sizes. 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 $\phi_0$ is enhanced, $n_0$ ($z = \pm h$) rotate in opposite directions leaving $n_0$ ($z = 0$) 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 $n_0$ at $z = - h$ were fixed along $(1, 0, 0)$ and $n_0$ 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 $\phi_0$) 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 $\phi_0$ 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 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, $B_\theta \sin^2 \theta - B_\theta \theta^2$ 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 $t = \cos T z, \sin T z, 0$; $T h = \phi_L$; $\phi_L + (B_\phi h/2 K_2) \sin (2 \phi_L - 2 \phi_0) = 0 \ldots$ (15)

where $B_\phi$ is the anchoring strength for twist. To study PD in the context of weak director anchoring, perturbations have to be imposed on $n_0$ given in (15); this will be treated elsewhere.

From the point of view of an experiment the effect of an electric field $E$ 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 $E$ 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 $E'$ as new infinitesimal variables. Thus the picture is not merely an extension of the case of $H$ by a replacement of $\chi_s$ by $\epsilon_s/4 \pi$, for it is no longer possible to factor out $\epsilon_s$; as the individual dielectric susceptibilities $\epsilon_1$ and $\epsilon_2$ enter the picture it is necessary to study the effect of varying an additional parameter such as the ratio $\epsilon_1/\epsilon_2$. The Maxwell equations, which provide relations between director fluctuations and $E'$, 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 \( n_0 = (1, 0, 0) \). 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 \( n_0 \) destroys the symmetry transformation. A field \( H_y \) annihilates the uniformity of twist in \( n_0 \) and this happens without a threshold; the director field will then be given by \( n_0 = (\cos \varphi, \sin \varphi, 0) \) where \( \varphi \) 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 \( H_y \).

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References