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Stability of the periodic deformations in planar nematic layers

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The periodic deformations induced by external fields have been analysed by means of the Taylor expansion method based on the theorems of catastrophe theory. The analysis is restricted to the planar nematic slab influenced by a magnetic field. Two different configurations of the field which lead to periodic deformations with prevailing splay or twist we considered. The ranges of material constants at which the periodic state is stable and the threshold magnetic field strength have been found. The problem of transitions between the undeformed, uniformly deformed and periodic states is discussed.

1. Introduction

The periodic distortions induced by external fields in nematic liquid crystal layers are an interesting alternative to the uniform deformations of the Freedericksz type usually found. They have been observed experimentally in various geometries [1–4] and analysed in several theoretical works [4–13]. Generally, they can be expected in materials with great elastic anisotropy, for example in liquid-crystalline polymers. The linearized Euler–Lagrange equations have been used to analyse these problems. In this paper, planar nematic layers subjected to a magnetic field are considered. Two directions of the field are used: normal to the layer and parallel to the layer but normal to the initial director orientation. The method employed is based on a Taylor expansion of the free energy G of the layer, truncated according to the rules which stem from catastrophe theory [14]; this approach yields qualitative information. The number of equilibrium states of the system and their disposition is revealed. The same method was applied earlier to the effects of the external fields on liquid crystals, for instance [15, 16]. Therefore it will only be briefly sketched in the next section; the results agree with other works. Some new details concerning the stability of the periodic deformations are found. They are presented in section 3, and discussed in section 4.

2. Method

The idea of the method applied here is as follows. The free energy of the layer, G is expressed as a function of the angles, which are sufficient for the qualitative determination of the director distribution. The degenerate critical point of G is found and, in its vicinity, G is reduced to the catastrophe, i.e. to the topologically equivalent function of a standard form. The catastrophe yields a qualitative picture of the behaviour of the system at small deformations, since it gives the number and disposition of the equilibrium states of the system in the neighbourhood of its critical points. The procedure used for the determination of a suitable catastrophe includes an expansion in a Taylor series in the neighbourhood of the chosen critical point, the elimination of the inessential variables and limitation of the resulting power series to the order necessary for a proper description of the system.

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It is assumed that the nematic material, characterized by elastic constants k_{11}, k_{22} and k_{33}, and positive diamagnetic anisotropy $\Delta\chi$, is confined between two plates placed parallel to the (xy) plane at $z=\pm d/2$. The director is aligned along y. Strong surface anchoring is assumed. The magnetic field of strength B is used for the sake of simplicity. Two configurations are considered:

(i) $\mathbf{B}\|z$, when the periodic distortion with prevailing splay occurs,
(ii) $\mathbf{B}\|x$, when twist is predominant in the periodic distortion.

The director orientation within the layer is determined by two angles: θ, between the director and its projection onto the (xy) plane, and ω, between this projection and the y axis. The director components are $n_x=\cos\theta\sin\omega$, $n_y=\cos\theta\cos\omega$ and $n_z=\sin\theta$. They are assumed to depend on z and to vary periodically along x. This is justified by the experimental results and allows us to avoid complications which arise when a generalized case of arbitrary patterns direction is taken into account. The free energy density of the layer is

$$\begin{aligned} g=&(1/2)(k_{11}[\sin\theta\sin\omega(\partial\theta/\partial x)+\cos\theta\cos\omega(\partial\omega/\partial x)-\cos\theta(\partial\theta/\partial z)]^2\\ &+k_{22}[\cos\theta^2(\partial\omega/\partial z)+\cos\omega(\partial\theta/\partial x)-\sin\theta\cos\theta\sin\omega(\partial\omega/\partial x)]^2\\ &+k_{33}\{[-\cos\theta\cos\omega(\sin\theta\cos\omega(\partial\theta/\partial x)+\sin\omega\cos\theta(\partial\omega/\partial x))\\ &-\sin\theta(-\sin\theta\sin\omega(\partial\theta/\partial z)+\cos\theta\cos\omega/\partial z)\\ &-\cos\theta(\partial\theta/\partial x))]^2\\ &+[-\sin\theta(\sin\theta\cos\omega(\partial\theta/\partial z)+\sin\omega\cos\theta(\partial\omega/\partial z))\\ &-\cos\theta\sin\omega(\sin\theta\cos\omega(\partial\theta/\partial x)+\sin\omega\cos\theta(\partial\omega/\partial x))]^2\\ &+[\cos\theta\sin\theta(\partial\theta/\partial z)+\cos\theta^2\sin\omega(\partial\theta/\partial x)]^2\})\\ &+g_{\text{magnetic}}. \end{aligned} \tag{1}$$

The two configurations of the magnetic field are related with two different components of the free energy density

$$g_{\text{magnetic}}=-(1/2)\Delta\chi B^2\sin^2\theta \tag{2}$$

for case 1, and

$$g_{\text{magnetic}}=-(1/2)\Delta\chi B^2\cos^2\theta\sin^2\omega \tag{3}$$

for case 2.

If small deformations are assumed, then the functions $\theta(xz)$ and $\omega(xz)$ can be approximated by appropriate trial functions. According to the discussion given in [10], they should vary periodically in the x direction but should be shifted in phase by $\pi/2$. The adopted functions

$$\theta(xz)=\xi f(z)\cos(qx/d), \tag{4}$$

$$\omega(xz)=\psi g(z)\sin(qx/d), \tag{5}$$

where ξ and ψ are the amplitudes of the deformations, possess all of the essential topological features of the real director distribution. The functions $f(z)$ and $g(z)$ describe the dependence of the corresponding angles on z. Their forms were also discussed in [10] and are given further by equations (13), (14), and (23), (24). The dimensionless wavevector is defined as

$$q-2\pi d/\Lambda=\pi d/\lambda, \tag{6}$$

where Λ is the spatial period of the deformed structure. The stationary states of the deformed layer in an external field can be found by minimization of the catastrophe function, equivalent to the total free energy per unit area of the layer with respect to ξ, ψ, and q. In order to calculate $G(\xi\psi q)$, the energy density g is expanded in a Taylor series in powers of ξ and ψ in the vicinity of the undeformed state ($\xi=0$, $\psi=0$), and then integrated

$$G=\frac{1}{\lambda}\int_0^{\lambda}\int_{-d/2}^{d/2} g\,dx\,dz. \tag{7}$$

The resulting series can be expressed as

$$G=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_{ij}\xi^i\psi^j \tag{8}$$

or in the form giving explicitly the dependence on q

$$G=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} b_{ijk}\xi^i\psi^j q^k, \tag{9}$$

which stems from equation (8), since some of the coefficients a_{ij} can be written as a sum of two parts

$$a_{ij}=b_{ij0}+b_{ijk}q^k. \tag{10}$$

It follows from formula (1) that $k\leqslant 2$. The undeformed state ($\xi=0$, $\psi=0$) is a critical point of G for arbitrary q since $\partial G/\partial\xi=\partial G/\partial\psi=0$ at this point. It is also evident that $G(\xi=0, \psi=0, q)=0$ for every q and for arbitrary values of the parameters h, k_b and k_t. This means that there is no point to take q as a variable during the determination of the catastrophe type and only ξ and ψ need be considered. The free energy of the states predicted by the catastrophe should be a minimum with respect to q. To assure this, the function $q(\xi, \psi)$ is determined by means of the minimization condition $\partial G/\partial q=0$

$$q=-\frac{1}{2}\frac{\sum_i\sum_j b_{ij1}\xi^i\psi^j}{\sum_l\sum_m b_{lm2}\xi^l\psi^m} \tag{11}$$

and substituted into equation (9). The resulting function $G(\xi, \psi)$ can be expressed as the power series in which q does not appear explicitly and $i+j$ takes only even values

$$G=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} c_{ij}\xi^i\psi^j. \tag{12}$$

The limiting value of q,

$$q_0=\lim_{\xi\to 0,\psi\to 0} q,$$

is required for the expansion. It can be obtained from the set of equations which arise when two of the minimization conditions are considered in the limit $\xi\to 0$, $\psi\to 0$. Further procedures will be described separately for each geometry in the next section.

3. Results

3.1. B||z

In this case the function $f(z)$ should be even and the function $g(z)$ odd [10]. They are approximated by

$$f(z)=\cos(\pi z/d), \tag{13}$$

$$g(z)=\sin(2\pi z/d). \tag{14}$$

The coefficients of the initial expansion (9) which are important in further calculations are

$$\left.\begin{aligned}
b_{200}&=(k_{11}\pi^2/8d)(1-h),\\
b_{111}&=(2k_{11}/3d)(1-k_t),\\
b_{020}&=(k_{11}\pi^2/2d)k_t,\\
b_{400}&=(3k_{11}\pi^2/128d)(k_b-1+h),\\
b_{220}&=(k_{11}\pi^2/16d)(k_b-2k_t),\\
b_{202}&=(k_{11}/8d)k_t,\\
b_{022}&=k_{11}/8d,\\
b_{040}&=0,\\
b_{311}&=(k_{11}/15d)(k_b-4+3k_t),\\
b_{131}&=(2k_{11}/105d)(2k_b-3+k_t),\\
b_{222}&=(k_{11}/128d)(6k_b-16-k_t),\\
b_{042}&=(3k_{11}/128d)(k_b-1).
\end{aligned}\right\} \tag{15}$$

The reduced quantities $h=B^2d^2\Delta\chi/\pi^2k_{11}$, $k_b=k_{33}/k_{11}$ and $k_t=k_{22}/k_{11}$ have been introduced in these formulae. The minimization conditions $\partial G/\partial q=0$ and $\partial G/\partial\psi=0$ considered in the limit $\xi\to0$, $\psi\to0$, give two solutions for q_0.

3.1.1. *Uniform deformation*, $q_0=0$

In this case G can be expressed by the series which contains only the coefficients b_{ij0}.

$$G=b_{200}\xi^2+b_{020}\psi^2+b_{400}\xi^4+b_{220}\xi^2\psi^2+\dots. \tag{16}$$

Since b_{020} is never zero, whereas $b_{200}=0$ for $h=1$, the essential variable is ξ. Since $b_{400}\neq0$ at $h=1$ for any acceptable k_b and k_t, the cusp catastrophe arises [14]. The minimization gives the undeformed state $\xi=0$, $\psi=0$ for $h<1$ and a uniformly deformed state $\xi=\pm(-b_{200}/2b_{400})^{1/2}$, $\psi=0$, for $h>1$. The typical $\xi(h)$ dependence is illustrated in figure 1.

3.1.2. *Periodic deformations*

The non-zero value of the initial wavevector

$$q_0=2\pi\{[4-(4+3\pi)k_t]/3\pi\}^{1/2} \tag{17}$$

exists only for sufficiently low twist to splay elastic constant ratio

$$k_t<4/(3\pi+4)=k_{t1}. \tag{18}$$

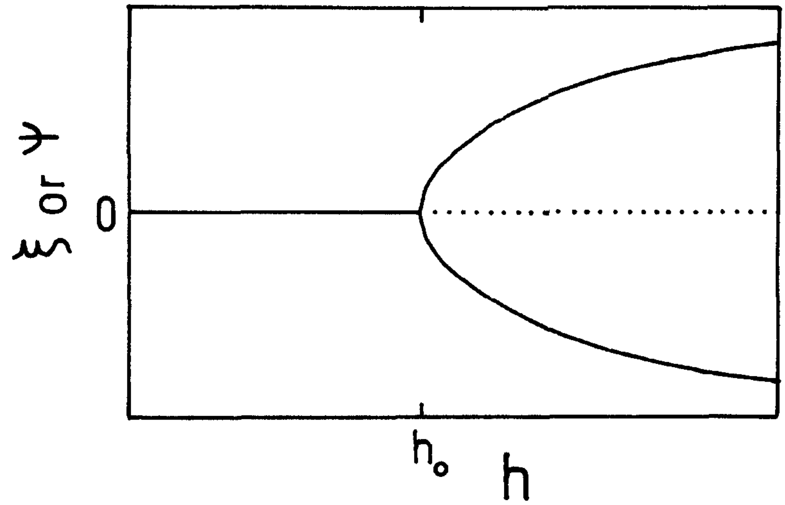

Figure 1. The typical shape of the $\xi(h)$ or $\psi(h)$ functions corresponding to the states of the layer predicted by the cusp catastrophe. h_0 is the threshold field; the full line shows the minima of G and the dotted line the other extremes.

This limit takes the value of 0·298; this is close to 0·303 which was obtained in earlier works [4, 7]. The power series has the form in equation (12) where the coefficients c_{ij} are combinations of b_{ijk}. The determinant of the second derivative matrix vanishes for suitable choice of parameters

$$4c_{20}c_{02}-c_{11}^2=0, \tag{19}$$

where

$$c_{20}=b_{200}+b_{202}q_0^2, \quad c_{02}=b_{020}+b_{022}q_0^2, \quad c_{11}=b_{111}q_0.$$

This determines the threshold magnetic field h_c

$$h_c=1-4\{[4-(4+3\pi)k_t]/3\pi\}^2 \tag{20}$$

or

$$h_c=1-4(q_0/2\pi)^4. \tag{21}$$

It does not depend on k_b and is less than 1. This means that periodic deformations occur instead of a uniform deformation. The series can be reduced to the catastrophe after the normalisation procedure by means of a suitable change of variables [14]

$$G=d_{20}u^2+d_{02}\omega^2+d_{40}u^4+\dots . \tag{22}$$

The calculations must be performed numerically because of the complicated analytical form of the resulting expressions; it is useless to give them explicitly. As previously, only the fourth degree terms must be retained to give rise to the cusp catastrophe. Minimization gives two stable states: $\omega=0$, $u=0$ and $\omega=0$, $u=\pm(-d_{20}/2d_{40})^{1/2}$. The former is due to the undeformed layer and the latter to the periodic distortion. They can be used to determine the values of ξ, ψ and q. The angles ξ and ψ arise continuously as shown in figure 1. The wavelength of the periodic distortion is finite at the threshold and varies weakly with the field. For $k_t=0{\cdot}25$ the initial value of the wavelength Λ is about $4d$.

Periodic deformations exist for some particular ranges of h, k_b and k_t. This is illustrated in figure 2, in the coordinates (h, k_t), where the regions corresponding to the undeformed (I), uniformly deformed (II) and periodically deformed (III) states are distinguished for various k_b. The curve separating (I) and (III) results from equation (20). The boundary between regions due to (II) and (III) is determined by the equality of the free energies of the layer in both states.

3.2. **B**||**x**

In this case the symmetry of the functions $f(z)$ and $g(z)$ is interchanged [10]

$$f(z) = \sin(2\pi z/d), \tag{23}$$

$$g(z) = \cos(\pi z/d). \tag{24}$$

The coefficients of the expansion (9) which are important in further calculations are

$$\left.\begin{aligned}
b_{200} &= k_{11}\pi^2/2d,\\
b_{111} &= (2k_{11}/3d)(1-k_t),\\
b_{020} &= (k_{11}\pi^2/8d)(k_t-h),\\
b_{400} &= (3k_{11}\pi^2/32d)(k_b-1),\\
b_{220} &= (k_{11}\pi^2/64d)(k_b-2k_t),\\
b_{202} &= (k_{11}/8d)k_t,\\
b_{022} &= k_{11}/8d,\\
b_{040} &= (3k_{11}\pi^2/128d)h,\\
b_{311} &= (4k_{11}/105d)(4-k_b-3k_t),\\
b_{131} &= (k_{11}/30d)(3-2k_b-k_t),\\
b_{222} &= (k_{11}/128d)(6k_b-16-k_t),\\
b_{042} &= (3k_{11}/128d)(k_b-1).
\end{aligned}\right\} \tag{25}$$

Two minimisation conditions $\partial G/\partial q=0$ and $\partial G/\partial\xi=0$ are taken in the limit $\xi\to0$, $\psi\to0$, to give two solutions for q_0.

3.2.1. *Uniform deformations*, $q_0=0$

The resulting power series (9) contains only the coefficients b_{ij0};

$$G = b_{200}\xi^2 + b_{020}\psi^2 + b_{040}\psi^4 + b_{400}\xi^4 + b_{220}\xi^2\psi^2 + \dots. \tag{26}$$

It is equivalent to the cusp catastrophe with the essential variable ψ. The undeformed state $\xi=0$, $\psi=0$ is stable for $h<k_t$ and the uniformly deformed state $\psi=\pm(-b_{020}/2b_{040})^{1/2}$, $\xi=0$, for $h>k_t$.

3.2.2. *Periodic deformations*

These deformations arise with the initial wavevector value

$$q_0 = 2\pi\{[4(k_t-1)-3\pi]/3\pi k_t\}^{1/2}. \tag{27}$$

This is possible only for

$$k_t > (3\pi+4)/4 = k_{t2}. \tag{28}$$

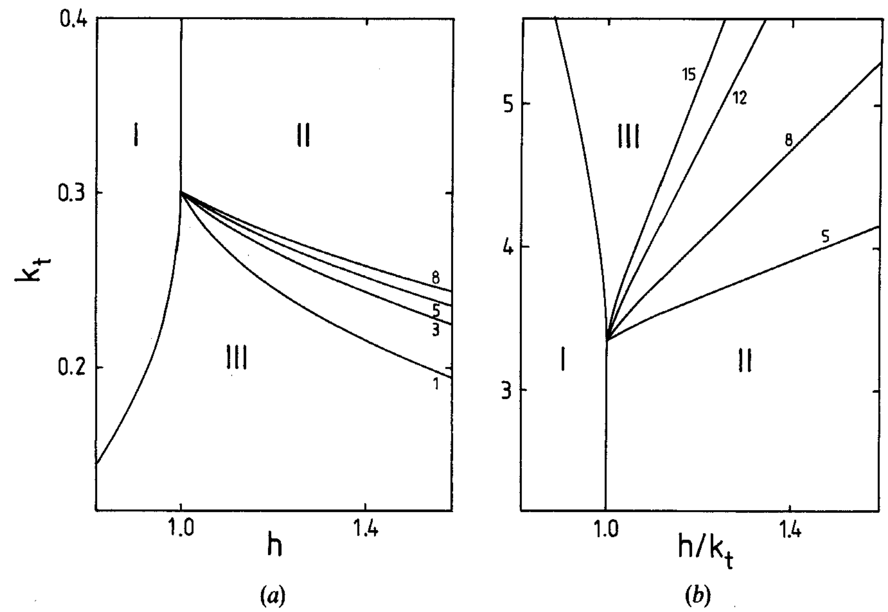

Figure 2. The phase diagram showing existence of the stable states of the layer. I, undeformed state; II, uniformly distorted state; III, periodically deformed state. Four boundary lines between II and III are given for various values of k_b as indicated. (*a*) **B**||**z**, (*b*) **B**||**x**.

The relation $k_{t2}=1/k_{t1}$ and the value $k_{t2}=3{\cdot}356$ agree with earlier work [4, 7]. The threshold field h_c obtained from an analogous equation to (19) is lower than k_t and does not depend on k_b

$$h_c=k_t(1-4\{[4(1-k_t)+3\pi]/3\pi k_t\}^2). \tag{29}$$

It can be expressed in a form similar to equation (21)

$$h_c/k_t=1-4(q_0/2\pi)^4, \tag{30}$$

where q_0 is given by equation (27). As before the cusp catastrophe arises and similar results are obtained. The region of existence of the periodic distortion is shown in figure 2 in coordinates $(h/k_t, k_t)$. The boundaries between various regions are determined in the same way as before. The initial value of the wavelength Λ is about $4d$ for $k_t=4$. Equation (27) can be transformed into equation (17) when the substitution $k_t \to 1/k_t$ is made; the same holds for equations (30) and (20).

4. Discussion

The periodic distortions induced by a magnetic field in a planar nematic slab have been considered in two configurations. Due to the qualitative character of the method applied, the numerical results are only approximate but acceptable in the vicinity of the critical point. The discrepancies arise from the adoption of the functions (13), (14) or (23), (24) and from neglecting the higher order terms in the Taylor expansion. However, the qualitative features are predicted correctly. The typical behaviour is presented in figure 1. The diagrams in figure 2 show the ranges of parameters for which periodic deformations occur. Two characteristic limiting values k_{t1} and $k_{t2}=1/k_{t1}$ agree with earlier results. The threshold field for the perodic deformations is well approximated. The deformations arise continuously when the field increases. The shape of the phase diagrams agrees with that predicted in [13] containing the Lifschitz point. In both cases the right boundary due to the transition between uniform and periodic distortions was predicted to occur when the free energies of the layer are equal in the neigbouring states. This approach is justified in many thermodynamic systems where the fluctuations play a role. Liquid crystal layers belong to mechanical systems which obey the perfect delay convention. They remain in one equilibrium state as long as it exists. Applying this rule to the present case shows that the periodic deformations should be stable with increasing field.

The elastic constant ratios which are used in the computations have moderate magnitudes. The values of d_{40} or d_{04} are positive, i.e. the system is described by the cusp catastrophe. The coefficients d_{40} or d_{04} can be taken to be zero at the threshold field only for some combinations of extreme values of k_b and k_t. In such a case the sixth degree of the Taylor expansion would be necessary. The butterfly catastrophe would arise and the transition between states (I) and (III) could be first order. Since such material constants do not seem to be plausible and since the corresponding calculations are rather laborious, the cusp catastrophe is adopted as sufficient. For reasons of simplicity the full form of the catastrophe function is not considered, i.e. the effects which could lead to the odd terms are not taken into account.

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