Periodic Fréedericksz transition for nematic-liquid-crystal cells with weak anchoring

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(Received 18 June 1986)

Lonberg and Meyer [Phys. Rev. Lett. 55, 718 (1985)] have recently discovered in polymer nematics the existence of a critical value $r_c = 0.303$ for the ratio $r = K_2/K_1$ between the twist and splay Frank elastic constants, below which a periodic splay-twist distortion is energetically favored with respect to the well-known aperiodic splay distortion which appears in a Fréedericksz transition. In this paper the effect of weak-anchoring conditions on the critical r value and on the other parameters of interest is theoretically investigated. Analytical expressions between these parameters are given. It is shown that the periodic transition is not allowed in the range $0.5 < r < 2$. Outside this range either the periodic or aperiodic transition appears, according to the surface treatment, the sample thickness, and the direction of the magnetic field. Hence the critical value of r can be controlled in a wide range.

I. INTRODUCTION

One of the most interesting effects in the physics of nematic liquid crystals, from both the fundamental and practical points of view, is the Fréedericksz transition.[1] As is well known, it is a kind of second-order phase transition from a static uniform director configuration to a distorted one, under the action of an external magnetic (or electric) field. The most interesting cases are those where the initial distortion is pure splay, pure twist, or pure bend. In these cases the critical field depends only on one of the three elastic constants K_1, K_2, and K_3.

In Fig. 1 the distorted director configurations are shown, in the case of initially pure-splay transition. In the distorted configuration the (x,y) plane is no longer a symmetry plane of the system, and two equivalent mirror-symmetric distortions may exist. The maximum distortion angle θ_0 plays the role of an order parameter, which continuously decreases by decreasing the field, going to zero for $H \to H_c$, where H_c is the critical field. Recently, the existence of a new form of transition has been found by Lonberg and Meyer,[2] where other symmetry elements are broken. In particular, the full translational symmetry along the y axis is substituted by a periodic one, in which the angle θ_0 is a harmonic function of y. In this distorted configuration the director is no longer parallel to the (x,z) plane, and its orientation depends on the y and z coordinates. Since it is a periodic function of y, a new order parameter is present, the wave vector q associated with the periodicity along y.

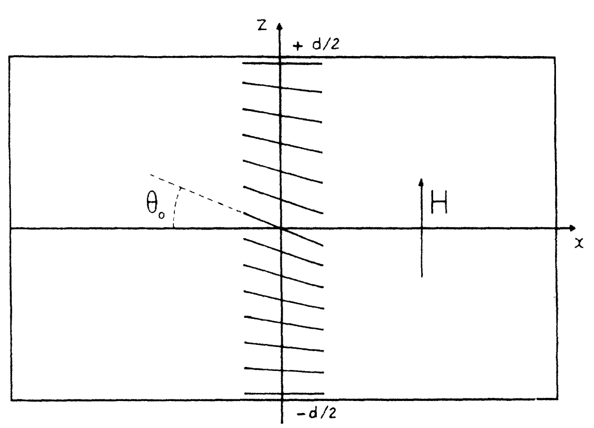

FIG. 1. Director configuration in the case of pure-splay Fréedericksz transition.

This configuration has been theoretically studied in Ref. 2 only in the limit of small distortions, i.e., for the value 0^+ of the previous order parameter. In this case it is found that a new kind of second-order phase transition exists between the periodic and the aperiodic distortion. In fact, the latter deformation is simply the limit for $q \to 0$ of the periodic one. In the case of strong-anchoring conditions (and within the limits of small distortion amplitudes) this transition is only controlled by the ratio $r = K_2/K_1$, since the distortion is splay and twist. The critical value of this parameter is found to be, according to a numerical computation, $r_c = 0.303$. In a very recent paper[3] the analysis given by Lonberg and Meyer is extended to the case of oblique director orientation and oblique magnetic field. The periodic distortion is of great interest from both theoretical physics and practical application. The former comes from the discovery of a new critical parameter. From this point of view, our analysis, considering a weak-anchoring situation, is particularly devoted to the relation between the parameters of interest in the proximity of the critical point and to the possible dependence of the critical value r_c on the anchoring constants.

The practical interest, potentially very great, seems to be limited by two facts.

(a) The first is related to the quite low value of the critical parameter r_c, and to the difficulty of controlling this parameter. As long as strong-anchoring conditions are imposed, r_c may only be changed (for a given nematic) by temperature control.

(b) The second is related to the response time for the occurrence of the periodic configuration that has been found to be very long (on the order of an hour, see Lonberg and Meyer). Further, the spatial periodicity seems to be be quite irregular. The possibility of reducing the response time and of obtaining a regular pattern is under study.

In this paper the point (a), and in particular the dependence of r_c on the anchoring conditions, is considered. In fact, it is evident that r_c must depend on the anchoring forces, and more specifically on the ratios between the extrapolation lengths and the sample thickness. At least in principle, this could provide a simple way of controlling the critical r_c value and the pitch $2\pi/q$ of the periodic patterns.

Some of the results presented in this paper, and more precisely Eqs. (16) and (19) of Sec. V, have already been published previously,[4] without demonstration. Here a more complete analysis of the problem is given.

II. PHYSICAL MODEL AND EQUATION SYSTEM

A nematic slab between plane-parallel walls of area S at $z=\pm d/2$ is considered, in the limit $S\rightarrow\infty$. The director is parallel to the x axis in the undistorted configuration (planar homogeneous alignment), while in the distorted one it makes angles θ_1 and θ_2 with the (x,y) and the (x,z) planes, respectively. Rotations of the director in correspondence to the surfaces of the sample are allowed. It is assumed that the restoring torque at a surface point only depends on the angles θ_1 and θ_2 at this point, and is equal to $(-w_1\theta_1-w_2\theta_2)$, where w_1 and w_2 are the anchoring constants for deformations of splay and twist, respectively. In the distorted configuration θ_1 and θ_2 only depend on the coordinates (y,z). An x dependence, which implies bend distortion, is possible but is not considered here. The initial form of the distortion is evaluated by use of linearized equations, and more precisely by assuming that the free-energy expression is given by

$$F=\tfrac{1}{2}\int dx\int dy\int_{-d/2}^{d/2}[K_1(\theta_{2,y}+\theta_{1,z})^2+K_2(\theta_{2,z}-\theta_{1,y})^2-\chi_a H^2\theta_1^2]$$
$$+\tfrac{1}{2}\int dx\int dy[(w_1\theta_1^2+w_2\theta_2^2)_{z=-d/2}+(w_1\theta_1^2+w_2\theta_2^2)_{z=d/2}]\ , \qquad (1)$$

where $\chi_a=\chi_{\parallel}-\chi_{\perp}$ is the magnetic anisotropy, which in the following is assumed to be positive, and H is the magnetic field, assumed as parallel to the z axis.

In the case of a magnetic field parallel to the y axis the free energy F^* is given by a similar equation, with $-\chi_a H^2\theta_2^2$ instead of $-\chi_a H^2\theta_1^2$. One may notice that F and F^* become identical by interchanging θ_1 and $-\theta_2$, K_1 and K_2, and w_1 and w_2. For any director configuration which minimizes F there exists a director configuration which minimizes F^*, and is obtained by rotating H by $\pi/2$ and interchanging the indices of the quantities θ,K,w. This analytically trivial fact is of great practical interest, since values of the parameter r_c giving such periodic distortion are found near a nematic-smectic transition.

The variational problem gives the bulk equations:[5]

$$\begin{aligned}&K_2\theta_{1,yy}+K_1\theta_{1,zz}+(K_1-K_2)\theta_{2,yz}+\chi_a H^2\theta_1=0\ ,\\&K_1\theta_{2,yy}+K_2\theta_{2,zz}+(K_1-K_2)\theta_{1,yz}=0\end{aligned} \qquad (2)$$

and the boundary conditions

$$\begin{aligned}&\pm K_1(\theta_{2,y}+\theta_{1,z})+w_1\theta_1=0\\&\pm K_2(\theta_{2,z}-\theta_{1,y})+w_2\theta_2=0\ ,\end{aligned} \qquad (3)$$

where the signs $+$ and $-$ correspond to $z=+d/2$ and $-d/2$, respectively.

III. APERIODIC SOLUTION

Let us first consider solutions of the type

$$\theta_1=a\cos(q_a z),\ \ \theta_2=0\ . \qquad (4)$$

A solution of this type does exist[6] for a critical field strength

$$H_c=u_c\frac{\pi}{d}\left[\frac{K_1}{\chi_a}\right]^{1/2}, \qquad (5)$$

where u_c satisfies the equation[7]

$$l_1\pi u_c\tan\left[\frac{\pi}{2}u_c\right]=1 \qquad (6)$$

and where l_1 is the reduced extrapolation length for a pure-splay deformation, i.e.,

$$l_1=\frac{1}{d}\frac{K_1}{w_1}\ . \qquad (7)$$

The distortion amplitude a is arbitrary, since linearized equations have been used and q_a is given by

$$q_a=\frac{\pi}{d}u_c\equiv h_c\ , \qquad (8)$$

where h_c is the critical value of the quantity

$$h=H(\chi_a/K_1)^{1/2} \qquad (9)$$

which gives a measure of the magnetic field, and has the meaning of an inverse magnetic coherence length. As is well known, aperiodic distortions are found for any $H>H_c$, but are not given by the approximated equations (2) and (3). In Sec. IV we consider periodic solutions of the type given in Ref. 2. We stress the fact that in both cases the linearized equations, which come from a free-energy expression where higher-order terms are neglected, only give the initial slope of the distortion.

IV. PERIODIC SOLUTIONS

The procedure used to find more general solutions is the following.

First we search for solutions of the bulk equations (2) of the type

$$\begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix}=\begin{bmatrix}c_1\\ c_2\end{bmatrix}\exp[i(qy+q_0z)]\ . \qquad (10)$$

For any value of q, four solutions are found, with

$$q_0^2=\tfrac{1}{2}h^2-q^2-\tfrac{1}{2}h^2\left[1+4\frac{1-r}{r}q_x^2/h^2\right]^{1/2}, \qquad (11)$$

$$\frac{c_1}{c_2}=-\frac{rq_0^2+q^2}{(1-r)qq_0}=-\frac{(1-r)qq_0}{rq^2+q_0^2-h^2}\ . \qquad (12)$$

The two values of q_0^2 are real and of opposite signs in the whole r interval where a periodic solution exists. The four solutions are therefore given by $\pm q_a$ and $\pm iq_b$, where q_a and q_b are real quantities. A linear superposition of these solutions gives the functions considered in Ref. 2, i.e.,

$$\begin{aligned}\theta_1&=[a_1\cos(q_az)+b_1\cosh(q_bz)]\cos(qy)\ ,\\ \theta_2&=[a_2\sin(q_az)+b_2\sinh(q_bz)]\sin(qy)\ ,\end{aligned} \qquad (13)$$

where b_1/b_2 coincides with the ratio c_1/c_2 given by Eq. (10) (with $q_0=q_b$), and a_1/a_2 coincides with $-c_1/c_2$ (with $q_0=q_a$). A second independent solution is that obtained by interchanging the parity with respect to z of the functions θ_1 and θ_2. It seems evident that the solution given by Eq. (13), where θ_1 is an even function of z, is the one which minimizes the energy of the magnetic field, hence giving a lower critical field.

By inserting Eq. (13) in the boundary conditions (3) one obtains

$$\begin{aligned}&K_1\{q[a_2\sin(q_ad/2)+b_2\sinh(q_bd/2)]-a_1q_a\sin(q_ad/2)+b_1q_b\sinh(q_bd/2)\}+w_1[a_1\cos(q_ad/2)+b_1\cosh(q_bd/2)]=0\ ,\\ &K_2\{a_2q_a\cos(q_ad/2)+b_2q_b\cosh(q_bd/2)+q[a_1\cos(q_ad/2)+b_1\cosh(q_bd/2)]\}+w_2[a_2\sin(q_ad/2)+b_2\sinh(q_bd/2)]=0\ .\end{aligned} \qquad (14)$$

From these equations, together with Eqs. (11) and (12), the ratios between the four parameters a_1,a_2,b_1,b_2 can be calculated and, further, the parameter q can be obtained as a function of the external field H. The latter is considered as an implicit definition of the function $H=H(q)$. The minimum value of the function $H(q)$ is evidently the critical field for the Fréedericksz transition. The corresponding value of q is the initial periodicity.

The curve $H=H(q)$ has indeed an enhanced minimum for small values of $r=K_2/K_1$. By increasing r, the minimum is shifted towards lower q values, and a critical value $r=r_c$ is found, such that for $r\geq r_c$ only the solution with $q=0$ exists. The corresponding field strength is the critical field H_c for the aperiodic distortion. For $r>r_c$ only the aperiodic distortion is allowed. We recall that the corresponding critical field is independent of K_2 and therefore of r.

Equations (13) and (14) have been solved numerically. In Figs. 2–4 the quantities H, q, q_b, q_a, a_1/b_1, a_2/b_1, and a_2/b_2 (corresponding to the initial distortion) are plotted as a function of r for different values of the anchoring constants. These figures remind us of a second-order phase transition, where q plays the role of the order parameter and r the role of the temperature. Figure 2(a) shows that the critical exponent for q is $\frac{1}{2}$.

The same curves show that the critical value strongly depends on the anchoring constants w_1 and w_2, and is an increasing function of the extrapolation length l_2 and a decreasing one of l_1. The practical interest of this fact,

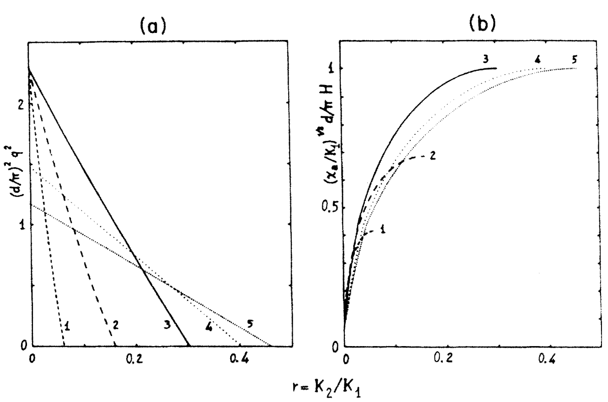

FIG. 2. Computed values of $(qd/\pi)^2$, where q is the in-plane wave vector for the periodic splay-twist deformation [Fig. (2a)], and of the critical field [Fig. (2b)], for different values of the reduced extrapolation lengths: (1) $l_1=1$, $l_2=0$; (2) $l_1=0.25$, $l_2=0$; (3) $l_1=l_2=0$; (4) $l_1=0$, $l_2=0.25$; (5) $l_1=0$, $l_2=1$, where $l_1=K_1/(dw_1)$ and $l_2=K_2/(dw_2)$, and w_1 and w_2 are the anchoring constants for splay and twist deformation, respectively.

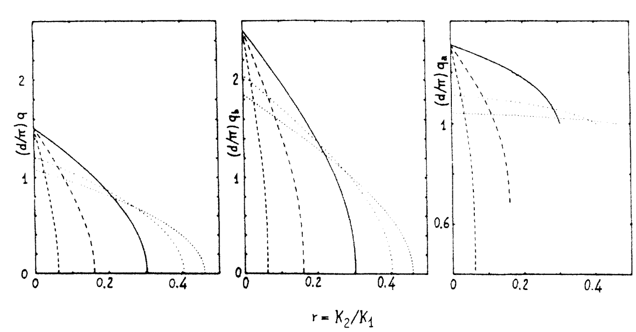

FIG. 3. Plots of the wave vectors q,q_b,q_a in units of π/d for the same values of the anchoring constants reported in Fig. 2.

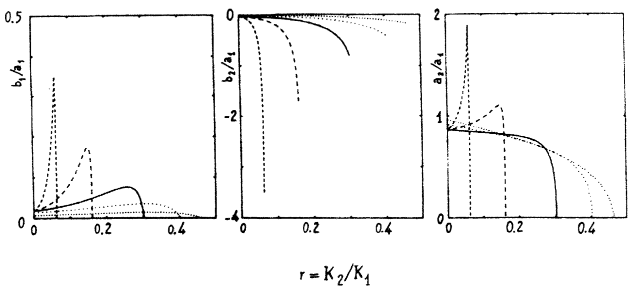

FIG. 4. Plots of the ratios between the amplitudes defined by Eq. (12), for the same values of the anchoring constants as those given in Fig. 2.

and the intrinsic interest of the critical point in any second-order transition, suggests that the dependence of r_c and of the other critical parameters on the anchoring constants should be studied in great detail.

V. ANALYSIS OF THE CRITICAL POINT

In any second-order transition the relation between the various parameters near to the critical point is particularly interesting and simple. In this type of transition, integer or semi-integer exponents are to be expected. In fact, Fig. 2(a) shows that in the limit $r \to r_c$, the quantity $(r_c - r)$ depends quadratically on q, and Fig. 2(b) suggests that $(H_c - H)$ depends quadratically on $(r_c - r)$. Therefore a relation of the type $(H_c - H) \propto q^4$ is expected. This is shown in Fig. 5(a). Figures 5(b) and 5(c) show the q dependence of the quantities q_b and $(q_a - h_c)$. The analytical expressions relating the various parameters may be found by expanding the free energy as a power series of the order parameter q. The calculations are quite long. Here only an expansion up to q^2 of some quantities is given, to obtain the critical value r_c of the ratio $r = K_2/K_1$ as a function of the quantities w_1, w_2, and d. In such an expansion the magnetic field must be considered as a constant and equal to H_c. This gives $h = h_c$, where h_c is defined by Eq. (8). Equations (11) and (12) give

$$q_a = h_c + \frac{1-2r}{2rh_c} q^2 ,\qquad q_b = qr^{-1/2} ; \tag{9'}$$

$$\frac{a_2}{a_1} = \frac{1-r}{r}\frac{q}{h_c} ,\qquad \frac{b_1}{b_2} = (1-r)r^{-1/2}\left[\frac{q}{h_c}\right]^2 . \tag{10'}$$

By inserting Eqs. (9′) and (10′) in the boundary conditions ratio (14), and taking into account the approximated expression

$$\cot(q_a d/2) \simeq \pi l_1 u_c - \frac{1-2r}{\pi r u_c}(qd/2)^2[1+(\pi l_1 u_c)^2] , \tag{15}$$

one obtains a relation between r_c and q, which in the limit $q \to 0$ gives $A/(B - r_c) = (C - r_c)/(D - Er_c)$, i.e.,

$$r_c^2 + (AE - C - B)r_c - (AD - BC) = 0 , \tag{16}$$

where

$$\begin{aligned} A &= u_c^2 \pi (l_2 + \tfrac{1}{2}) , \\ B &= 1 - \pi^2 l_1 u_c^2/2 , \\ C &= 1 + \pi^2 l_1 l_2 u_c^2 , \\ D &= -\frac{\pi}{2} l_1 + \frac{\pi}{4}[1+(\pi l_1 u_c)^2] , \\ E &= \frac{\pi}{2}[1+(\pi l_1 u_c)^2] . \end{aligned} \tag{17}$$

If one of the constants l_1, l_2 is equal to zero, Eq. (16) greatly simplifies, giving

$$r_c^2 + 2Fr_c - F = 0 , \tag{18}$$

where

$$F = \frac{\pi^2}{8}(2l_2 + 1) - 1 \tag{19}$$

for $l_1 = 0$, and

$$F = \frac{\pi^2}{8} u_c^2 [2l_1 + 1 + (\pi l_1 u_c)^2] - 1 \tag{19'}$$

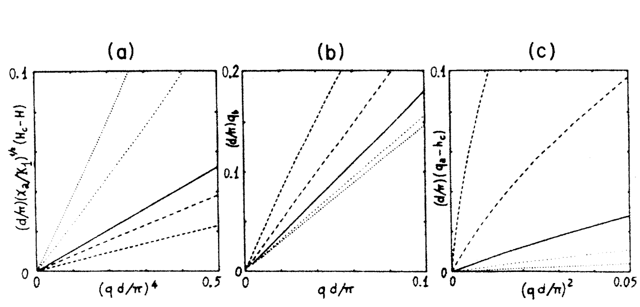

FIG. 5. Plots of the quantities $(H_c - H)(d/\pi)(\chi_a/K_1)^{1/2}$, $(d/\pi)q_a$, and $(d/\pi)(q_b - h_c)$, for the same values of the anchoring constants as those given in Fig. 2.

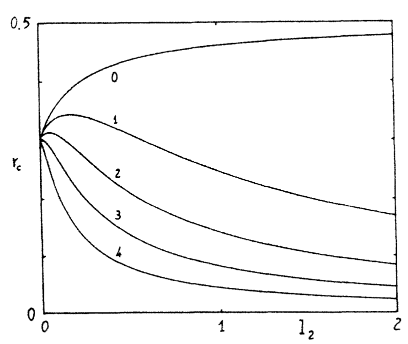

FIG. 6. Plots of the critical values of the ratio $r = K_2/K_1$ as a function of the reduced extrapolation length l_2, for different values of the ratio l_1/l_2: the curves 0, 1, 2, 3, and 4 correspond to $l_1/l_2 = 0$, 0.2, 0.5, 1, and 2, respectively.

for $l_2=0$.

For $l_1=l_2=0$, i.e., in strong-anchoring conditions, one obtains $F=\pi^2/8-1$. This gives

$$r_c=\left[\left(\frac{\pi^2}{8}-1\right)^2+\left(\frac{\pi^2}{8}-1\right)\right]^{1/2}-\left(\frac{\pi^2}{8}-1\right)$$

$$=0.303\,25\ldots .$$

The value is very close to the value $r_c=\frac{1}{3.3}$ given in Ref. 2, which has been obtained by a numerical computation of the distortion. Some plots of r_c versus l_2 for different values of the ratio l_1/l_2 are shown in Fig. 6. They show that r_c may be changed in the range 0—0.5 by suitably controlling the surface conditions and the sample thickness.

VI. CONCLUDING REMARKS

The analysis of Lonberg and Meyer for the Fréedericksz transition giving a periodic twist-splay distortion is extended to the case of weak anchoring, with particular emphasis on the critical value r_c of the ratio r between the Frank twist and splay constants. A simple analytic expression which relates r_c to the anchoring constants and the sample thickness is given. It shows that, at least in principle, r_c may be changed over a wide range by suitable surface treatment of the cell. This fact increases the potential interest of the periodic distortion, since the r_c value corresponding to strong anchoring is not easily obtained with the currently known thermotropic liquid crystals. Although the practical interest of the given analysis is, at present, considerably limited by the fact that no procedures for obtaining reasonably controlled weak anchoring have yet been developed, this problem is under study in many laboratories. It is not unreasonable to hope that it may be solved in the next few years.

Note added in proof. After submission of this paper, a communication was published [W. Zimmermann and L. Kramer, Phys. Rev. Lett. **56**, 2655 (1986)] reporting some results consistent with the present ones, obtained in the particular case $l_1 \ll 1$.

ACKNOWLEDGMENTS

This work was supported by the Ministero della Publica Istruzione of the Italian Government, and by the Italian Consiglio Nazionale delle Ricerche under research contract No. 84.01186.11. C.O. acknowledges support from the Gruppo Nazionale di Struttura della Materia, Consiglio Nazionale delle Ricerche (Unità di Ricerca No. 24).

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