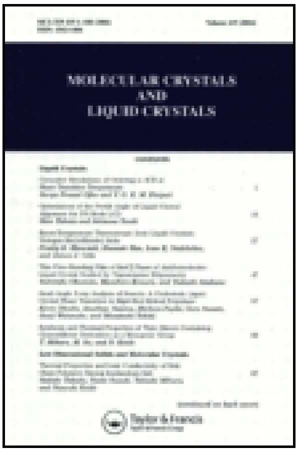

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Freedericksz Transition in a Planar Nematic Cell and the Surfacelike Elastic Constant Problem

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FREEDERICKSZ TRANSITION IN A PLANAR NEMATIC CELL AND THE SURFACELIKE ELASTIC CONSTANT PROBLEM

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Abstract On the basis of local stability analysis we have studied how the splay-bend term, that is known as the K_{13}-term, influences Freedericksz transition in a nematic liquid crystal (NLC) sandwiched between two parallel plates. Two cases are considered: (a) the homeotropic anchoring is favored at both walls and magnetic field is assumed to be parallel to the confining surfaces; (b) the boundary conditions are planar and the magnetic field is normal to the walls. Under certain conditions it is found that the splay-bend term can change the order of the Freedericksz transition. In particular, we encounter the bistability induced by the term.

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INTRODUCTION

In our recent papers[1-3] we have studied how the surface-like elastic terms, known as the K_{24}- and K_{13}-terms, affect stability of the axial director configuration of a nematic liquid crystal (NLC) confined to cylindrical cavity within the approach given in[4].

It was shown that the K_{24}-term plays a significant part in the theory and can be easily incorporated into the framework of the Euler-Lagrange formalism.[5-6]

The latter is not the case as far as the K_{13}-term is concerned. The free energy functional with the K_{13}-term is unbounded from below[4], what accounts for the infinitely strong subsurface director deformations (Oldano-Barbero paradox)[7].

Leaving aside the discussion of different approaches to the problem, we briefly address the theory that will be employed in this paper.

The starting point of the approach under consideration is that the discontinuous behavior of the director field is an artifact of the elastic first-order theory and higher-order terms make the free-energy functional bounded from below. According to [4], the main effect of the higher-order terms can be reduced to the requirement for the director field to be smooth. Roughly speaking, it means that a naive application of the Euler-Lagrange formalism gives the correct recipe. It is supposed that the recipe does not lead to strong subsurface director deformations that are rather difficult to accommodate in the continuum approach. If so, we can get rid of a discontinuity in the surface angle searching for the director distribution minimizing the free-energy functional among the solutions of the Euler-Lagrange equations.

This work is aimed to study influence of the K_{13}-term on the Freedericksz transition in the planar NLC cell. Note that the problem was previously investigated in [8] on the basis of local stability analysis for the homogeneous director state aligned perpendicular to applied magnetic field. The following results have been obtained:

1 If K_{13} falls within the range between $-K_{11}$ and K_{33}, the splay-bend term just shifts the critical field of the Freedericksz transition renormalizing the relevant bulk elastic constants.

2 Otherwise, an anomalously deformed director state is predicted to occur in sufficiently thin layers. The existence of this anomalously deformed regime greatly affects the Freedericksz transition, leading to a rather exotic phase diagram where the applied field alternatively enhances and inhibits distortions. In particular, it was shown that a magnetic field tends to align a nematic, having positive magnetic anisotropy, perpendicular to itself in this case.

Notice that our definition of the K_{13}-term in Eq.(2) is slightly different from that in[8] ($K_{13}/2$ instead of K_{13}).

Some of the above results look very unusual and the idea behind our study is to take into account the fact that the K_{13}-term can result in effects that look like bistability[2,3].

In Sec. 2 local stability of the homeotropic and planar director configurations is investigated taking into consideration the out-of-plane director fluctuations. It is shown that the existence of the anomalously deformed director state is tantamount to the statement that a magnetic field fails to stabilize the director structure aligned along the field direction. It implies the restriction $-K_{11} < K_{13} < K_{33}$, imposed on K_{13}.

In Sec. 3, by using the results of Sec.2, it is found that, under certain conditions, the K_{13}-term leads to the existence of the bistability region where both structures are locally stable. The exact solutions to the Euler-Lagrange equation obtained in the one-constant approximation are exploited to show the K_{13}-term can change the order of the Freedericksz transition.

Discussion of the results is given in Sec. 4.

STABILITY ANALYSIS

Let us consider NLC sandwiched between two identical parallel plates, $z = \frac{d}{2}$ and $z = -\frac{d}{2}$, and suppose that the homeotropic anchoring is favored at both surfaces and the magnetic field is applied along the x-axis, $\mathbf{H} = H\,\mathbf{e}_x$. The anchoring energy density is assumed to be taken in the Rapini-Papoular form [9]:

$$F_S = -\frac{W}{2}(\mathbf{n}\cdot\mathbf{e}_z)^2 \tag{1}$$

where W is the anchoring strength; $\mathbf{e}_z$ is the unit vector directed along the axis of easy orientation (z-axis). As in[8] Eq.(1) suggests no azimuthal anchoring (for more details, see Sec. 4). Note that planar geometry of the Freedericksz transition with the magnetic field applied along the z-axis and the axis of easy orientation parallel to the x-axis will be discussed at the end of this section.

The splay-bend term reads

$$\mathbf{F}_{13} = \frac{K_{13}}{2}\int_V \mathbf{dv}\,\mathrm{div}[\,\mathbf{n}\,\mathrm{div}\,\mathbf{n}\,] \tag{2}$$

where $\mathbf{n}$ is the director field.

Stability Of The Homeotropic Director Configuration

Let us define the NLC director field in terms of two angles, Θ and Φ,

$$\mathbf{n} = \cos\Theta\cdot\cos\Phi\cdot\mathbf{e}_z + \cos\Theta\cdot\sin\Phi\cdot\mathbf{e}_y + \sin\Theta\cdot\mathbf{e}_x \tag{3}$$

so that the homeotropic configuration can be obtained from Eq.(3) by setting $\Theta = \Phi = 0$. Denote small deviations of the angles Θ and Φ from zero by θ and ϕ, respectively. In what follows we shall restrict ourselves to the case of the structures invariant under the translations along the x- and y-axis, so that all the angles are functions of z.

To find out whether the configuration is locally stable or not, one has to derive the second-order variation of free-energy functional, $\delta^2 F$, solve the linearized Euler-Lagrange equations and substitute the solutions into $\delta^2 F$. As a result we have a quadratic form that must be positive definite under the configuration is locally stable.

By making use Eqs.(1, 2) and the standard expression for the bulk free energy[10], the second order variation of the free-energy functional can be obtained as a bilinear part of the energy per unit area in θ and ϕ:

$$F \approx F_h + \delta^2 F = -W + \delta^2 F_\theta + \delta^2 F_\phi \tag{4}$$

$$\delta^2 F_\theta = \frac{K_{33}}{2} \cdot \int_{-\frac{d}{2}}^{\frac{d}{2}} f_\theta \, dz - \frac{K_{13}}{2} \cdot \theta \cdot \theta' \Bigg|_{-\frac{d}{2}}^{\frac{d}{2}} + \frac{W}{2} \cdot \theta^2 \Bigg|_{\pm\frac{d}{2}} \tag{5}$$

$$\delta^2 F_\phi = \frac{K_{33}}{2} \cdot \int_{-\frac{d}{2}}^{\frac{d}{2}} \left(\phi'\right)^2 dz - \frac{K_{13}}{2} \cdot \phi \cdot \phi' \Bigg|_{-\frac{d}{2}}^{\frac{d}{2}} + \frac{W}{2} \cdot \phi^2 \Bigg|_{\pm\frac{d}{2}} \tag{6}$$

where $f_\theta = \left(\theta'\right)^2 - (q_3 \cdot \theta)^2$, $q_i^2 = \dfrac{\chi_a H^2}{K_{ii}}$ and F_h is energy of the homeotropic director configuration. It is straightforward to solve the linearized Euler-Lagrange equations and to insert the solutions in Eqs.(5, 6). As a result we come to the stability conditions that ensure the positive definiteness of $\delta^2 F$ (local stability):

$$\begin{cases} Wd \sin^2 u_3 + (K_{33} - K_{13}) u_3 \sin 2u_3 > 0 & (7) \\ Wd \cos^2 u_3 - (K_{33} - K_{13}) u_3 \sin 2u_3 > 0 & (8) \\ Wd + 2(K_{33} - K_{13}) > 0 & (9) \end{cases}$$

Eqs.(7, 8) are identical to those given in[8] and come from $\delta^2 F_\theta$. Eq.(9) provides stability of the structure with respect to fluctuations in the angle Φ. According to[8], violating of this condition leads to the appearance of so-called anomalously deformed director state which loses its stability after magnetic field exceeded its critical value determined from Eq.(7). But, as it can be seen from Eq.(9), the homeotropic configuration is absolutely unstable in this case. The reason why the case where $K_{13} > K_{33}$ should be eliminated from the consideration will be discussed later.

If $K_{13} < K_{33}$ Eq.(8) gives the equation for the stability threshold (generalized Rapini-Papoular equation):

$$Wd = 2(K_{33} - K_{13})u_k \tan u_k \qquad (10)$$

so that the structure in question is locally stable at $u_3 < u_k$.

Stability Of The Planar Director Configuration

In this subsection we deal with stability of the planar director configuration (NLC molecules are aligned along the magnetic field). Stability analysis requires different parametrization of the director field to start from:

$$\mathbf{n} = \sin\Theta \cdot \cos\Phi \cdot \mathbf{e}_x + \sin\Theta \cdot \sin\Phi \cdot \mathbf{e}_y + \cos\Theta \cdot \mathbf{e}_z \qquad (11)$$

The planar structure is defined by Eq.(11) with $\Theta = \frac{\pi}{2}$ and $\Phi = 0$, so that θ and ϕ now stand for small angle deviations from $\frac{\pi}{2}$ and 0, respectively. In exactly the same manner as for the homeotropic structure we have:

$$F \approx F_p + \delta^2 F = \frac{\chi_a H^2}{2} \cdot d + \delta^2 F_\theta + \delta^2 F_\phi \qquad (12)$$

$$\Delta F = F_p - F_h = 2K_{11}(w - u_1^2)/d \qquad (13)$$

$$\delta^2 F_\phi = \frac{K_{22}}{2} \cdot \int_{-\frac{d}{2}}^{\frac{d}{2}} \left[\left(\phi'\right)^2 + (q_2\phi)^2 \right] dz \qquad (14)$$

$$\delta^2 F_\theta = \frac{K_{11}}{2} \cdot \int_{-\frac{d}{2}}^{\frac{d}{2}} f_\theta \, dz + \frac{K_{13}}{2} \cdot \theta \cdot \theta' \Bigg|_{-\frac{d}{2}}^{\frac{d}{2}} - \frac{W}{2} \cdot \theta^2 \Bigg|_{\pm\frac{d}{2}} \qquad (15)$$

where $f_\theta = \left(\theta'\right)^2 + (q_1 \cdot \theta)^2$, $w = \dfrac{Wd}{2K_{11}}$ and F_p is energy of the planar director configuration. Since $\delta^2 F_\phi$ is positive definite, it is clear that fluctuations in Θ govern stability of the structure. Stability conditions can be written in the form:

$$\begin{cases} -Wd\,\sinh^2 u_1 + (K_{11}+K_{13})\,u_1 \sinh 2u_1 > 0 & (16) \\ -Wd\,\cosh^2 u_1 + (K_{11}+K_{13})\,u_1 \sinh 2u_1 > 0 & (17) \end{cases}$$

In the case of $K_{13} > -K_{11}$, from Eq.(17) we get the equation for the stability threshold:

$$Wd = 2(K_{11}+K_{13})\,u_p \tanh u_p \qquad (18)$$

so that the planar structure is locally stable at $u_1 > u_p$. For $K_{13} < -K_{11}$, the left-hand sides of Eqs.(16, 17) are negative. It follows that a magnetic field fails to stabilize the structure in this case. If one takes the physically reasonable assumption that a sufficiently strong magnetic field makes the NLC molecules aligned along the field direction (magnetic anisotropy is assumed to positive, $\chi_a > 0$) then we have the restriction imposed on K_{13}. Stability analysis for the Freedericksz transition in planar geometry can be made in the same fashion and the stability conditions for the planar and homeotropic director configurations can be derived from Eqs.(7, 8) and Eqs.(16, 17) by making the substitution: $K_{11} \leftrightarrow K_{33}$, $K_{13} \to -K_{13}$. Clearly, we have another restriction imposed on K_{13}. In summary, we can say that K_{13} must be within the range between $-K_{11}$ and K_{33}.

BISTABILITY INDUCED BY THE SPLAY-BEND TERM

Throughout this section we suppose that $-K_{11} < K_{13} < K_{33}$. Then there are two thresholds, u_h and u_p, that govern local stability of the homeotropic and planar structures (see Eqs.(10, 18)).

The Freedericksz transition under consideration is known to be a second-order transition provided that the K_{13}-term is disregarded (normal regime of the Freedericksz transition). It means that after the homeotropic structure is deformed at $u_3 > u_h$ the director field goes towards the planar configuration as magnetic field increases. Clearly, it implies that u_p is greater than u_h.

It is of interest to consider how the thresholds depend on w at positive K_{13}. The w-dependencies of the thresholds for $K_{13} = 0.8K_{33}$, depicted in Fig.1, suggest that there is a value of w, $w = w_1$, such that $u_p < u_h$ at $w < w_1$. Notice that, in order to facilitate the subsequent discussion, the plots are displayed in the one-constant approximation, $K_{11} = K_{33} = K$, but numerical calculations show that elastic anisotropy does not change the result qualitatively. In other words, we encounter bistability region of the $w - u$ plane where both of the structures are locally stable and a first-order transition can be expected to occur. When K_{13} is negative, we arrive at the same conclusion for the Freedericksz transition in planar geometry.

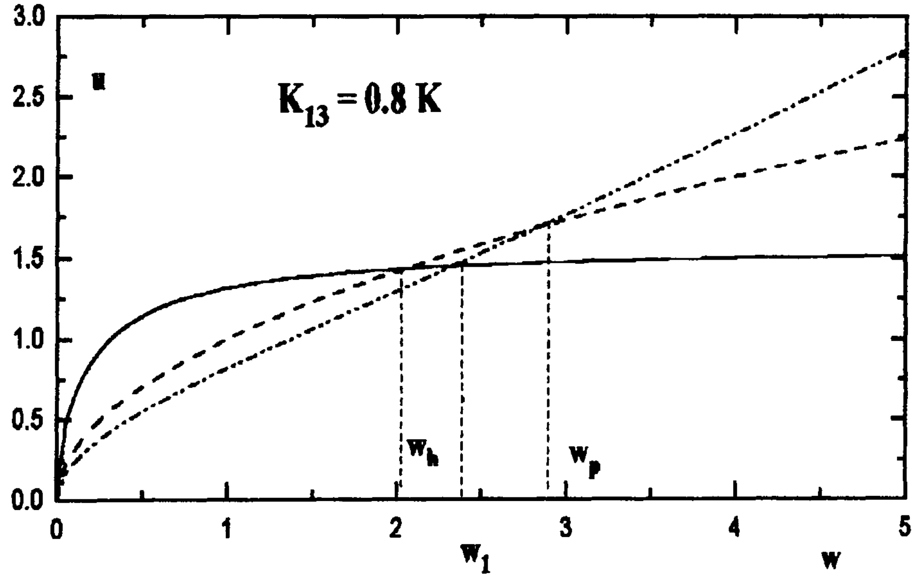

FIG.1 Thresholds u_h (solid line) and u_p (line marked as -..-..-) vs w at $K_{13} = 0.8K$. The homeotropic (planar) configuration is locally stable at $u < u_h$ ($u > u_p$). The planar structure is favorable in energy over the homeotropic one above the line $u = \sqrt{w}$ (dashed line).

Let us make use of some experimentally obtained data to see if the bistability region can be encountered in real systems. Of special interest are the estimates reported in[11], where submicron nematic films were studied to verify the status of the K_{13}-term. Since K_{13} was found to be negative, $K_{13} \approx -0.4K_{11}$, we proceed with the Freedericksz transition in planar geometry assuming the relevant constants take the following values (5CB): $K_{11} = 6.3 \times 10^{-12}$N, $K_{33} = 1.41K_{11}$, $W = 8.3 \times 10^{-6}$J/m^2 and $d = 0.5\mu$m. The dimensionless parameter w then can be estimated at about 0.234 and, as shown in Fig.2, its value is less than $w_1 \approx 1.2$. Thus the bistability region is found to exist under the specified conditions.

To get some idea of what are the director states involved in transition it is instructive to make comparison between its energies based on explicit solutions to the Euler-Lagrange equation within the one-constant approximation $(u_1 = u_3 = u)$.

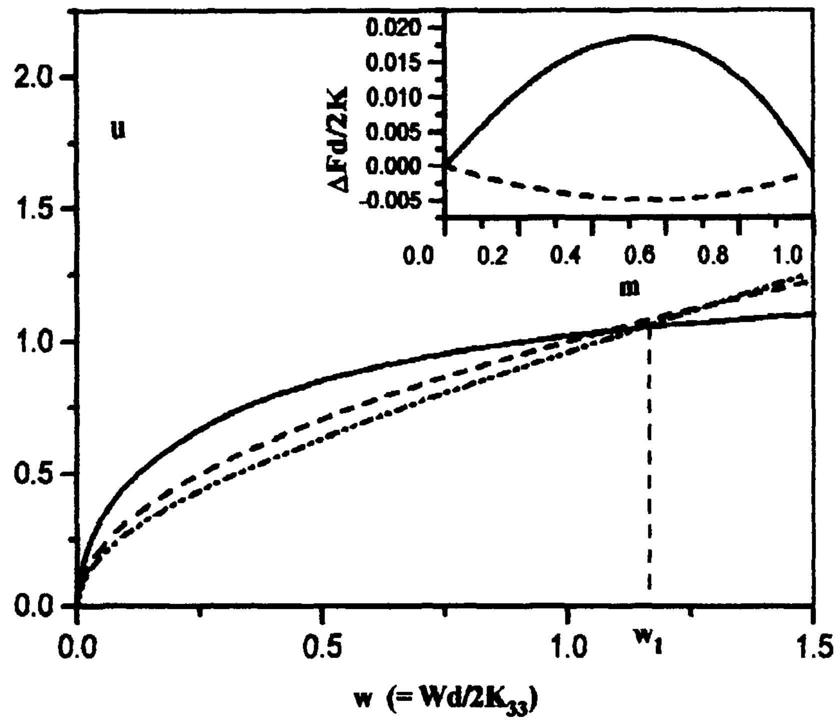

FIG.2 Thresholds u_h (line marked as -..-..-) and u_p (solid line) vs w at $K_{13} = -0.4K_{11}$ and $K_{33} = 1.41K_{11}$. The planar (homeotropic) configuration is locally stable at $u_3 < u_p$ $(u_3 > u_h)$. Above the curve $u = \sqrt{w}$ (dashed line) the homeotropic structure is favorable in energy over the planar director configuration. Right inset: m-dependence of the free energy at $w = 0.234$ and $u = 0.484$ for $K_{13} = -0.4K$ (solid line) and $K_{13} = 0$ (dashed line).

(For brevity, detailed calculations behind the analytical and numerical treatment of this case are omitted.) In the case we are interested in, $|K_{13}| < K$, the angle Φ can be excluded from the consideration and the director field is

$$\mathbf{n} = \cos\Theta(z) \cdot \mathbf{e}_z + \sin\Theta(z) \cdot \mathbf{e}_x \tag{19}$$

In the one-constant approximation the Euler-Lagrange equation can be solved analytically and the solution of interest reads

$$\cos\Theta(z) = \mathrm{dn}(q\,z + K(m)|m) \qquad (20)$$

where $\mathrm{dn}(x|m)$ is a Jacobian elliptic function and $K(m)$ is the complete elliptic integral of the first kind [12]. Notice that $m \in [0;1]$, so that Eq.(20) gives the homeotropic (planar) configuration at $m = 0$ $(m = 1)$. Let us consider the energy of the structure (19, 20) as a function of m at $K_{13} = 0.8K$ for various values of w ($\sim W$) and u ($\sim H$). (It is convenient to count the energy from F_h, $\Delta F(m) = F(m) - F_h$). Referring to Fig.1, it can been seen that, in addition to $w_1 = 2.332$, there are two characteristic values of

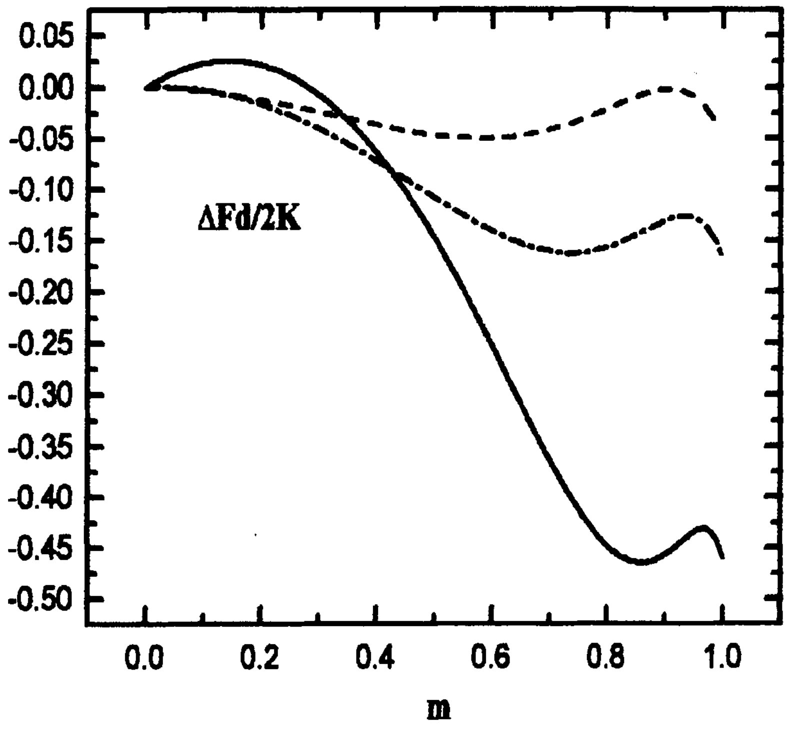

FIG.3 The free energy of the deformed director configuration (20), counted from the homeotropic structure energy, as a function of m at $K_{13} = 0.8K$ for various values of w and u: $w = 3.0$, $u = 1.86$ (solid line); $w = 2.2$, $u = 1.5$ (dashed line); $w = 2.5$, $u = 1.633$ (line marked as -..-..-).

w, $w_k = 2.051$ and $w_p = 2.819$ related to the intersection points of the curve $u = \sqrt{w}$ and the threshold lines.

For small w, $w < w_k$, at $u = \sqrt{w}$ m-dependence of the energy looks like that presented in right inset of Fig.2 (solid line). So we have two structures of the same energy separated by energy barrier. Under the field further increases, the homeotropic structure becomes metastable. Notice that there is no metastable deformed director states in this case.

At $w > w_k$ and $u > u_c$ $\Delta F(m)$ has local minimum within the interval $(0; 1)$. This point represents the deformed director state that can be metastable depending on whether the energy reaches its minimum at the point or not. The plots depicted in Fig.3 show that, even if $w > w_1$, there is a value of u (magnetic field), such that the energies of two structure (the planar structure and the deformed director configuration) are equal.

DISCUSSION

The results given in Sec.3 show the K_{13}-term may change regime of the Freedericksz transition. Under certain conditions the Freedericksz transition is indicated as a first-order transition. It should be emphasized that, as a matter of fact, it does not mean jump-like reorientation of the director in real systems. Study of the reorientation dynamics requires more comprehensive and extended analysis with hydrodynamic motions taken into account. But it seems to be unlikely that the effects of this kind are not detectable. Thus we have the effects to be tested experimentally to verify the status of the K_{13}-term within the theory[4] that have been employed throughout this paper.

Eq.(1) implies no azimuthal anchoring in the system under investigation (substrates are assumed to be isotropic), so that the system is identical with that considered in[8]. It eases a comparison between the results. Note that Eqs.(7, 8) are coincident with the key equations obtained in [8]. On the other hand, azimuthal anchoring can be shown not to change the results of Sec.2 qualitatively.

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