

Spontaneous deformations of the uniform director ground state induced by the surfacelike elastic terms in a thin planar nematic layer

V. M. Pergamenschchik*

Institute of Physics, Prospekt Nauki 46, Kiev 03039, Ukraine

(Received 9 June 1999; revised manuscript received 1 August 1999)

We study the effect of the divergence (surfacelike) K_{24} and K_{13} terms on stability of the uniform ground state of a nematic phase. It is shown that the K_{13} term can effectively boost the action of the K_{24} term. As a result, even if the two Ericksen stability conditions are satisfied, spontaneous deformations can occur in geometries with a sufficiently small volume-to-surface ratio. For a specific example, we show that this mechanism can destabilize the uniform planar director field in a thin nematic layer with planar anchoring and produce spontaneous periodic director modulation. The critical thickness below which the predicted modulated phase occurs is found to be $h_c = -2L_a[1 - (1 - 2K_{24}/K_{11})^2 + K_{13}^*/K_{11}]$, where L_a is the polar anchoring extrapolation length, K_{11} and K_{24} are the standard Nehring-Saupe elastic constants, and K_{13}^* is the effective elastic constant of the layer.

PACS number(s): 61.30.Gd, 64.70.Md

I. INTRODUCTION

The very definition of a liquid crystalline nematic phase involves the idea that in the ground state its vector order parameter \mathbf{n} , called director, is uniform, i.e., $\mathbf{n}(\mathbf{x}) = \text{const}$ [1], [2]. However, the derivation of the deformation free energy (FE) only presupposes that the director deformations associated with its derivatives ∂n are weak [2]. For this reason, the fundamental stability condition of the uniform ground state must follow from the FE itself and can be nontrivial. The nematic deformation FE is of the form [2]

$$F_d = \frac{1}{2} \int dV \left\{ \frac{1}{2} K_{11} (\nabla \cdot \mathbf{n})^2 + \frac{1}{2} K_{22} (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2} K_{33} (\mathbf{n} \times \nabla \times \mathbf{n})^2 - K_{24} \nabla \cdot [\mathbf{n}(\nabla \cdot \mathbf{n}) + \mathbf{n} \times \nabla \times \mathbf{n}] + K_{13} \nabla \cdot [\mathbf{n}(\nabla \cdot \mathbf{n})] \right\}. \quad (1)$$

This expression was derived for a spatially unrestricted body. Recently, it was shown that the FE of a spatially restricted nematic body has exactly the same form but with rescaling of the constants K_{24} and K_{13} [3] (see Sec. II).

In a nematic phase the elastic constants K_{11} , K_{22} , and K_{33} are positive. Then the first three terms are positive definite and thus describe elastic resistance to any director deformation ∂n . To characterize these terms it is sufficient to describe a specific deformation to which each of them resists. As the three positive terms show the FE cost of the splay, twist, and bend deformations, respectively, they are called the splay, twist, and bend terms, respectively. Clearly, in a nematic liquid crystal free of any external torque, the sum of these term that is minimized by a uniform director cannot be a source of spontaneous deformations.

The last two terms in (1) are total divergencies. They are often called surfacelike as their FE can be converted to a surface integral. In contrast to the splay, twist, and bend terms, the divergence K_{13} and K_{24} terms are not positive definite for all values of the constants K_{13} and K_{24} , and, in principle, the FE can be reduced at the expense of their finite contributions. Therefore, the K_{13} and K_{24} terms can be a source of spontaneous deformations. To characterize these terms one has to describe possible patterns of the director field that can be spontaneously induced by this source in different geometries [4]. Ericksen [1] addressed this problem. He pointed out that the uniform director ground state can be unstable if the magnitude of the K_{24} term exceeds the elastic resistance of the positive definite terms. However, in this analysis both anchoring and the K_{13} term were not incorporated in the stability condition. That the K_{24} term can induce a spontaneous pattern formation has been recognized [5,6], and an essential role of the K_{13} term in this pattern formation has been reported [7,8]. Under these conditions it is natural to ask what is a joint effect of both divergence terms and anchoring on the stability of the uniform director ground state in a finite-size body. Addressing this problem one should realize that it cannot be considered in the general form of Ref. [1]. In [1] the analysis was not restricted to a specific geometry of the nematic sample because it reduced to the local condition that the FE density is non-negative in each spatial point. Incorporating anchoring and the K_{13} term makes dealing with an arbitrary geometry practically impossible. Indeed, whereas the volume elasticity gives rise to the bulk torques, the anchoring produces a torque at the nematic surface. Therefore, locally these two torques cannot balance one another, and the stability of the uniform director ground state can be realized only as a global requirement that the sum of the bulk and surface FE of the sample cannot be reduced for finite ∂n . This requirement cannot be derived in general, and the problem reduces to investigating spontaneous pattern formation in different geometries with a specific anchoring potential. Anchoring, which is a major mechanism of aligning the director, is a director-dependent part of the

*Electronic address: pergam@i.kiev.ua

surface tension. The anchoring potential consists of two terms. The first one, called polar anchoring, gives the surface energy as a function of the polar angle θ between the director and surface normal ν , while the second one, called azimuthal anchoring, gives the surface energy as a function of the azimuthal angle ϕ between the director and some preferred direction on the surface.

In this paper we consider stability of the uniform director ground state in a plane layer with planar polar anchoring that favors the surface director to be tangential to the surfaces, and zero azimuthal anchoring on both substrates. On the one hand, this geometry is one of the most widely used in the physics of liquid crystals. On the other hand, in this particular geometry the K_{24} term has the strongest effect [9] while an azimuthal anchoring would severely suppress it. The obvious ground state of such a layer is a uniform planar director field $\theta = \pi/2$ with zero FE. The main result of this paper is a prediction of instability of this ground state induced by joint action of the K_{24} and K_{13} terms. It is shown that in sufficiently thin layers, a periodic director modulation can lower the FE under certain condition between elastic constants. This condition can hold even if the two well-known Ericksen inequalities [1] (see Sec. II for details) are not violated. The critical thickness of the layer is proportional to the polar anchoring extrapolation length and thus is larger for weaker anchoring. Estimates show that the predicted effect—spontaneous formation of periodic domains in a thin planar layer—can be observed in a polarizing microscope since the period of the structure is larger than the layer thickness, and is to be sought in the range of film thicknesses of order of a micrometer.

The paper is organized as follows. In Sec. II, general statements of the elastic theory [10], incorporating the K_{13} term, are given in the form instructive to our task. In Sec. III, the general theory is applied to a periodic instability of the uniform director in a planar layer. In Sec. IV, the obtained results are discussed and summarized.

II. GENERAL STATEMENTS OF THE ELASTIC THEORY

Let the layer of thickness h be normal to the z axis and parallel to the (x, y) plane. Measuring length in units h , the bulk V occupied by the layer can be written as $0 < x, y < L/h, 0 < z < 1$, where $L \gg h$ is the size in the x and y directions. It is known that the sum of the first three terms in the FE (1) also contains certain total divergence. To study the intrinsic mechanisms of spontaneous deformations in a nematic phase, it is relevant to rewrite its FE separating this divergence term with the aid of the identity

$$(\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2 = (\partial_i n_j)^2 + \nabla \cdot [\mathbf{n}(\nabla \cdot \mathbf{n}) + (\mathbf{n} \times \nabla \times \mathbf{n})],$$

where $\partial_i = \partial/\partial x_i$ and summation over repeating subscripts is implied. Converting the divergence terms to surface integrals, the nematic FE per unit square of the layer can be represented as the sum of the irreducible bulk and surface terms, i.e.,

$$F = \frac{2h^2}{L^2} \left(\int dV f_b + \int dS \sum f_s \right), \quad (2)$$

where

$$f_b = (\partial_i n_j)^2 + (t-1)(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + (b-1)(\mathbf{n} \times \nabla \times \mathbf{n})^2, \quad (3)$$

$$f_s = p_{\parallel} f_{\parallel} + p_{\perp} f_{\perp} + d f_a. \quad (4)$$

Here F is the FE in units $K_{11}/4h$; $\sum f_s = f_s(z=1) + f_s(z=0)$ is the sum of the surface FE densities on the surface $z=0$ and $z=1$; $t = K_{22}/K_{11}$ and $b = K_{33}/K_{11}$ are the reduced twist and bend constants, $d = h/L_a$ is the thickness normalized on the anchoring extrapolation length $L_a = K_{11}/W$, and $\frac{1}{2} W f_a(n_z^2)$ is the anchoring potential. The surface densities f_{\parallel} and f_{\perp} with the director derivatives, respectively, tangential and normal to the surface S [11] take the form

$$f_{\parallel} = \nu_z [n_z (\partial_x n_x + \partial_y n_y) - (n_x \partial_x + n_y \partial_y) n_z], \quad (5)$$

$$f_{\perp} = \nu_z n_z \partial_z n_z, \quad (6)$$

where ν_z is the z component of the outer surface normal, $\nu_z(0) = -1$, $\nu_z(1) = 1$, and their coefficients are $p_{\parallel} = 1 - (2K_{24}^* - K_{13}^*)/K_{11}$ and $p_{\perp} = K_{13}^*/K_{11}$. The constants K_{13}^* and K_{24}^* derived in [3] are the effective quantities that in a finite body replace elastic constants K_{13} and K_{24} calculated by Nehring and Saupe in [2] for the infinite nematic medium. The constant K_{13}^* is determined by the behavior of the scalar order parameter η at the surface [3]: for smooth changes, $K_{13}^* \sim (\eta_b - \eta_s) K_{13}$, where η_b and η_s are the bulk and surface values, respectively [12]. The constant K_{24}^* is the sum $K_{24}^* = K_{24} + \frac{1}{2} K_{13}^*$ [14]. As a result p_{\parallel} takes the value

$$p_{\parallel} = 1 - 2K_{24}/K_{11}, \quad (7)$$

where K_{24} is the material parameter of a nematic medium alone (the infinite medium constant). At the same time the quantity p_{\perp} is determined by both the nematic medium and details of subsurface behavior.

The constant p_{\parallel} is the total coefficient of the FE term, functionally similar to the K_{24} term, which like p_{\perp} can be of any sign. If the anchoring and K_{13} term are neglected, i.e., $p_{\perp} = d = 0$, the uniform state is stable under the conditions

$$|p_{\parallel}| < 1, \quad (8)$$

$$-2t < 1 - p_{\parallel} - 2t < 0, \quad (9)$$

derived by Ericksen in [1]. These inequalities imply that both the K_{24} and K_{22} mechanisms should be restricted (not too large p_{\parallel} and not too small t). In contrast, for any finite p_{\perp} the director is known to be distorted very close to the surface [15]. Nonetheless, since this subsurface mode cannot be directly observed, the assumption of a homogeneous ground state remains valid for the *observable bulk* director. For a finite p_{\perp} , the bulk director is determined by the standard Euler-Lagrange equations for F and the effective boundary conditions derived in [10]. These equations determine the angles θ and ϕ the director makes with the z and x axes. In terms of these angles the director takes the form $\mathbf{n} = (\sin \theta \cos \phi \sin \theta \sin \phi, \cos \theta)$, and the boundary conditions [10] can be written as

$$\nu_z \left(\frac{\partial f_b}{\partial \theta'} + p_\perp \frac{\partial f_\perp}{\partial \theta} \right) + p_{||} \left(\frac{\partial f_{||}}{\partial \theta} - \partial_x \frac{\partial f_{||}}{\partial (\partial_x \theta)} - \partial_y \frac{\partial f_{||}}{\partial (\partial_y \theta)} \right) + d \frac{\partial f_a}{\partial \theta} = 0, \quad (10)$$

$$\nu_z \frac{\partial f_b}{\partial \phi'} + p_{||} \left(\frac{\partial f_{||}}{\partial \phi} - \partial_x \frac{\partial f_{||}}{\partial (\partial_x \phi)} - \partial_y \frac{\partial f_{||}}{\partial (\partial_y \phi)} \right) = 0, \quad (11)$$

where the prime stands for the z derivative. Note that the divergence terms do not alter the Euler-Lagrange equations and affect the director configuration only through boundary conditions.

In terms of the angle θ one has $f_\perp = -\frac{1}{2}\theta' \sin 2\theta$, and the contribution of the K_{13} term to the boundary condition (10) is $-\nu_z p_\perp \theta' \cos 2\theta$. The θ equation (10) can be formally obtained from F if a variation of the term $f_\perp = -\frac{1}{2}\theta' \sin 2\theta$ is taken in the form

$$\bar{\delta} f_\perp = -\theta' \cos 2\theta \delta \theta \quad (12)$$

as if θ' would be constant. This reflects the fact that for $p_\perp \neq 0$, the standard FE (1) or (2) has no minimum [16,11], and the boundary condition (10) gives the extremum of the *true* FE functional introduced in [10]. This true FE takes into account that the nematic density vanishes at the surface, which provides the minimum for $p_\perp \neq 0$ [10]. Of course, $\bar{\delta}$ is not a real variation, and Eq. (12) only expresses a convenient rule showing how to write the extremum conditions for the true FE functional dealing with the expression for F alone.

In spite of a formal status of the standard functional F in obtaining the extremum bulk director field for $p_\perp \neq 0$, the equilibrium value of the FE can be calculated by substituting this field in the functional F [10]. This enables one to select the director field with the lowest FE among different solutions of the system of the Euler-Lagrange equations and boundary conditions (10), (11). Thus, the closed procedure of finding the observable bulk director can be formulated solely in terms of F without resorting to the true FE functional [10].

In order to anticipate possible effects of the K_{13} term, let us consider a simplified situation when $K_{11} = K_{22} = K_{33}$. In this case, dividing by $1 - p_\perp \cos 2\theta$, the θ equation (10) can be rewritten as

$$\nu_z K_{11} \theta' + \frac{p_{||}}{1 - p_\perp \cos 2\theta} \left(\frac{\partial f_{||}}{\partial \theta} - \partial_x \frac{\partial f_{||}}{\partial (\partial_x \theta)} - \partial_y \frac{\partial f_{||}}{\partial (\partial_y \theta)} \right) + \frac{d}{1 - p_\perp \cos 2\theta} \frac{\partial f_a}{\partial \theta} = 0. \quad (13)$$

We see that compared to the case $p_\perp = 0$, the coefficient $p_{||}$ is replaced by $p_{||}/(1 - p_\perp \cos 2\theta)$. Since the magnitude of this last quantity can be larger than that of $p_{||}$, Eq. (13) suggests that the K_{13} term can boost the action of the surface elastic FE density $f_{||}$ associated with the K_{24} term. We are to note here another possible and apparently more straight interpretation of the role a nonzero p_\perp plays in strengthening the pure K_{24} mechanism of spontaneous deformations. In the original form of the one constant version of Eq. (10) [which

is obtained from Eq. (13) by multiplying by $1 - p_\perp \cos 2\theta$], the constant K_{11} is replaced by $K_{11} - K_{13}^* \cos 2\theta$, whereas $p_{||}$ remains unchanged. Then, instead of attributing the effect of K_{13}^* to the increase of $p_{||}$, one may say that the K_{24} mechanism becomes more effective because the constant K_{11} , which resists the spontaneous deformations, is effectively reduced. However, this interpretation is not consistent with the fact that it is K_{11} that enters the Euler-Lagrange equations, for these are not altered by the divergence terms, and we attribute the role of a nonzero p_\perp to the rescaling of $p_{||}$. Calculations performed in Sec. III confirm the qualitative consideration given above. It will be found that the director in the ground state of a planar layer can be periodically modulated even if inequalities (8) and (9) hold, but the factor $1 - p_\perp \cos 2\theta < 1$, and the ratio d is sufficiently small.

III. JOINT K_{13} - AND K_{24} -TERM-INDUCED INSTABILITY OF THE UNIFORM DIRECTOR FIELD

Analysis of patterns in thin nematic films with hybrid boundary conditions (the polar anchoring favors director orientation normal on one and planar on the other surface) [5] shows that in the thinnest films only stripe domains occur [17,9,7,8]. The period L of these surfacelike elasticity-induced periodic patterns is much larger than the film thickness h so that the dimensionless wave number $\chi = 2\pi h/L \ll 1$. Although a hybrid film differs from a pure planar one, in the last case a periodic modulation with small χ can be expected to appear at least at the instability point. To describe such an instability in a planar layer we can use the theory [9] developed for hybrid films for $p_\perp = 0$.

The uniform ground state of a planar layer with zero FE is described by the angles $\theta_0 = \pi/2$ and $\phi_0 = 0$. Consider periodic perturbations thereof in the form

$$\theta = \pi/2 + f(z) \sin(\chi y/h), \quad (14)$$

$$\phi = g(z) \cos(\chi y/h). \quad (15)$$

After the x, y integration, the layer FE (2) of the two leading orders in the small χ , f , and g takes the form

$$F = \int_0^1 dz \bar{f}_b + \sum \bar{f}_s, \quad (16)$$

where

$$\bar{f}_b = f'^2 + \chi^2 t f^2 + \chi^2 g^2 + t g'^2 - 2\chi(1-t)g'f, \quad (17)$$

$$\bar{f}_s = \nu_z 2(\chi p_{||} g f + p_\perp f f') + d f^2 - \frac{1}{4} \nu_z \chi p_{||} f g^3. \quad (18)$$

The Euler-Lagrange equations for the functional (16) can be readily written. However, since the K_{13} term does not alter them, the solution thereof is obtained from that of Ref. [9] by setting the unperturbed value of θ to $\pi/2$. Following Ref. [9], the small perturbations f and g are represented in the form of a power series in χ . Then, in the leading orders, the solution of the Euler-Lagrange equations has the form

$$f = \chi^2 (\xi - \zeta z), \quad (19)$$

$$g = \chi\gamma + \chi^3 \left[\frac{1}{2} \gamma z + (1-t) \left(\xi - \frac{1}{2} \zeta z \right) + \delta \right] \frac{z}{t},$$

where $\xi, \zeta, \gamma, \delta$ are constants to be found from the boundary conditions.

To obtain the boundary conditions for the functional (16) from Eqs. (10) and (11), it is sufficient to note that now $f_{\perp} = ff'$ and in the surface density (18) f and g play the role of θ and ϕ , respectively. To the leading order, this yields the following boundary conditions for f and g :

$$\nu_z(1+p_{\perp})f' + \nu_z\chi^2 p_{\parallel}\gamma + df = 0, \quad (20)$$

$$tg' - (1-t-p_{\parallel})f = 0.$$

In the context of (19) these equations written for $z=0$ and $z=1$ constitute the system

$$-(1+p_{\perp})\zeta + p_{\parallel}\gamma + d(\xi - \zeta) = 0,$$

$$(1+p_{\perp})\zeta - p_{\parallel}\gamma + d\xi = 0, \quad (21)$$

$$\gamma + \delta + p_{\parallel}(\xi - \zeta) = 0,$$

$$-\delta - p_{\parallel}\xi = 0.$$

A nontrivial solution of system (21) exists if its determinant vanishes. This condition reduces to the equality

$$d = -2(1-p_{\parallel}^2+p_{\perp}), \quad (22)$$

and the solution of (21) is obtained in the form

$$\zeta = \frac{\gamma}{p_{\parallel}}, \quad \xi = \frac{\gamma}{2p_{\parallel}}, \quad (23)$$

$$\delta = -\frac{\gamma}{4}.$$

It now remains to find γ and χ . This can be done from the condition that the variation of the *true* FE [10] calculated for the above solution is equal to zero. As described above, *instead* of dealing with the complicated true FE functional, one can apply the rule (12) to the term $p_{\perp}ff'$ in the functional F (16). To this end we substitute (19) and (23) in all the terms in F except $p_{\perp}ff'$. As for this last term, in order to set the variation of f' to zero, we may explicitly separate this derivative f' as an individual variable substituting solutions (19),(23) only in f . Such a form of F is obtained as

$$\begin{aligned} F[\chi, \gamma, f'(0), f'(1)] &= \chi^4 \frac{d+2(1-p_{\parallel}^2)}{2p_{\parallel}^2} \gamma^2 \\ &- \chi^2 \frac{p_{\perp}\gamma}{2p_{\parallel}} [f'(1) + f'(0)] \\ &+ \chi^6 \left(P\gamma^2 + \frac{1}{4}\gamma^4 \right), \end{aligned} \quad (24)$$

where

$$P = \frac{(1-p_{\parallel})(p_{\parallel}+2t-1)}{4p_{\parallel}^2 t}. \quad (25)$$

Varying (24) in γ and χ^2 and then substituting solutions (19),(23) in f' gives, respectively,

$$\chi^4 \frac{d+2(1-p_{\parallel}^2+p_{\perp})}{2p_{\parallel}^2} \gamma + \chi^6 \left(P\gamma + \frac{1}{2}\gamma^3 \right) = 0, \quad (26)$$

$$\chi^2 \frac{d+2(1-p_{\parallel}^2+p_{\perp})}{2p_{\parallel}^2} \gamma^2 + \chi^4 \left(\frac{3}{2}P\gamma^2 + \frac{3}{8}\gamma^4 \right) = 0. \quad (27)$$

Solution χ and γ of system (26) and (27) along with Eqs. (19), (23) and (14), (15) determines the periodic director field extremizing the true FE functional. However, as was described above, the FE of this extremum field can be calculated by substituting this field in the standard functional F . Substituting (19), (23) in F (16) reduces to substituting these formulas in f' in the expression for $F[\chi, \gamma, f'(0), f'(1)]$ (24). This gives

$$F(\chi, \gamma) = \chi^4 \frac{d+2(1-p_{\parallel}^2+2p_{\perp})}{2p_{\parallel}^2} \gamma^2 + \chi^6 \left(P\gamma^2 + \frac{1}{4}\gamma^4 \right). \quad (28)$$

For χ and γ satisfying system (26),(27) this $F(\chi, \gamma)$ gives the equilibrium FE of the periodic state.

Note that Eqs. (26) and (27) can be formally obtained as extrema of the following generating function:

$$F^*(\chi, \gamma) = \chi^4 \frac{d+2(1-p_{\parallel}^2+p_{\perp})}{2p_{\parallel}^2} \gamma^2 + \chi^6 \left(P\gamma^2 + \frac{1}{4}\gamma^4 \right). \quad (29)$$

The function F^* coincides with the equilibrium FE F (28) only for $p_{\perp}=0$, which reflects the formal status of the rule (12) described in the Introduction. We stress that introduction of F^* is not necessary as the equilibrium equations (26) and (27) are known anyway. However, having it can be useful, e.g., for finding the sign of the FE F (28) without actually calculating its value for χ and γ satisfying system (26), (27). This will be demonstrated below.

Let us assume that Ericksen inequalities (8) and (9) are satisfied and hence $P > 0$ (the opposite case will be discussed in Sec. IV). Then a nonzero solution of system (26),(27), which has the form

$$\chi = \left(-\frac{d+2(1-p_{\parallel}^2+p_{\perp})}{6Pp_{\parallel}^2} \right)^{1/2}, \quad (30)$$

$$\gamma = 2P^{1/2}, \quad (31)$$

exists only if

$$d+2(1-p_{\parallel}^2+p_{\perp}) < 0, \quad (32)$$

when $\min F^* < 0$.

Now we can compare the FE $F(\chi=0, \gamma=0)=0$ of the uniform state with the FE (28) of the periodic solution for χ

and γ (30), (31). Instead of calculating this FE, we observe that if inequalities (8) and (9) are satisfied, and, in particular, $1 - p_{\parallel}^2 > 0$, then the condition (32) can take place only at the expense of negative p_{\perp} . Then the first term in F (28) is smaller than the first term in F^* . Therefore, as soon as the nonzero solution (30),(31) appears and $F^* < 0$, one has $F < F^* < 0$. Thus, if the condition (32) is satisfied, the periodic solution has a lower FE than that of the naive uniform director field.

The obtained periodic director field has all three deformations similar to the case when the K_{24} mechanism of chiral symmetry breaking produces periodic domains in a hybrid layer considered for $1 - p_{\parallel}^2 > 0$ and $p_{\perp} = 0$ in [9]. The term $p_{\perp} f_{\perp}$ amplifies this mechanism so that the condition (32) is satisfied. This is possible only for negative p_{\perp} when the factor $1 - p_{\perp} \cos 2\theta_0 = 1 + p_{\perp} < 1$ and

$$\frac{|p_{\parallel}|}{1 - p_{\perp} \cos 2\theta_0} > |p_{\parallel}|$$

in accordance with the qualitative prediction derived from the form of Eq. (13). In addition, the term $p_{\perp} f_{\perp}$ also breaks parity of the director field. Indeed, it is easy to verify that the perturbations of θ on both surfaces are not equal, $f(0) = -f(1)$, and the solution $f(z)$ is antisymmetric with respect to the middle plane in the symmetric geometry. Some divergence mechanisms of parity violation has already been reported [18].

IV. DISCUSSION

Thus, even if the inequalities (8) and (9) are not violated but the condition (32) is satisfied, the periodic state has FE lower than that of the simple uniform state. This means that a nematic liquid crystal in a planary anchored layer is spontaneously modulated if

$$1 - p_{\parallel}^2 + p_{\perp} < 0 \quad (33)$$

and the layer thickness is smaller than

$$h_c = -2L_a(1 - p_{\parallel}^2 + p_{\perp}). \quad (34)$$

This can happen only if $p_{\perp} < 0$ (note that a negative value of p_{\perp} is reported in [7,8]). We see that h_c is proportional to the anchoring extrapolation length and thus is larger for a weaker anchoring. In the absence of p_{\perp} the factor $1 - p_{\parallel}^2$ can be negative only if the coefficient p_{\parallel} of the surface elastic term f_{\parallel} is sufficiently large and the fundamental inequalities (8) and (9) are violated. Hence the term $p_{\perp} f_{\perp}$ with the normal-to-surface derivative can effectively renormalize p_{\parallel} , thus amplifying the ability of the surface elastic terms with the tangential-to-surface derivatives to spontaneously produce director deformations. This was suggested by the form of boundary condition (13).

Consider the conditions when the predicted effect of spontaneous director modulation can be observed. A strong anchoring can make the effect practically inaccessible for observations. For instance, for $W \sim 10^{-3} - 10^{-4}$ erg cm⁻², the critical thickness can be in the range $h_c \sim 1 - 10$ μ m. Modern technology allows for making such thin planar samples with no azimuthal anchoring [19]. However, for W

$\sim 10^{-2}$ erg cm⁻², the maximum thickness becomes as small as $h_c \sim 0.1$ μ m, which is hardly accessible. The relevant data can be taken from works (Refs. [7,8]) on stripe domains in hybrid films of a nematic liquid crystal 5CB between air and glycerin. The anchoring extrapolation length on both surfaces was found to be of order of 1 μ m, $p_{\perp} < 0$, and the factor $1 - p_{\parallel}^2 + p_{\perp} \approx -0.4$. For these data one obtains $h_c \approx 0.8$ μ m.

The periodic structure is of long wavelength if the thickness $h < h_c$ is sufficiently close to h_c so that formula (30) gives $\chi \ll 1$. In contrast, the instability that could occur if one of the inequalities (8) and (9) was violated would be of short wavelength. Indeed, then $P < 0$, Eq. (25), and the function F^* (29) is minimized by a large χ . Of course, in this case our approach cannot give a quantitative result since the restriction of the FE to χ^6 is not justified. Nonetheless, two important qualitative points can be made.

The first point is concerned with the role the anchoring plays for the pure K_{24} and joint K_{24} - K_{13} mechanisms of instability of the uniform ground state. In the last case, the extrapolation length L_a enters the leading χ^4 terms in F^* and F and crucially influences the critical condition of the instability. The situation is different in the case of the pure K_{24} mechanism when one of the inequalities (8) and (9) is violated, χ is large, and the leading negative term in F and F^* is $\chi^6 P$. Since L_a does not enter this term, the role of anchoring is much weaker. Of course, for a very large W , L_a is very small, the χ^4 term dominates, and the instability is suppressed, too.

The second point is about the very possibility of adopting spontaneous deformations of the ground state within the conventional idea of a nematic phase. For vanishing W this would be impossible since the nematic would have been spontaneously distorted even in very thick samples, which contradicts the experiment. For a finite W , however, it is possible. The critical condition (32) suggests that the quantity $d = (\text{smallest system size})/L_a$, which is in fact the natural dimensionless parameter characterizing the ratio volume/surface, plays an important role both in the case of a layer and in more general geometries. In thick samples with $d \gg 1$, the joint K_{24} - K_{13} mechanism produces no instability. This practically means that in samples thicker than a few microns, the uniform ground state is intact. Thus, the possibility can be adopted that in geometries with $d < 1$ the nematic director can be spontaneously distorted due to the predicted joint mechanism.

It is much more difficult to answer the question if inequalities (8) and (9) can be violated in a nematic material. The problem is not just that the deformation would then appear in samples much thicker than L_a . An additional problem is that because of a large χ , the FE of such a state can be much lower than for a long wavelength instability. In this case the result of a linear analysis that may be performed also for large χ cannot be conclusive because it is not able to take into account a possible spontaneous defect creation (as in the model of a blue phase [20]).

To conclude we emphasize that the intrinsic ability of a nematic material to produce deformations without external sources is much less exotic than it might look at first sight. Indeed, the same intermolecular forces that give rise to the K_{13} term also produce an intrinsic anchoring. But if the sur-

face is curved, the intrinsic anchoring favors director deformations that are totally due to the interaction between nematic molecules. We showed that divergence terms can violate the chiral symmetry and parity of the uniform director field even in a sample with plane surfaces without contradiction to the basic idea of a nematic phase. The above estimates show that the predicted effect of spontaneous periodic structure in a thin planar layer can be observed in experiments with standard nematics, e.g., 5CB. This would give an important in-

sight into the intermolecular interaction in nematogens, the role of surfacelike elasticity, and intrinsic mechanisms of pattern formation in liquid crystals.

ACKNOWLEDGMENTS

This work was supported by CRDF Grant No. UE1-310 and STCU Grant No 637.

-
- [1] J.L. Ericksen, *Phys. Fluids* **99**, 1205 (1966).
 [2] J. Nehring and A. Saupe, *J. Chem. Phys.* **54**, 337 (1971); **56**, 5527 (1972).
 [3] V.M. Pergamenschchik and S. Žumer, *Phys. Rev. E* **59**, R2531 (1999).
 [4] The analysis of Refs. [1,2] shows that the K_{24} term does not represent an individual deformation mode independent of the splay, twist, and bend. There are five independent first-order director derivatives in the vicinity of any spatial point: two of them contribute to the splay term, another two contribute to the twist term, one gives rise to the bend term, and only the last one does not contribute to the K_{24} term. As for the K_{13} term, it is independent because of the second-order director derivatives and thus can be associated only with derivatives of the conventional modes.
 [5] O.D. Lavrentovich and V.M. Pergamenschchik, *Int. J. Mod. Phys. B* **12**, 2389 (1995).
 [6] G.P. Crawford and S. Žumer, *Int. J. Mod. Phys. B* **12**, 2469 (1995).
 [7] O.D. Lavrentovich and V.M. Pergamenschchik, *Phys. Rev. Lett.* **73**, 979 (1994).
 [8] V. M. Pergamenschchik, O.V. Lobov, and O. D. Lavrentovich, (unpublished).
 [9] V.M. Pergamenschchik, *Phys. Rev. E* **47**, 1881 (1993).
 [10] V.M. Pergamenschchik, *Phys. Lett. A* **243**, 167 (1998); *Phys. Rev. E* **58**, R16 (1998).
 [11] V.M. Pergamenschchik, *Phys. Rev. E* **48**, 1254 (1993).
 [12] The effective constant K_{13}^* has another contribution $K_{13,W}$ from the homogeneous part of the FE usually associated solely with anchoring terms. This contribution was introduced in [11] and recently considered in [13]. However, if the ratio molecular length/anchoring extrapolation length is small, $K_{13,W}$ is also small compared to a typical elastic constant [11]. As we are interested in the case of a weak anchoring with extrapolation length of order of a micrometer, $K_{13,W}$ is not expected to give a notable effect. Of course, predictions of the elastic approach are irrespective of the nature of the effective K_{13}^* .
 [13] M. Faetti and S. Faetti, *Phys. Rev. E* **57**, 6741 (1998).
 [14] There is a sign misprint in the formula for K_{24}^* in Ref. [3] [last line in Eq. (20)]: it should read $K_{24}^* = \frac{1}{4}(K_{11}^* + K_{22}^* + 2K_{13}^*)$.
 [15] G. Barbero, N.V. Madhusudana, and C. Oldano, *J. Phys. (France)* **50**, 2263 (1989).
 [16] G. Barbero and C. Oldano, *Nuovo Cimento D* **6**, 479 (1985).
 [17] O.D. Lavrentovich and V.M. Pergamenschchik, *Mol. Cryst. Liq. Cryst.* **179**, 125 (1990).
 [18] V.M. Pergamenschchik, P.I.C. Teixeira, and T.J. Sluckin, *Phys. Rev. E* **48**, 1265 (1993); V.M. Pergamenschchik, *Ukr. Fiz. Zh. (Russ. Ed.)* **38**, 59 (1993).
 [19] I. Dozov *et al.*, in *Proceedings of the European Conference on Liquid Crystals, Hersonissos, Greece, April 1999* (University, of Patras, 1999).
 [20] S. Meiboom, M. Sammon, and W.F. Brinkman, *Phys. Rev. A* **27**, 438 (1983).