Periodic deformations in nematic liquid crystals

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We reconsider the possibility of periodic deformations in nematic liquid crystal samples, and present a simple method to analyze their stability near the threshold. Our method consists in finding the matrix characterizing the total energy in terms of the integration constants of the linearized solutions of the variational problem. In the undeformed state all the integration constants are identically zero. Hence the analysis of the stability of the undeformed state reduces to the analysis of the sign of the determinants of the principal minors of the matrix of the quadratic form representing the total energy of the nematic sample. We discuss the role of the saddle-splay elastic constant and of the anchoring energy strength in the stability of the modulated structure. The role of the thickness of the sample, as well as of the polar and azimuthal anchoring energies, in the phenomenon is also considered.

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I. INTRODUCTION

The possibility of stable periodic deformations in nematic liquid crystal samples has been analyzed long ago by Lonberg and Meyer [1]. In their analysis the nematic sample, with a planar orientation, submitted to an external magnetic field perpendicular to the initial orientation was considered. They have shown that if the twist elastic constant is smaller than a critical value, the magnetic field induces a periodic deformation, instead of the aperiodic one. This problem has been theoretically analyzed by different authors [2,3]. Periodic deformations in hybrid nematic cells, in the absence of magnetic or electric field, have been considered by Strigazzi and co-workers [4–6]. In all the cases considered above, an external field, electric, magnetic, or mechanical, is responsible for the periodic instability. Recently, Pergamenshchik [7,8] has considered the possibility of a spontaneous appearance of periodic deformation in planar samples, induced by surfacelike terms. He has shown that if the elastic constant of saddle splay, K_{24}, is large enough, the ground state of a nematic sample characterized by planar easy axes on both surfaces could be periodically distorted. In our paper we reconsider the possibility of periodic deformations in nematic samples, and present a simple way to analyze their stability near the threshold. Our method consists in finding the matrix characterizing the total energy in terms of the integration constants of the linearized solution of the variational problem. Since in the nondeformed state all the integration constants are zero, the analysis of the stability of the nondeformed state reduces to the study of the sign of the determinants of the principal minors of the matrix of the quadratic form representing the total energy of the nematic sample.

Our paper is organized as follows. In Sec. II the elastic energy density of a nematic sample close to the homogeneous planar alignment is obtained. In Sec. III the bulk differential equations and the boundary conditions are deduced. The particular case of small periodic distortions around the planar configuration, where the solutions of the bulk differential equations depend linearly on the integration constants, is considered in the same section. In this framework, the quadratic form expressing the total energy in terms of the integration constants is deduced, and a new form of the system determining the integration constants, equivalent to the boundary conditions, is derived. Section IV is devoted to the explicit solution of the problem treated, in general, in Sec. III, by considering a well defined form for the elastic energy density and for the anisotropic part of the surface energy. In Sec. V the critical thickness for the periodic instability is obtained by analyzing the cases considered by Pergamenshchik [7,8]. The possibility to observe modulated structures in nematic samples with large thickness, and the role of the polar and azimuthal anchoring energies in the predicted phenomenon are discussed in the same section. The main results of our paper are reported in Sec. VI. The Appendix is devoted to the derivation of the surfacelike contribution to the energy density.

II. ELASTIC ENERGY DENSITY

We consider the stability of the uniform planar alignment with respect to periodic deformations. To this end, it is necessary to obtain the elastic energy density in terms of the director components n_i. In our analysis we consider a nematic sample in the shape of a slab of thickness d. The Cartesian reference frame has the z axis normal to the bounding surfaces, at $z=0$ and $z=d$, and the (x,y) plane parallel to the surfaces. The unit vectors along the axes x, y, and z are indicated by $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$, respectively. The nematic director $\mathbf{n}$, or the polar angles defining it with respect to our reference frame, is supposed to depend on (y,z) coordinates. If $\mathbf{n}=\mathbf{n}(z)$ only, the corresponding nematic deformation is called aperiodic. On the contrary, if $\mathbf{n}=\mathbf{n}(y,z)$, the y dependence will be assumed periodic, i.e., $\mathbf{n}(y,z)=\mathbf{n}(y+\lambda,z)$, where $\lambda=2\pi/q$ is the spatial period of the deformation. The spatial derivatives are indicated by $X_{,y}=\partial X/\partial y$. We assume that in the uniform state $n_x(0)=1$ and $n_y(0)=n_z(0)=0$. For small fluctuations around the planar orientation, described by n_y and n_z, considered small quantities of first order, n_x differs from 1 for a quantity of second order. In fact, from the condition $n_x^2+n_y^2+n_z^2=1$, it follows that $n_x \sim 1-(1/2)(n_y^2+n_z^2)=1+O(2)$. From the hypothesis $\mathbf{n}=\mathbf{n}(y,z)$, $\nabla\cdot\mathbf{n}=n_{y,y}+n_{z,z}$ and $\nabla\times\mathbf{n}=(n_{z,y}-n_{y,z})\mathbf{e}_x+O(2)$. Consequently, $\mathbf{n}\cdot(\nabla\times\mathbf{n})=n_{z,y}-n_{y,z}+O(2)$ and $\mathbf{n}\times(\nabla\times\mathbf{n})=O(2)$.

The elastic energy density of the nematic liquid crystal is given by [9]

$$f_e=\frac{1}{2}\{K_{11}(\nabla\cdot\mathbf{n})^2+K_{22}[\mathbf{n}\cdot(\nabla\times\mathbf{n})]^2+K_{33}[\mathbf{n}\times(\nabla\times\mathbf{n})]^2\}$$

$$-(K_{22}+K_{24})\nabla\cdot[\mathbf{n}\nabla\cdot\mathbf{n}+\mathbf{n}\times(\nabla\times\mathbf{n})], \tag{1}$$

which at the second order in the variations n_y and n_z reads

$$f_e=\frac{1}{2}\{K_{11}(n_{y,y}+n_{z,z})^2+K_{22}(n_{z,y}-n_{y,z})^2$$

$$-4(K_{22}+K_{24})(n_{y,y}n_{z,z}-n_{y,z}n_{z,y})\}. \tag{2}$$

The contribution of the surfacelike term to the energy density is deduced in the Appendix. Using polar coordinates we have $n_y=\cos\theta\sin\phi$ and $n_z=\sin\theta$, that for $\phi\to 0$ and $\theta\to 0$ become $n_y=\phi$ and $n_z=\theta$. In terms of θ and ϕ, f_e can be rewritten as

$$f_e=\frac{1}{2}K_{22}\{\nu(\phi_{,y}+\theta_{,z})^2+(\theta_{,y}-\phi_{,z})^2$$

$$-2\mu(\phi_{,y}\theta_{,z}-\phi_{,z}\theta_{,y})\}, \tag{3}$$

where

$$\nu=\frac{K_{11}}{K_{22}} \quad \text{and} \quad \mu=2\frac{K_{22}+K_{24}}{K_{22}}. \tag{4}$$

f_e is a quadratic form of $\phi_{,y}$, $\phi_{,z}$, $\theta_{,y}$, and $\theta_{,z}$. In the absence of surface constraint the homogeneous planar orientation corresponds to a minimum of f_e only if the quadratic form is positive definite. This happens if the determinants of the principal minors of the matrix

$$\mathcal{Q}=\begin{pmatrix} \nu & 0 & 0 & \nu-\mu \\ 0 & 1 & \mu-1 & 0 \\ 0 & \mu-1 & 1 & 0 \\ \mu-\nu & 0 & 0 & \nu \end{pmatrix} \tag{5}$$

are positive. Simple calculations give

$$\nu>0, \quad \nu[1-(\mu-1)^2]>0,$$

$$[1-(\mu-1)^2][\nu^2-(\nu-\mu)^2]>0. \tag{6}$$

Since $\nu>0$, from Eqs. (6) it follows that the uniform planar orientation is stable if $\mu(\mu-2)<0$ and $\mu(\mu-2\nu)<0$, giving

$$0<\mu<2 \quad \text{or} \quad 0<\mu<2\nu, \tag{7}$$

depending on the value of ν. In the nematic phase $\nu>1$, and the first inequality is the dominant one. However, close to the nematic-smectic temperature transition, the twist elastic constant diverges, whereas the splay elastic constant remains practically temperature independent [10]. Consequently, in this limit $\nu\to 0$, and the second inequality becomes dominant. The discussion reported above is relevant to the stability of the planar orientation in a nematic sample of infinite thickness, in the absence of surface energy fixing the planar orientation. Of course, if the sample is of finite thickness, and the anchoring energy strength different from zero, the range of μ for which the planar orientation is stable differs from the one reported above, as we will show in the following.

If the nematic sample is submitted to a magnetic field $\mathbf{H}=H\mathbf{e}_z$, the magnetic energy density connected with the diamagnetic anisotropy $\chi_a=\chi_\parallel-\chi_\perp$, where $\parallel$ and $\perp$ refer to $\mathbf{n}$, is

$$f_h=-\frac{1}{2}\chi_a n_z^2H^2=-\frac{1}{2}\chi_a H^2\theta^2, \tag{8}$$

at the second order in θ. The total bulk energy density is then $f=f_e+f_h$.

We assume that the surface energy, characterized by an easy axis along the x axis, is of the type

$$g_S=\frac{1}{2}\sum_{\alpha,\beta}[w_{\alpha\beta}(0)n_\alpha(0)n_\beta(0)+w_{\alpha\beta}(d)n_\alpha(d)n_\beta(d)]. \tag{9}$$

In the simple case where $w_{\alpha\beta}(0)=w_0\delta_{\alpha\beta}$ and $w_{\alpha\beta}(d)=w_1\delta_{\alpha\beta}$ we have, at the second order in the polar angles,

$$g_S=\frac{1}{2}w_0[\phi^2(0)+\theta^2(0)]+\frac{1}{2}w_1[\phi^2(d)+\theta^2(d)]. \tag{10}$$

A possible generalization of g_S, that will be considered in the following, corresponds to the case in which the two eigenvalues of the matrix $\mathcal{W}$ of elements $w_{\alpha\beta}$ are different. In this case the effective anchoring energy in terms of the polar angles reads

$$g_S=\frac{1}{2}[w_{0\phi}\phi^2(0)+w_{0\theta}\theta^2(0)]$$

$$+\frac{1}{2}[w_{1\phi}\phi^2(d)+w_{1\theta}\theta^2(d)]$$

$$=g_0+g_1. \tag{11}$$

Expression (11) for g_S is more realistic than Eq. (10) because splay-bend deformation, involving just θ angle imply a variation of the anisotropic part of the van der Waals interaction due to the change of the average distance between the surface nematic molecule and the substrate. On the contrary, in a pure twist deformation, where only ϕ is changing, the average distance does not change. As a particular case of Eq. (11), we will consider $w_{0\phi}=w_{1\phi}=0$, corresponding to no-azimuthal anchoring energy.

III. BULK DIFFERENTIAL EQUATIONS AND BOUNDARY CONDITIONS

The average total energy, per unit length along the y axis, is given, in general, by

$$F=\frac{1}{\lambda}\left\{\int_0^\lambda\int_0^d f(\theta,\phi;\theta_{,i},\phi_{,i})dy\,dz+\int_0^\lambda g_0(\theta_0,\phi_0)dy+\int_0^\lambda g_1(\theta_1,\phi_1)dy\right\},\qquad(12)$$

where $\theta_0=\theta(0)$, $\theta_1=\theta(d)$, and $\theta_{,i}$ means $\theta_{,y}$ and $\theta_{,z}$ and ϕ_0, ϕ_1, and $\phi_{,i}$ have similar meanings. In Eq. (12) λ is the wavelength of the periodic deformation we are looking for. The actual director orientation is the one minimizing F given by Eq. (12). By imposing that the functional derivatives of F with respect to θ and ϕ vanish, routine calculations give

$$\frac{\partial f}{\partial\theta}-\sum_\alpha\partial_\alpha\frac{\partial f}{\partial\theta_{,\alpha}}=0,\quad \frac{\partial f}{\partial\phi}-\sum_\alpha\partial_\alpha\frac{\partial f}{\partial\phi_{,\alpha}}=0,\qquad(13)$$

for $0\leqslant z\leqslant d$ and $0\leqslant y\leqslant\lambda$, where $\alpha=y,z$, and

$$-\frac{\partial f}{\partial\theta_{,z}}+\frac{\partial g_0}{\partial\theta_0}=0,\quad -\frac{\partial f}{\partial\phi_{,z}}+\frac{\partial g_0}{\partial\phi_0}=0\quad\text{at}\quad z=0,\qquad(14)$$

and

$$\frac{\partial f}{\partial\theta_{,z}}+\frac{\partial g_1}{\partial\theta_1}=0,\quad \frac{\partial f}{\partial\phi_{,z}}+\frac{\partial g_1}{\partial\phi_1}=0\quad\text{at}\quad z=d.\qquad(15)$$

Equations (14) and (15) are the boundary conditions of the bulk differential equations (13). Note that the other boundary conditions at y and $y+\lambda$ are automatically satisfied if we look for a periodic deformation along y. In fact, if $\mathbf{n}(y,z)=\mathbf{n}(y+\lambda,z)$ we have also $\delta\mathbf{n}(y,z)=\delta\mathbf{n}(y+\lambda,z)$.

In a linearized analysis around the nondeformed state, the periodic solutions of the bulk differential equations are chosen of the form $\theta(y,z)=\Theta(z)\cos(qy)$ and $\phi(y,z)=\Phi(z)\sin(qy)$. In this case $\Theta(z)$ and $\Phi(z)$ are solutions of two coupled differential equation of the second order. The differential equation determining $\Theta(z)$ is a linear differential equation of the fourth order. It follows that $\Theta(z)$ contains four integration constants C_i'. The same procedure can be used to determine $\Phi(z)$, that contains also four integration constants C_i. Since $\theta(y,z)$ and $\phi(y,z)$ have to satisfy also the coupled second order differential equations, it is possible to obtain the integration constants C_i' in terms of C_i. Consequently, in the linearized case, the solutions of Eqs. (13) are of the kind

$$\theta=\theta(C_i;y,z)\qquad\text{and}\qquad\phi=\phi(C_i;y,z),\qquad(16)$$

where $i=1, 2, 3,$ and 4 are four integration constants determined by the boundary conditions (14),(15), which form a linear and homogeneous system. The critical parameter defining the threshold is deduced by putting the determinant of the coefficients of this system equal to zero.

The analysis of the stability of the nondeformed state has to be performed by considering the total energy F. As it is well known, the nondeformed state is stable if it corresponds to a minimum of F.

As discussed above, in a linearized analysis θ and ϕ depend linearly on the integration constants C_i. Consequently, F is a quadratic form of these integration constants. To know if the nondeformed state is stable, it is necessary to analyze the sign of the quadratic form representing F, which is symmetric. In other words, by substituting Eq. (16) into Eq. (12) we obtain for F an expression of the type

$$F=\frac{1}{2}\sum_{i,j}M_{ij}C_iC_j,\qquad(17)$$

where $M_{ij}=M_{ji}$, because the asymmetric part of the matrix $\mathcal{M}$, of elements M_{ij}, does not contribute to F. The quantities C_i are obtained by minimizing F with respect to C_i, $\partial F/\partial C_i=0$. We obtain

$$\sum_j M_{ij}C_j=0.\qquad(18)$$

System (18) is equivalent to the boundary conditions (14), (15), but the knowledge of the matrix $\mathcal{M}$ allows a simpler investigation of the stable state. In fact, the undeformed state $C_i=0$, for $i=1, 2, 3,$ and 4 corresponds to a minimum of F if all four determinants of the principal minors of the matrix $\mathcal{M}$, $m_1=M_{11}$, $m_2=M_{11}M_{22}-M_{12}^2$, and so on, are positive. On the contrary, the knowledge of the system obtained by Eqs. (14) and (15) does not allow to conclude anything about the stability of the undeformed state.

The elements of the matrix $\mathcal{M}$ can be easily obtained by substituting solutions (16) into Eq. (13). In this way F is transformed in an ordinary function of the integration constants C_i, $F=F(C_i)$. From this function we obtain

$$\frac{\partial F}{\partial C_i}=\frac{1}{\lambda}\int_0^\lambda\left\{\left[\left(-\frac{\partial f}{\partial\theta_z}+\frac{\partial g_0}{\partial\theta_0}\right)\frac{\partial\theta_0}{\partial C_i}+\left(-\frac{\partial f}{\partial\phi_z}+\frac{\partial g_0}{\partial\phi_0}\right)\frac{\partial\phi_0}{\partial C_i}\right]_{z=0}+\left[\left(\frac{\partial f}{\partial\theta_z}+\frac{\partial g_1}{\partial\theta_1}\right)\frac{\partial\theta_1}{\partial C_i}+\left(\frac{\partial f}{\partial\phi_z}+\frac{\partial g_1}{\partial\phi_1}\right)\frac{\partial\phi_1}{\partial C_i}\right]_{z=d}\right\}dy,\qquad(19)$$

because $\theta(y,z)$ and $\phi(y,z)$ are solutions of the bulk equations (13). As it is evident from Eq. (19), $\partial F/\partial C_i$ is obtained by means of a linear combination of the boundary conditions (14), (15). To proceed further, it is necessary to consider a special system described by defined f, g_0, and g_1.

IV. PERIODIC INSTABILITY IN THE ABSENCE OF EXTERNAL FIELDS

The analysis presented above is valid even in the case in which the nematic sample is in an external field, and hence f includes f_h. In the following we limit our investigation to the case in which external fields are absent, where $f=f_e$, given by Eq. (3) and g_0 and g_1 by Eq. (11). In this framework, the bulk differential equations read [5]

$$\theta_{,yy}+\nu\theta_{,zz}+(\nu-1)\phi_{,yz}=0,$$

$$\nu\phi_{,yy}+\phi_{,zz}+(\nu-1)\theta_{,yz}=0, \tag{20}$$

whose solutions are

$$\theta(y,z)=[C_1'\cosh(qz)+C_2'z\cosh(qz)+C_3'\sinh(qz)+C_4'z\sinh(qz)]\cos(qy),$$

$$\phi(y,z)=[C_1\cosh(qz)+C_2z\cosh(qz)+C_3\sinh(qz)+C_4z\sinh(qz)]\sin(qy), \tag{21}$$

where $q=2\pi/\lambda$, and

$$C_1'=AC_2-C_3,\quad C_2'=-C_4,$$

$$C_3'=AC_4-C_1,\quad C_4'=-C_2, \tag{22}$$

with

$$A=\frac{\nu+1}{q(\nu-1)}. \tag{23}$$

In order to rewrite system (19) in a more tractable form, we put

$$\theta_0=X_1\cos(qy),\quad \phi_0=X_2\sin qy,$$

$$\theta_1=X_3\cos(qy),\quad \phi_1=X_4\sin(qy), \tag{24}$$

where, as it follows from Eqs. (21), X_i are linear combinations of C_i. We put, furthermore,

$$\left(-\frac{\partial f}{\partial\theta_z}+\frac{\partial g_0}{\partial\theta_0}\right)_{z=0}=V_1\cos(qy),$$

$$\left(-\frac{\partial f}{\partial\phi_z}+\frac{\partial g_0}{\partial\phi_0}\right)_{z=0}=V_2\sin(qy),$$

$$\left(\frac{\partial f}{\partial\theta_z}+\frac{\partial g_1}{\partial\theta_1}\right)_{z=d}=V_3\cos(qy),$$

$$\left(\frac{\partial f}{\partial\phi_z}+\frac{\partial g_1}{\partial\phi_1}\right)_{z=d}=V_4\sin(qy), \tag{25}$$

where also the quantities V_i are linear combinations of C_i. By substituting Eqs. (24) and (25) into Eq. (19), we obtain

$$\frac{\partial F}{\partial C_i}=\frac{1}{2}\sum_k V_k\frac{\partial X_k}{\partial C_i}, \tag{26}$$

Since, as stated above, $V_k=\Sigma_m A_{km}C_m$, by indicating with $B_{ik}=\partial X_k/\partial C_i$, the condition $\partial F/\partial C_i=0$ reads

$$\frac{\partial F}{\partial C_i}=\frac{1}{2}\sum_{k,m}B_{ik}A_{km}C_m=0. \tag{27}$$

By comparing Eqs. (27) with Eqs. (18) we deduce

$$M_{ij}=(1/2)\sum_k B_{ik}A_{kj}. \tag{28}$$

Using Eqs. (21) we obtain for matrix $\mathcal{B}$, of elements B_{ik} defined above,

$$\mathcal{B}=\begin{pmatrix} 0 & 1 & -S & C \\ A & 0 & AC-dS & dC \\ -1 & 0 & -C & S \\ 0 & 0 & AS-dC & dS \end{pmatrix}, \tag{29}$$

where $S=\sinh(qd)$ and $C=\cosh(qd)$. We have, furthermore, for the elements A_{km} of the matrix $\mathcal{A}$,

$$A_{11}=\mu q,\quad A_{12}=\frac{\nu A}{L_{0\theta}},\quad A_{13}=-\frac{\nu}{L_{0\theta}},\quad A_{14}=\nu(1-qA),$$

$$A_{21}=\frac{1}{L_{0\phi}},\quad A_{22}=qA(\mu-1)-1,\quad A_{23}=-\mu q,\quad A_{24}=0,$$

$$A_{31}=-\left(q\mu C+\frac{\nu}{L_{1\theta}}S\right),$$

$$A_{32}=\nu\left[(qA-1)S+\frac{AC-dS}{L_{1\theta}}\right]-\mu q\,dC,$$

$$A_{33}=-\left(q\mu S+\frac{\nu}{L_{1\theta}}C\right),$$

$$A_{34}=\nu\left[(qA-1)C+\frac{AS-dC}{L_{1\theta}}\right]-\mu q\,dS,$$

$$A_{41}=\mu qS+\frac{C}{L_{1\phi}},$$

$$A_{42}=(1+qA)C+\frac{Cd}{L_{1\phi}}-\mu q(AC-dS),$$

$$A_{43}=\mu qC+\frac{S}{L_{1\phi}},$$

$$A_{44}=(1+qA)S+\frac{Sd}{L_{1\phi}}-\mu q(AS-dC), \tag{30}$$

where $L_{0\theta}=K_{11}/w_{0\theta}$, $L_{1\theta}=K_{11}/w_{1\theta}$, $L_{0\phi}=K_{22}/w_{0\phi}$, and $L_{1\phi}=K_{22}/w_{1\phi}$ are extrapolation lengths.

V. CRITICAL THICKNESS FOR THE PERIODIC INSTABILITY

We can now evaluate, by means of our formalism, the critical thickness to observe periodic instabilities. The critical thickness is obtained, for Cramer's rule, by putting $\det\mathcal{M}=m_4=0$. In this case system (18) can have solutions different from the trivial ones, $C_i=0$. The condition $\det\mathcal{M}=0$, for Eq. (28), is equivalent to $\det\mathcal{B}\cdot\det\mathcal{A}=0$. Since

$$\det\mathcal{B}=\left\{\frac{\nu+1}{q(\nu-1)}\sinh(qd)\right\}^2-d^2>0, \tag{31}$$

for $d>0$, the critical thickness is given by the equation $\det\mathcal{A}=0$, which coincides with the same condition of instability deduced by means of the boundary conditions (14), (15).

A. No azimuthal anchoring energy

As an example, we consider the case in which $w_{0\phi}=w_{1\phi}=0$, already analyzed by Pergamenshchik [7,8], corresponding to $L_{0\phi}$ and $L_{1\phi}\to\infty$. In this case, as it follows from Eq. (30), we have $A_{21}=0$, and

$$A_{41}=\mu qS,\quad A_{42}=(1+qA)C-\mu q(AC-dS),$$

$$A_{43}=\mu qC,\quad A_{44}=(1+qA)S-\mu q(AS-dC). \tag{32}$$

Our aim is to analyze the stability of the homogeneous planar orientation.

Let us first consider the matrix $\mathcal{M}$ in the limit $q\to 0$. By using Mathematica we obtain for the determinants of the principal minors of the matrix $\mathcal{M}$ the expressions

$$m_1=\left(\frac{\nu d}{L_1}+2\mu\right)dq^2+O(3),$$

$$m_2=\frac{\nu(1+\nu)^2d[\nu d+2(L_0+L_1)\mu]}{(\nu-1)^2L_0L_1}+O(1),$$

$$m_3=\frac{4\nu^3d^2[\nu d+2(L_0+L_1)\mu]}{(\nu-1)^2L_0L_1}q^2+O(3),$$

$$m_4=\frac{16\nu^3d^3}{(\nu-1)^4L_0L_1}[\nu^2d+2\nu(L_0+L_1)\mu-(L_0+L_1)\mu^2]q^2+\mathcal{O}(3), \tag{33}$$

where $L_0=L_{0\theta}$ and $L_1=L_{1\theta}$. The condition $\det\mathcal{M}=m_4=0$ gives

$$d_c=(L_0+L_1)\mu\frac{\mu-2\nu}{\nu^2}. \tag{34}$$

Since $\nu>0$, $d_c>0$ implies $\mu(\mu-2\nu)>0$, from which we obtain $\mu>2\nu$, or $\mu<0$, which correspond to $K_{24}>K_{11}-K_{22}$ and to $K_{24}<-K_{22}$. The critical thickness given by Eq. (34) coincides with the one obtained by Pergamenshchik in the case $L_0=L_1=L$ [7,8].

If $d_c>0$, for $d>d_c$ the quadratic form is positive definite, and the homogeneous state stable. For $d<d_c$ the planar orientation is unstable with respect to the periodic deformation,

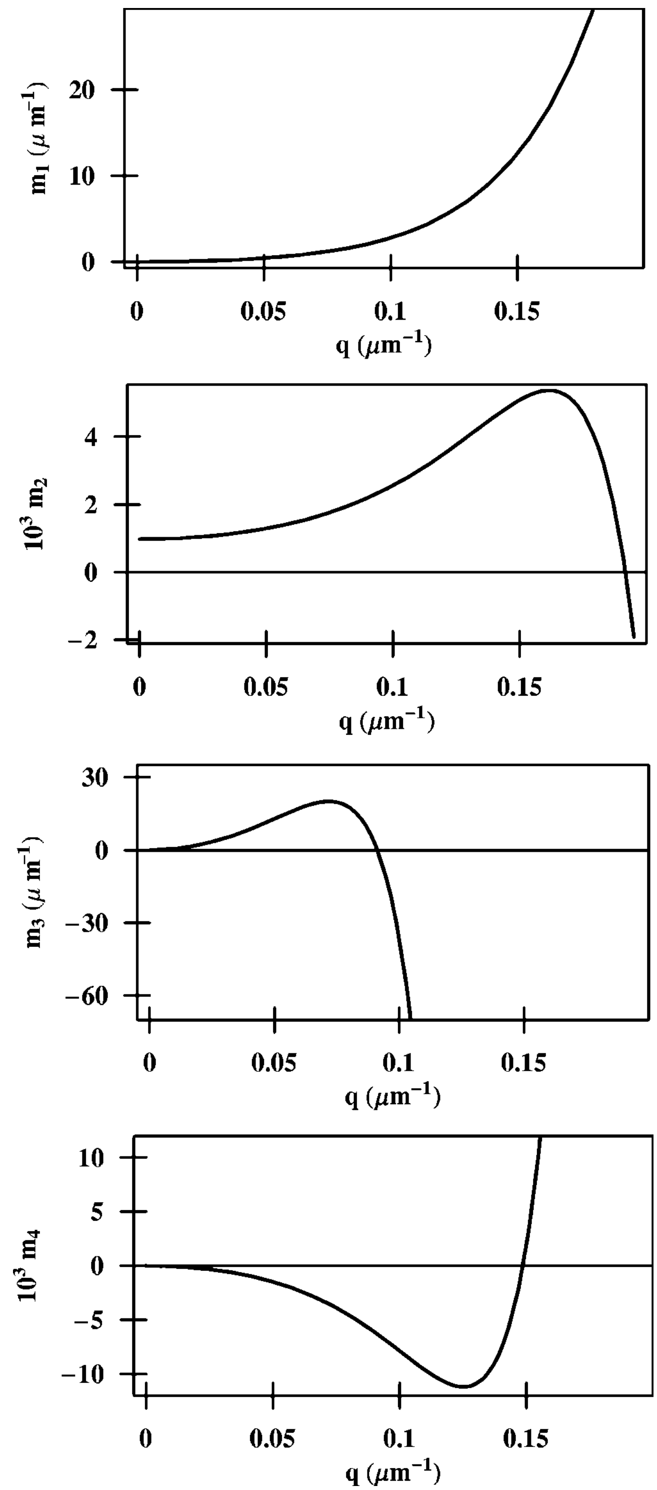

FIG. 1. $m_1(q), m_2(q), m_3(q), m_4(q)$ in the case of a symmetric cell without azimuthal anchoring, for $\mu=3$, $\nu=0.5$, $L_\theta=1$ μm, and $d=12$ μm$<d_c=48$ μm. The planar orientation is never stable.

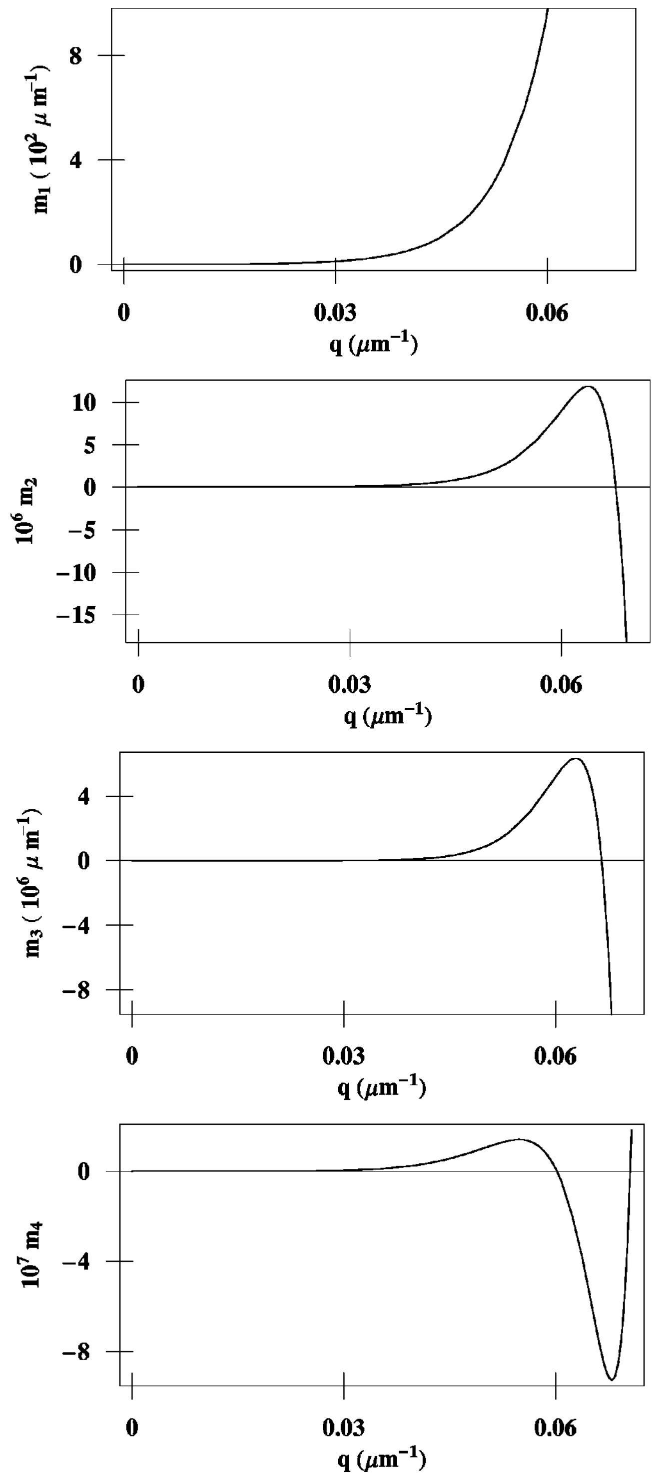

FIG. 2. $m_1(q), m_2(q), m_3(q), m_4(q)$ in the case of a symmetric cell without azimuthal anchoring ($\mu=3, \nu=0.5, L_\theta=1$ μm), for $d=70$ μm$>d_c=48$ μm. The planar orientation is stable for $q<q_0^*=0.0602$ μm^{-1}. q_0^* goes to $q_0^*=0.0667$ μm^{-1} with increasing thickness.

for every polar anchoring energy strength. In this case our linear analysis does not allow to determine the wave vector of the periodic deformation.

In Fig. 1 and Fig. 2 we show the determinants of the principal minors of the matrix $\mathcal{M}$ for arbitrary q, for the set of physical parameters $\mu=3$ and $\nu=0.5$. According to the value of the thickness of the sample we have two different behaviors of $m_4=m_4(q)$.

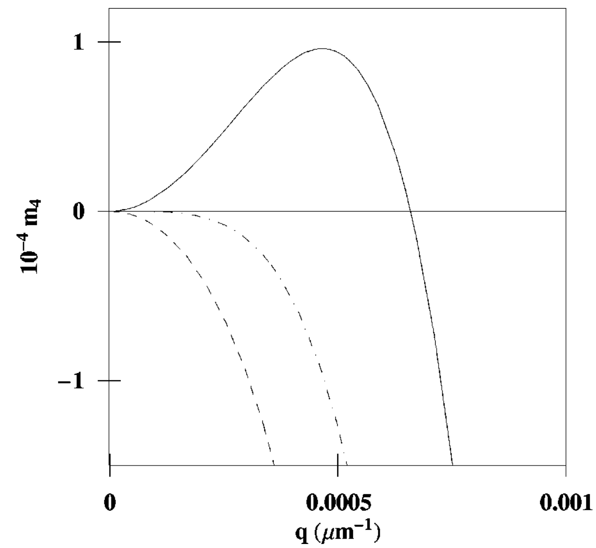

FIG. 3. $m_4(q)$ in the case of a symmetric cell without azimuthal anchoring, for $\mu=3$, $\nu=0.5$, and $L_\theta=1$ μm. The planar orientation becomes unstable when crossing d_c. $d_c=48$ μm (dot-dashed line), $d=d_c+1$ nm (solid line), and $d=d_c-1$ nm (dashed line).

For $d<d_c$ (Fig. 1), $m_4(q)$ has a maximum for $q=0$ and a negative minimum. It becomes positive for $q=q^*$. However, since m_3 remains negative for $q>q^*$, while m_2 becomes zero for a wave vector q larger than q^* and after remains negative, the planar orientation is never stable.

For $d>d_c$ (Fig. 2), $m_4(q)$ has a minimum for $q=0$, a positive maximum and it vanishes for $q=q_0^*$. Then it has a negative minimum, and becomes positive again for $q=q_1^*$. The determinants m_2 and m_3 become negative above q: $q_0^*<q<q_1^*$, and remain negative for $q>q_1^*$. We conclude that the planar orientation is stable only for $q<q_0^*$, since m_1, m_2, m_3, and m_4 are all positive in this range.

Figure 3 shows $m_4(q)$ around the transition from planar ($d>d_c$, solid line) to striped texture ($d<d_c$, dashed line). The dot-dashed line corresponds to the critical thickness, $d_c=48$ μm.

The case where $d\to\infty$ can be treated analytically. In this limit $qd \gg 1$ and consequently $\sinh(qd)\simeq\cosh(qd)$. We indicate by $x=(1/2)\exp(qd)$ their common value. Simple calculations give for the determinants of principal minors of matrix $\mathcal{M}$ the expressions

$$m_1=\frac{\nu+2L_1\mu q}{L_1}x^2,$$

$$m_2=-\frac{\mu(\nu+1)[\nu(\mu-4)+\mu]}{(\nu-1)^2}\left(1-\frac{q_1^*}{q}\right)x^4[1+O(x^{-2})],$$

$$m_3=-\frac{\mu(\nu+1)(\nu+2L_0\mu q)[\nu(\mu-4)+\mu]}{(\nu-1)^2L_0}$$
$$\times\left(1-\frac{q_1^*}{q}\right)x^4[1+O(x^{-2})],$$

$$m_4=\left\{\frac{(\nu+1)[\nu(\mu-4)+\mu]}{(\nu-1)^2}\right\}^2\left(1-\frac{q_0^*}{q}\right)\left(1-\frac{q_1^*}{q}\right)x^4, \tag{35}$$

where

$$q_0^*=\frac{2\nu^2}{L_0\mu[\mu(\nu+1)-4\nu]},$$

$$q_1^*=\frac{2\nu^2}{L_1\mu[\mu(\nu+1)-4\nu]}. \tag{36}$$

From the asymptotic expressions reported in Eq. (35) we derive that, if $L_0>L_1$, m_4 vanishes for q_0^*, and for $q_1^*>q_0^*$, and in the range $q_0^*<q<q_1^*$ it is negative. As regards the other determinants we have: m_1 is always positive, for $\mu>-\nu/(2L_1q)$, whereas m_2 and m_3 vanish for $q\sim q_1^*$, and are positive for $q<q_1^*$ and negative for $q>q_1^*$. Consequently, for $q<q_0^*$ the planar homogeneous orientation is stable, whereas it is unstable for $q>q_1^*$. From the discussion reported above it follows that, in the limit of thick sample, limited by two identical surfaces (which implies $L_0=L_1$, and hence $q_0^*=q_1^*=q^*$), the homogeneous planar orientation is unstable. Due to the presence of thermal fluctuations, the stable nematic orientation is modulated with a wave vector q^*.

The critical wave vector of the instability has to be positive. Consequently, the existence of modulated structures in thick sample in the presence of finite anchoring energy for the polar angles requires

$$\mu<0 \quad \text{or} \quad \mu>\frac{4\nu}{1+\nu}. \tag{37}$$

We note that for $\nu>1$,

$$\frac{4\nu}{1+\nu}>2, \tag{38}$$

as well as

$$\frac{4\nu}{1+\nu}>2\nu, \tag{39}$$

for $\nu<1$. This means that the range defined by Eq. (37) is larger than the one defined by Eq. (7), as expected. In fact, in the presence of finite anchoring for the θ angle, the K_{24} term, responsible for the mechanical instability, has to be larger than the term that can induce periodic structure in an unbounded sample.

B. Influence of the azimuthal anchoring energy on the modulated structure

In the preceeding subsection we have analyzed the possibility of periodic structures in nematic sample, in the hypothesis that the surface treatment was such to induce planar orientation. We have also assumed that no azimuthal anchoring energy was present in the anisotropic part of the surface

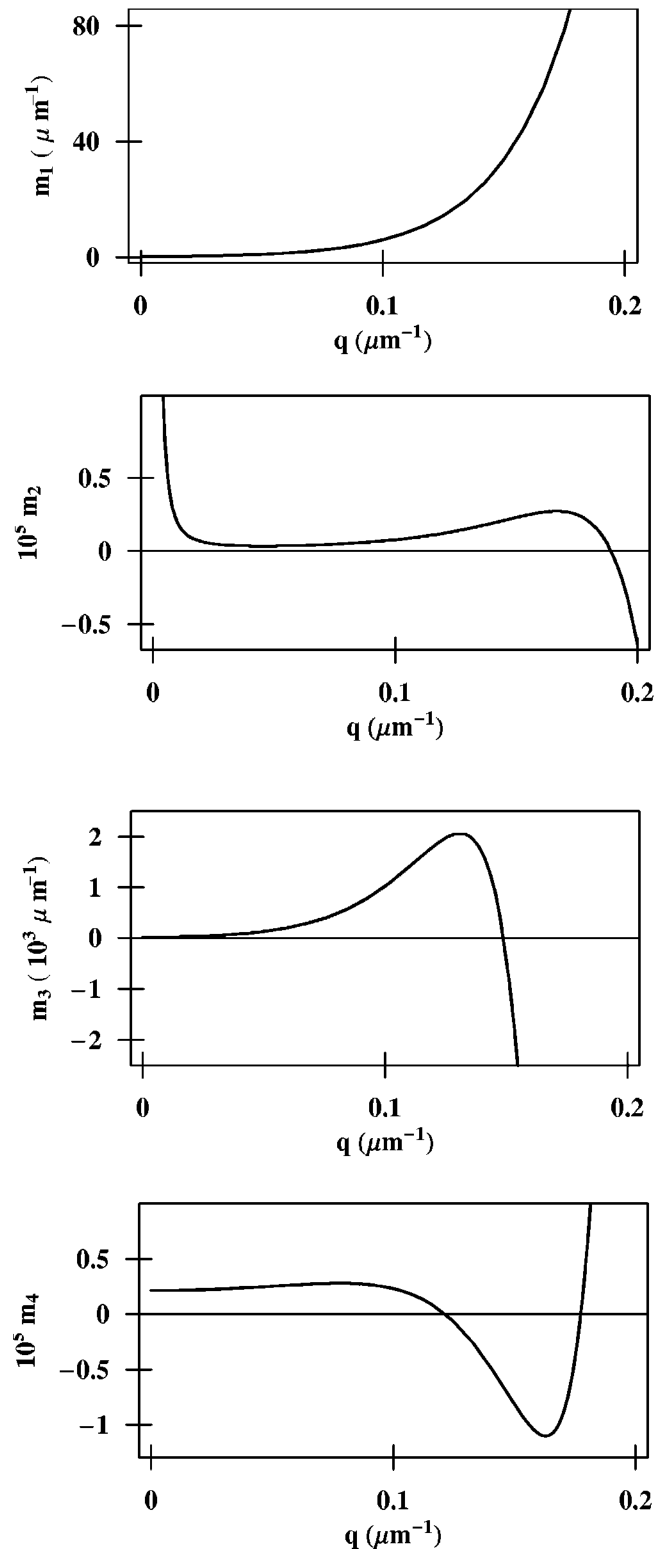

FIG. 4. $m_1(q), m_2(q), m_3(q), m_4(q)$ in the case of a symmetric cell with azimuthal anchoring ($L_\phi=10$ μm, the other parameters are the same as previously), for a thin sample: $d=12$ μm. Long wavelength deformations are forbidden, i.e., the uniform texture is stable, no critical thickness exists. An instability may appear when $m_4\leqslant 0$. q^* is the wave vector of the periodic instability in the limit of large d.

tension characterizing the interface between the nematic liquid crystal and the solid substrate. The aim of this subsection is to generalize the previous results to take into account a finite azimuthal anchoring energy. We limit our investigation to the case in which the two limiting surfaces are identical, and hence $L_{0\theta}=L_{1\theta}=L_\theta$, and $L_{0\phi}=L_{1\phi}=L_\phi$.

The trends of the determinants of the principal minors of the matrix $\mathcal{M}$, for the set of elastic parameters $\nu=0.5$ and $\mu=3$ are reported in Fig. 4. As it follows from this figure, m_1 is positive for every q. For what concerns m_4, it is positive for $q=0$. It has a positive maximum and a negative minimum. This minimum tends to zero for large d. The behaviors of m_2 and m_3 are also reported in the same figure. They are positive in the limit of $q\to 0$, and can change their sign, for large d, for a value of q close to the one for which m_4 vanishes.

In the limit of small q, it is possible to expand again m_1, m_2, m_3, and m_4 in power series of q. However, in the present case

$$\lim_{q\to 0} m_1(q)=\frac{2}{L_\phi},$$

$$\lim_{q\to 0} m_2(q)=4\frac{\nu}{L_\theta L_\phi}\left\{\frac{\nu+1}{q(\nu-1)}\right\}^2,$$

$$\lim_{q\to 0} m_3(q)=8\frac{\nu^3(d+2L_\phi)d}{(\nu-1)^2 L_\theta L_\phi^2},$$

$$\lim_{q\to 0} m_4(q)=16\left(\frac{\nu}{\nu-1}\right)^4\frac{d^2(d+2L_\theta)(d+2L_\phi)}{L_\theta^2 L_\phi^2}. \quad (40)$$

It follows that the critical thickness, as defined before, does not exist any longer. This means that if the azimuthal anchoring is not identically zero, it is impossible to find a d_c such that for $d<d_c$ the planar orientation is unstable with respect to periodic deformations for $q\to 0$. This result can be easily understood: if $w_\phi\neq 0$ a period deformation involving twist deformation costs also in surface energy. Consequently, long wave deformations, having $q\to 0$, are forbidden.

In the limit of large d (Fig. 5), where $\cosh(qd)\simeq\sinh(qd)$ the expressions for the determinants are

$$m_1=\frac{(\nu+2\mu L_\theta q)L_\phi+L_\theta}{L_\theta L_\phi}x^2[1+O(x^{-2})],$$

$$m_2=-\frac{(\nu+1)L_\theta[\nu(\mu-4)+\mu]}{(\nu-1)^2 L_\theta}\left(1-\frac{q_a^*}{q}\right)\times\left(1-\frac{q_b^*}{q}\right)x^4[1+O(x^{-2})],$$

$$m_3=-\frac{(\nu+1)L_\theta[\nu(\mu-4)+\mu]}{(\nu-1)^2 L_\theta^2}[\nu+(L_\theta/L_\phi)+2\mu q L_\theta]\times\left(1-\frac{q_a^*}{q}\right)\left(1-\frac{q_b^*}{q}\right)x^4[1+O(x^{-2})],$$

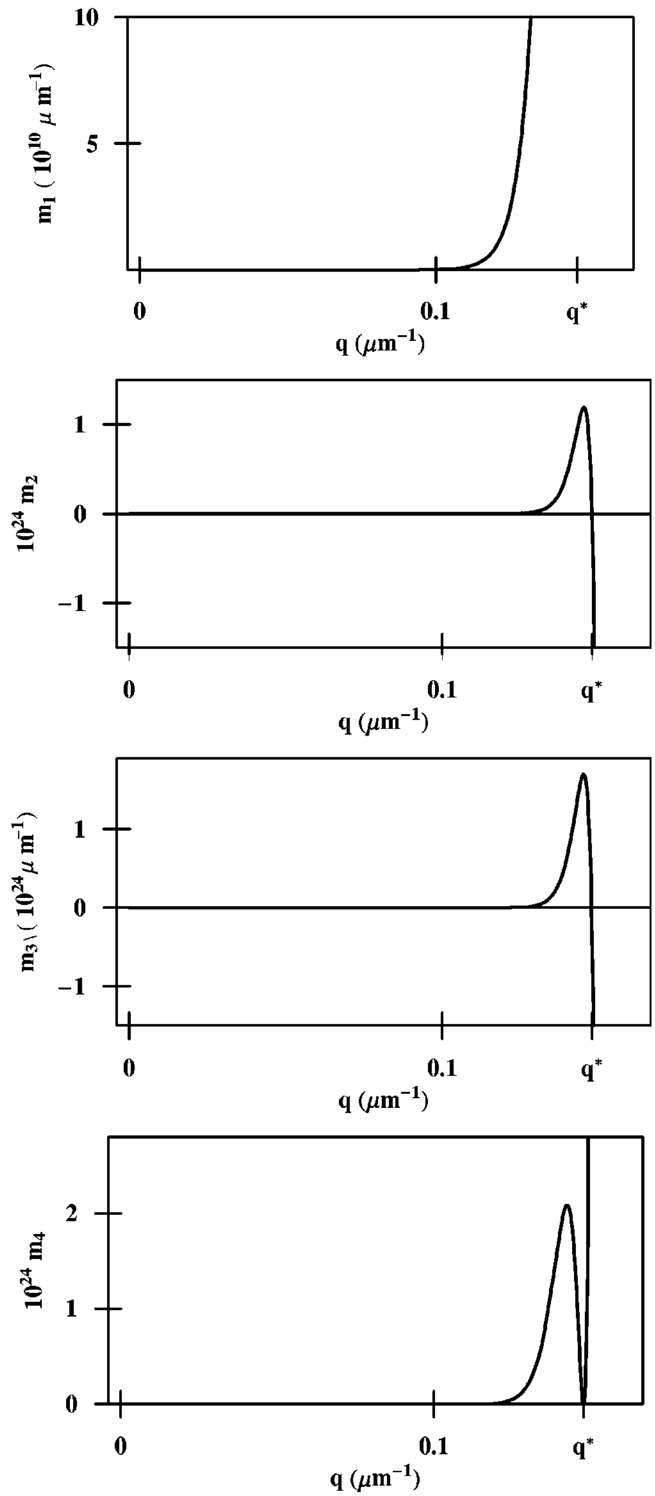

FIG. 5. Same conditions as Fig. 4. Thick sample: $d=100$ μm, the wave vector of the periodic instability goes to q^*.

$$m_4=\left\{\frac{(\nu+1)L_\theta[\nu(\mu-4)+\mu]}{(\nu-1)^2 L_\theta}\right\}^2\left(1-\frac{q_a^*}{q}\right)^2\left(1-\frac{q_b^*}{q}\right)^2 x^4, \quad (41)$$

where, as before, $x=(1/2)\exp(qd)$, and q_a^* and q_b^* are given by

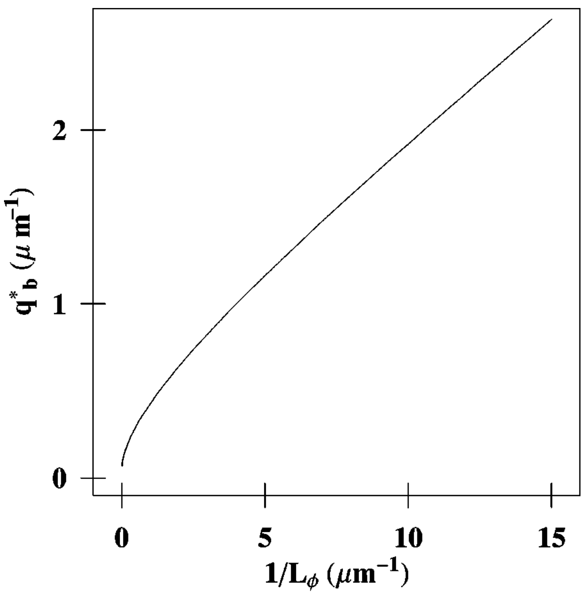

FIG. 6. Dependence of the periodic instability wave vector q_b^* on L_ϕ in the limit of large d. The periodicity tends to molecular dimensions with azimuthal anchoring energy.

$$q_a^* = \frac{\nu[\nu+(L_\theta/L_\phi)]}{L_\theta\mu[\nu(\mu-4)+\mu]} - \sqrt{\left(\frac{\nu[\nu+(L_\theta/L_\phi)]}{L_\theta\mu[\nu(\mu-4)+\mu]}\right)^2 + \frac{\nu(\nu+1)}{L_\theta L_\phi\mu[\nu(\mu-4)+\mu]}},$$

$$q_b^* = \frac{\nu[\nu+(L_\theta/L_\phi)]}{L_\theta\mu[\nu(\mu-4)+\mu]} + \sqrt{\left(\frac{\nu[\nu+(L_\theta/L_\phi)]}{L_\theta\mu[\nu(\mu-4)+\mu]}\right)^2 + \frac{\nu(\nu+1)}{L_\theta L_\phi\mu[\nu(\mu-4)+\mu]}}. \tag{42}$$

From Eqs. (42) it follows that even in the case of finite azimuthal anchoring energy the condition to have periodic deformations in nematic samples is that inequalities (37) hold.

The critical wave vectors q_a^* and q_b^*, in the limit of $w_\phi \to 0$, become 0 and q^*, respectively, as obtained in the preceding subsection. In the opposite case of $w_\phi \neq 0$, $q_a^* < 0$ and $q_b^* > 0$. Consequently, the wave vector of the instability is q_b^*. In this case the presence of a finite L_ϕ is responsible for an increase of the value of the critical wave vector, i.e., a reduction of the spatial periodicity of the deformation. If the azimuthal anchoring is strong, and hence $L_\phi \to 0$, the spatial periodicity tends to molecular dimensions (Fig. 6).

VI. CONCLUSION

We have shown that the analysis of stability of the uniform state, with respect to the periodically deformed one, is easily performed if the quadratic form representing the total energy in terms of the integration constant is known. We have indicated how to obtain the matrix of the coefficients of the quadratic form. As an application, we have used our formalism to obtain the critical thickness of a nematic sample characterized by planar easy axes on both surfaces to observe periodic deformations. We have also considered the possibility of periodic deformations in a thick sample, taking into account the presence of polar and azimuthal anchoring energy.

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APPENDIX

The aim of this appendix is to derive the contribution of the surfacelike term to the elastic energy density. We put $\mathbf{v} = \mathbf{n}\nabla\cdot\mathbf{n} + \mathbf{n}\times(\nabla\times\mathbf{n})$. In Cartesian coordinates $\nabla\cdot\mathbf{n} = n_{\gamma,\gamma}$, and $\nabla\times\mathbf{n} = \varepsilon_{\beta\gamma\alpha} n_{\alpha,\gamma}\mathbf{e}_\beta$, where $\varepsilon_{\beta\gamma\alpha}$ is the antisymmetric tensor (Levi-Civita tensor), and Einstein's convention has been used. Consequently, $\mathbf{n}\nabla\cdot\mathbf{n} = n_\mu n_{\gamma,\gamma}\mathbf{e}_\mu$, and

$$\mathbf{n}\times(\nabla\times\mathbf{n}) = \varepsilon_{\mu\nu\beta} n_\nu (\nabla\times\mathbf{n})_\beta \mathbf{e}_\mu = \varepsilon_{\mu\nu\beta} n_\nu \varepsilon_{\beta\gamma\alpha} n_{\alpha,\gamma}\mathbf{e}_\mu. \tag{A1}$$

Since $\varepsilon_{\mu\nu\beta} = \varepsilon_{\beta\mu\nu}$, we have $\varepsilon_{\mu\nu\beta}\varepsilon_{\beta\gamma\alpha} = \varepsilon_{\beta\mu\nu}\varepsilon_{\beta\gamma\alpha} = \delta_{\mu\gamma}\delta_{\nu\alpha} - \delta_{\mu\alpha}\delta_{\nu\gamma}$, and from Eq. (A1) we get

$$\mathbf{n}\times(\nabla\times\mathbf{n}) = (\delta_{\mu\gamma}\delta_{\nu\alpha} - \delta_{\mu\alpha}\delta_{\nu\gamma}) n_\nu n_{\alpha,\gamma}\mathbf{e}_\mu = (n_\alpha n_{\alpha,\mu} - n_\gamma n_{\mu,\gamma})\mathbf{e}_\mu. \tag{A2}$$

By taking into account that $|\mathbf{n}| = 1$, and hence $n_\alpha n_\alpha = 1$, a simple calculation gives $n_\alpha n_{\alpha,\mu} = 0$. Consequently, from Eq. (A2) we obtain $\mathbf{n}\times(\nabla\times\mathbf{n}) = -n_\gamma n_{\mu,\gamma}\mathbf{e}_\mu$. It follows that vector $\mathbf{v}$ can be written as $\mathbf{v} = (n_\mu n_{\gamma,\gamma} - n_\gamma n_{\mu,\gamma})\mathbf{e}_\mu$, and its divergence is found to be

$$\nabla\cdot\mathbf{v} = v_{\mu,\mu} = (n_\mu n_{\gamma,\gamma} - n_\gamma n_{\mu,\gamma})_\mu = n_{\mu,\mu} n_{\gamma,\gamma} - n_{\gamma,\mu} n_{\mu,\gamma}. \tag{A3}$$

In the case considered in our paper, $\mathbf{n} = \mathbf{n}(y,z)$. Hence,

$$n_{\mu,\mu} n_{\gamma,\gamma} = n_{y,y}^2 + 2n_{y,y} n_{z,z} + n_{z,z}^2,$$

$$n_{\gamma,\mu} n_{\mu,\gamma} = n_{y,y}^2 + 2n_{y,z} n_{z,y} + n_{z,z}^2. \tag{A4}$$

In this framework $\nabla\cdot\mathbf{v} = 2(n_{y,y}n_{z,z} - n_{y,z}n_{z,y})$, and the surfacelike contribution to the elastic energy density we are looking for, given by $-(K_{22}+K_{24})\nabla\cdot\mathbf{v}$, is

$$-(K_{22}+K_{24})\nabla\cdot\mathbf{v} = -2(K_{22}+K_{24})(n_{y,y}n_{z,z} - n_{y,z}n_{z,y}), \tag{A5}$$

as reported in Eq. (2).

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