PHYSICAL REVIEW E VOLUME 49, NUMBER 6 JUNE 1994

Anchoring energy for nematic liquid crystals: Contribution from the spatial variation of the elastic constants

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(Received 16 November 1993; revised manuscript received 2 February 1994)

The influence of the spatial variation of the elastic constants of a nematic liquid crystal on the detectable surface anchoring energy is analyzed. It is shown that, in the framework of the usual elastic approach, the apparent surface free energy connected with the spatial variation of the elastic constants is proportional to the difference between the average value of the elastic constant in the surface layer and the bulk value. The related extrapolation length is estimated to be of the order of the interaction range of the forces responsible for the nematic phase. When the spatial variation of the elastic constants is large and the usual elastic approach does not work, the same analysis is performed in the framework of the second-order elasticity. In this case a nonlocal form for the surface energy is used. By considering simple situations the equivalent surface anchoring energy is deduced. Our results generalize the conclusions obtained by other researchers for a similar problem.

PACS number(s): 61.30.Cz, 61.30.Gd

I. INTRODUCTION

The bulk elastic behavior of nematic liquid crystals (NLC's) is well described by the continuum theory proposed long ago by Frank [1]. According to this theory a distorted NLC is described by a vectorial field $\mathbf{n}=\mathbf{n}(\mathbf{r})$, called director. It is defined as the statistical average of the long axis of the rodlike molecules forming the NLC phase. The vectorial field $\mathbf{n}(\mathbf{r})$ is obtained by minimizing the total free energy F of the NLC sample under consideration. In the case in which the orientation of $\mathbf{n}$ on the limiting surface of the sample is fixed by the surface treatment, F can be written as

$$F=\int_\tau f(n_i,n_{i,j})d\tau \ , \tag{1.1}$$

where τ is the volume of the sample, n_i the i component of the director $\mathbf{n}$, $n_{i,j}=\partial n_i/\partial x_j$ its spatial derivatives, and f the NLC free-energy density. By minimizing F and taking into account that $\mathbf{n}^2=1$, one obtains that $\mathbf{n}(\mathbf{r})$ satisfies the differential equations

$$\frac{\partial f}{\partial n_i}-\partial_j\frac{\partial f}{\partial n_{i,j}}=\lambda n_i, \quad \forall \mathbf{r}\in\tau \ , \tag{1.2}$$

where $\partial_j=\partial/\partial x_j$, and λ is a Lagrange multiplier connected with the condition $\mathbf{n}^2=1$.

Equation (1.2) has to be solved with the boundary conditions

$$n_i(\mathbf{r})=n_{0_i}(\mathbf{r}), \quad \forall \mathbf{r}\in\Sigma \ , \tag{1.3}$$

where $\mathbf{n}_0(\mathbf{r})$ is the director imposed by the surface treatment, and Σ is the surface limiting the volume τ of the sample. The situation described above is known as the strong anchoring case, in which $\mathbf{n}_0(\mathbf{r}\in\Sigma)$ is independent on the bulk distribution of $\mathbf{n}(\mathbf{r})$.

In a more realistic situation the surface orientation of the director depends on the bulk NLC distortion. This case is known as weak anchoring case. In this case the total free energy of the NLC sample is given by

$$F=\int_\tau f(n_i,n_{i,j})d\tau+\int_\Sigma \psi(n_i)d\Sigma \ , \tag{1.4}$$

where the first term of the right-hand side is the bulk contribution, and the second one the surface contribution. $\psi(n_i)$ is the so-called surface free-energy density [2].

By minimizing (1)–(4) one obtains that $\mathbf{n}(\mathbf{r})$ is still a solution of Eq. (1.2), for which the boundary conditions are now given by

$$N_j\frac{\partial f}{\partial n_{i,j}}+\frac{\partial \psi}{\partial n_i}=0, \quad \forall \mathbf{r}\in\Sigma \ , \tag{1.5}$$

where $\mathbf{N}$ is a unit vector parallel to the normal to the surface $d\Sigma(\mathbf{r})$. In the case in which the NLC is undeformed (and hence $n_{i,j}=0$, $\forall \mathbf{r}\in\tau$), Eq. (1.5) gives

$$\frac{\partial \psi}{\partial n_i}=0, \quad \forall \mathbf{r}\in\Sigma \ , \tag{1.6}$$

which defines the surface easy axis $\boldsymbol{\pi}$, i.e., the surface orientation minimizing the surface free energy. In the case $|\mathbf{n}(\mathbf{r}\in\Sigma)-\boldsymbol{\pi}|\ll 1$, ψ can be written in the form

$$\psi(n_i)=-\frac{w}{2}(\mathbf{n}\cdot\boldsymbol{\pi})^2, \quad \forall \mathbf{r}\in\Sigma \ , \tag{1.7}$$

known as the Rapini-Papoular [2] expression of the surface energy density.

The previous discussion concerning the stable orientation of a deformed NLC is general and applies to all elastic problems [3]. However, it is important to stress that the analysis implies the possibility of separating the bulk contribution from the surface one. As it is well known, f is usually written in the Frank form

$$f=\frac{k_{11}}{2}(\mathrm{div}\mathbf{n})^2+\frac{k_{22}}{2}(\mathbf{n}\cdot\mathrm{rot}\mathbf{n})^2+\frac{k_{33}}{2}(\mathbf{n}\times\mathrm{rot}\mathbf{n})^2\;, \quad (1.8)$$

where k_{11}, k_{22}, and k_{33} are the splay, twist, and bend elastic constants, respectively. They are connected with the intermolecular forces giving rise to the NLC phase. They may be obtained, as shown, e.g., in Ref. [4], by expanding the interaction energy at the second order and integrating over a spherical volume, whose radius coincides with the molecular interaction range ρ. This interaction sphere is complete only if the distance between the molecule under consideration and the boundary surface of the sample is larger than ρ. Otherwise it is incomplete, and the elastic constants depend explicitly on the distance between the molecule and the surface. This implies that a simple elastic description of a NLC near a wall is no longer possible. To be more precise, the separation between bulk and surface contributions is, to some degree, arbitrary. The situation is even more complicated, because the surface may be responsible for "fields" giving rise to a bulklike interaction, localized near the surface, which modifies the expression of f. These aspects of the problem have been analyzed by different authors [5–7].

In this paper we analyze the connection between the spatial variation of the elastic constants and the anchoring energy by supposing that (i) the NLC scalar order parameter S is position independent, (ii) the function density d of the NLC is steplike, and (iii) the conductivity of the NLC is high enough to ensure that the Debye screening length is microscopic.

According to (i) and (ii) the free-energy density of the NLC reduces to the elastic energy given by (1). In the opposite case, in the free-energy density, terms proportional to the gradient of S and of d also appear, as well as contributions proportional to S and d. Of course, a gradient expansion of the free-energy density is possible only if the profiles of S and d are not very sharp. Otherwise the gradient expansion fails to converge, and an elastic description of the NLC free-energy density is no longer possible.

Hypothesis (i) is equivalent to supposing that the temperature of the NLC is sufficient to fix a bulk value of the scalar order parameter equal to the one (unknown) fixed by the surface.

Hypothesis (ii) is equivalent to supposing that the substrate density is equal to that of the NLC, and that packing effects do not cause large number density gradients near the surface limiting the NLC.

Hypothesis (iii) is important in order to neglect the flexoelectric polarization and the electric effect connected to it.

These hypotheses are very restrictive, and a more rigorous analysis also has to consider spatial inhomogeneities of S and d. However, in some special situations, like the one described above, the spatial variation of the elastic constants may be the most important effect due to the presence of the surface. This is true, in particular, when the range of forces giving rise to the NLC phase are long range.

In Sec. II, by considering simple situations, we will show that an apparent weak anchoring energy can be associated with a spatial variation of the elastic constants, even in the case in which the actual interaction energy between the NLC and the substrate is infinite. There we will discuss also the case in which the NLC-substrate interaction is finite, considering in detail the case in which the surface forces are short range. The more general case in which the NLC-substrate interactions has both long- and short-range contributions is also discussed.

In Sec. III it will be shown how it is possible to take into account the spatial variation of the elastic constants by modifying the surface energy density and the bulk elastic energy density. Then a model proposed long ago by Mada will be correctly applied [8–10].

Simple applications of our generalized model will be given in Sec. IV, in which the well-known Freedericksz transition will be reconsidered. The main results of our paper are emphasized in Sec. V.

II. SPATIAL VARIATION OF THE ELASTIC CONSTANT AND ANCHORING ENERGY

As we stressed in Sec. I, the NLC elastic constants are expected to be position dependent near a wall. Their behavior is shown in Fig. 1, which refers to a NLC limited by a flat surface localized at $z=0$. $k(0)$ is the surface value of the elastic constant, k_b the bulk value, and ρ the range of the intermolecular forces responsible for the NLC mesophase.

We underline that in general $k_b-k(0)$ is not negligible with respect to k_b. The aim of this section is to connect $k(z)$ with the anchoring energy. For this we suppose that (1) the NLC deformation is one dimensional, and that the NLC director is everywhere parallel to a given plane; (2) the NLC sample is a slab of thickness d, whose surfaces are localized at $z=0$ and d; (3) the surface at $z=0$ is characterized by strong anchoring, whose easy axis is parallel to the z axis (homeotropic alignment); (4) the surface at $z=d$ is characterized by strong anchoring, whose easy axis is at an angle Φ with the z axis (tilted

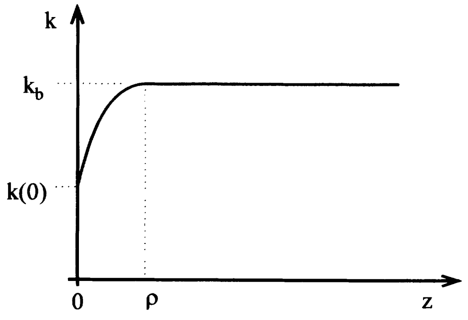

FIG. 1. Nematic elastic constant vs the distance from a flat surface. k_b and $k(0)$ are the bulk and surface values, respectively. The z dependence of the elastic constants is limited to a surface layer, whose thickness is of the order of the range of the intermolecular forces responsible for the nematic phase.

alignment); and (5) the deformation is small and hence $\Phi \ll 1$.

As follows from hypothesis (i), the twist contribution to the elastic energy is identically zero, because $\mathbf{n}\cdot\mathrm{rot}\mathbf{n}\equiv 0$. Consequently the Frank energy density reduces to

$$f=\tfrac{1}{2}k_{11}(z)(\mathrm{div}\mathbf{n})^2+\tfrac{1}{2}k_{33}(z)(\mathbf{n}\times\mathrm{rot}\mathbf{n})^2 ,$$

where $k_{11}(z)$ and $k_{33}(z)$ are the local elastic constants for splay and bend deformations. In terms of the tilt angle $\phi(z)=\cos^{-1}[\mathbf{n}(z)\cdot\hat{\mathbf{e}}_z]$, where $\hat{\mathbf{e}}_z$ is the z-axis unit vector, the expression for f writes

$$f=\tfrac{1}{2}[k_{11}(z)\sin^2\phi(z)+k_{33}(z)\cos^2\phi(z)]\phi'^2 ,$$

where $\phi'=d\phi/dz$. This expression shows that the effective elastic constant

$$k(z)=k_{11}(z)\sin^2\phi(z)+k_{33}(z)\cos^2\phi(z)$$

depends on the nematic tilt angle $\phi(z)$. In the event in which $\phi(z)\to 0$, a simple calculation gives $k(z)=k_{33}(z)+o(\phi^2)$, i.e., the effective elastic constant coincides with the bend elastic constant. In the limit of small tilt angles [hypothesis (5)] the elastic energy density, at the second order in $\phi(z)$, is then

$$f=\tfrac{1}{2}k(z)\phi'^2 . \tag{2.1}$$

As stated above, the $\phi(z)$ profile is obtained by minimizing the total free energy

$$F=\int_0^d \tfrac{1}{2}k(z)\phi'^2 dz , \tag{2.2}$$

with the boundary conditions

$$\phi(0)=0 \quad\text{and}\quad \phi(d)=\Phi . \tag{2.3}$$

Simple calculations give

$$\frac{d}{dz}[k(z)\phi']=0 , \tag{2.4}$$

from which

$$k(z)\phi'=c , \tag{2.5}$$

where c is a constant. By using (2.5) and (2.3), we obtain

$$c=\frac{k_b}{J(0,d)}\Phi , \tag{2.6}$$

where

$$J(\alpha,\beta)=\int_\alpha^\beta \frac{k_b}{k(z)}dz \tag{2.7}$$

is connected to the spatial variation of the elastic constant. By means of (2.6) and (2.7), Eq. (2.5) gives

$$\phi(z)=\Phi\frac{J(0,z)}{J(0,d)} , \tag{2.8}$$

which is the solution of our problem. In the case in which $k(z)=k_b$, Eq. (2.7) gives $J[\alpha,\beta;k(z)=k_b]=\beta-\alpha$, and (2.8) becomes the well-known linear solution for the distortion in the case of fixed boundary conditions:

$$\phi(z)=\Phi\frac{z}{d} . \tag{2.9}$$

In order to relate $k(z)$ to the surface energy, it is necessary to observe that

$$\begin{aligned} &k(z)\neq k_b, \quad \text{for } z\in(0,\rho) \text{ and } z\in(d-\rho,d) ,\\ &k(z)=k_b, \quad \text{for } z\in(\rho,d-\rho) . \end{aligned} \tag{2.10}$$

Consequently, Eq. (2.5) can be written as

$$\begin{aligned} &k(z)\phi'=c, \quad \forall z\in(0,\rho) \text{ and } \forall z\in(d-\rho,d) ,\\ &k_b\phi_b'=c, \quad \forall z\in(\rho,d-\rho) , \end{aligned} \tag{2.11}$$

where

$$\phi_b'=\frac{\phi(d-\rho)-\phi(\rho)}{d-2\rho} , \tag{2.12}$$

is the value of $\phi'(z)$ in the "bulk," i.e., in the region where $k(z)=k_b$ is constant.

From (2.11) we also deduce

$$\phi'(z)=\frac{k_b}{k(z)}\phi_b' . \tag{2.13}$$

By means of (2.13), (2.12), and (2.7), we obtain

$$\begin{aligned} &\phi(z)=\phi_b'J(0,z), \quad z\in(0,\rho) ,\\ &\phi(z)=\phi(\rho)+\phi_b'(z-\rho), \quad z\in(\rho,d-\rho) ,\\ &\phi(z)=\phi(d-\rho)+\phi_b'J(d-\rho,z), \quad z\in(d-\rho,d) . \end{aligned} \tag{2.14}$$

By imposing the continuity of $\phi(z)$ for $z=\rho$ and $z=d-\rho$, and taking into account the boundary conditions (2.3), from Eq. (2.14) we have

$$\begin{aligned} &\phi(\rho)=\phi_b'J(0,\rho) ,\\ &\phi(d-\rho)=\phi(\rho)+\phi_b'(d-2\rho) ,\\ &\Phi=\phi(d-\rho)+\phi_b'J(d-\rho,d) , \end{aligned} \tag{2.15}$$

from which we obtain

$$\begin{aligned} &\phi(\rho)=\frac{J(0,\rho)}{d-2\rho+J(0,\rho)+J(d-\rho,d)}\Phi ,\\ &\phi(d-\rho)=\frac{J(0,\rho)+d-2\rho}{d-2\rho+J(0,\rho)+J(d-\rho,d)}\Phi \end{aligned} \tag{2.16}$$

and hence

$$\phi_b'=\frac{\Phi}{d-2\rho+J(0,\rho)+J(d-\rho,d)} . \tag{2.17}$$

Let us suppose $k_b-k(z)\geq 0$. In this situation the trend of $\phi(z)$ is as shown in Fig. 2, where ϕ_{ex} are deduced by extrapolating the bulk trend of $\phi(z)$ up to the boundaries.

In the case considered, $\phi_{\mathrm{ex}}(0)>0$ and $\phi_{\mathrm{ex}}(d)<\Phi$.

A simple calculation for the extrapolated values of $\phi_{\mathrm{ex}}(0)$ and $\phi_{\mathrm{ex}}(d)$ gives the expressions

$$\begin{aligned} &\phi_{\mathrm{ex}}(0)=\frac{J(0,\rho)-\rho}{d-2\rho+J(0,\rho)+J(d-\rho,d)}\Phi ,\\ &\phi_{\mathrm{ex}}(d)=\frac{J(0,\rho)+(d-\rho)}{d-2\rho+J(0,\rho)+J(d-\rho,d)}\Phi . \end{aligned} \tag{2.18}$$

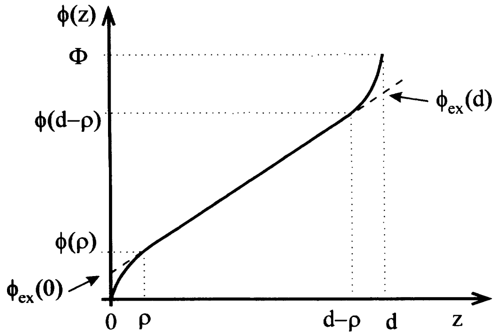

FIG. 2. Nematic tilt angle $\phi(z)$ in a slab characterized by strong anchoring on the two surfaces, whose easy axes are homeotropic and tilted at an angle Φ. In the bulk, where $k(z)=k_b$, $\phi'(z)$ is a constant. In the two boundary layers the z dependence of the elastic constant introduces a spatial variation of $\phi'(z)$.

The extrapolated values of f are the only ones which are experimentally detectable. They may be considered as the actual values of $\phi(z)$, different from $\phi(0)=0$ and $\phi(d)=\Phi$, because the effective anchoring energies are finite.

In order to relate $k(z)$ to the effective anchoring energies, we now have to consider the classical problem in which the elastic constants are position independent, but the surfaces at $z=0$ and d, characterized by easy axes 0 and Φ, have finite anchoring energies w_0 and w_d, respectively. In this frame the $\phi(z)$ profile is obtained by minimizing the quantity

$$F=\int_0^d \frac{k_b}{2}\phi'^2 dz+\frac{w_0}{2}\phi^2(0)+\frac{w_d}{2}[\Phi-\phi(d)]^2 \,, \tag{2.19}$$

where the surface contributions are supposed to be connected with interactions of very short range. Simple calculations give

$$\begin{aligned} &\phi'(z)=\text{const}, \quad \forall z\in(0,d) \,, \\ &-k_b\phi'(0)+w_0\phi(0)=0, \quad z=0 \,, \\ &k_b\phi'(d)+w_d[\phi(d)-\Phi]=0, \quad z=d \,. \end{aligned} \tag{2.20}$$

From the first equation of (2.20), we have

$$\phi'(z)=\frac{\phi(d)-\phi(0)}{d} \,, \tag{2.21}$$

and hence

$$\phi(0)=\frac{L_0}{d+L_0+L_d}\Phi \tag{2.22}$$

for the surface tilt angle on the $z=0$ wall, and

$$\phi(d)=\frac{L_0+d}{d+L_0+L_d}\Phi \tag{2.23}$$

for the surface tilt angle on the $z=d$ wall.

In (2.22) and (2.23), $L_0=k_b/w_0$ and $L_d=k_b/w_d$ are the usual extrapolation lengths.

By identifying $\phi_{\text{ex}}(0)$ and $\phi_{\text{ex}}(d)$ with $\phi(0)$ and $\phi(d)$, Eqs. (2.18) and (2.23) give

$$\begin{aligned} &L_0=J(0,\rho)-\rho \,, \\ &L_d=J(d-\rho,d)-\rho \,, \end{aligned} \tag{2.24}$$

from which it is possible to connect the effective extrapolation lengths with the spatial variation of the elastic constants. In the considered case we can put

$$J(0,\rho)=J(d-\rho,d)=J \tag{2.25}$$

at the lowest order in Φ. In this approximation, from (2.24) we obtain

$$L_0=L_d=J-\rho \,, \tag{2.26}$$

which it is possible to rewrite as

$$\begin{aligned} L_0=L_d=J-\rho&=\int_0^\rho \frac{k_b}{k(z)}dz-\rho \\ &=\int_0^\rho \frac{k_b-k(z)}{k(z)}dz=\rho\left\langle \frac{k_b-k(z)}{k(z)}\right\rangle . \end{aligned} \tag{2.27}$$

The effective surface energy is then

$$w=\left\{\rho\left\langle \frac{k_b-k(z)}{k_b k(z)}\right\rangle\right\}^{-1} . \tag{2.28}$$

Equation (2.27) shows that

$$L=\rho\left\langle \frac{k_b-k(z)}{k(z)}\right\rangle<\rho \,. \tag{2.29}$$

Consequently the extrapolation length connected to the spatial variation of the elastic constants is of the order of ρ, the range of the intermolecular forces responsible for the NLC phase, which is usually very small. It is important to stress that $w>0$ for $k_b\geq k(z)$.

The case considered above was connected with the situation shown in Fig. 3, in which one surface is characterized by homeotropic alignment and the other by tilted alignment. In this case the symmetry is broken in the sense that the surfaces are intrinsically different. For this reason it may be interesting to consider another situation, in which both surfaces are characterized by tilted alignments with antiparallel configurations, as shown in Fig. 4. In this case the easy axes are $\pm\Phi$ for $z=\pm d/2$. In this case the surfaces are identical, and therefore it is possible to give a simple analysis of the effective anchoring energy connected to $k(z)$. To analyze this case it is useful to use the Cartesian reference frame shown in Fig. 4.

The total free energy is still given by (2.2), and the boundary conditions are now

$$\begin{aligned} &\phi\left[-\frac{d}{2}\right]=-\Phi \,, \\ &\phi\left[\frac{d}{2}\right]=\Phi \,. \end{aligned} \tag{2.30}$$

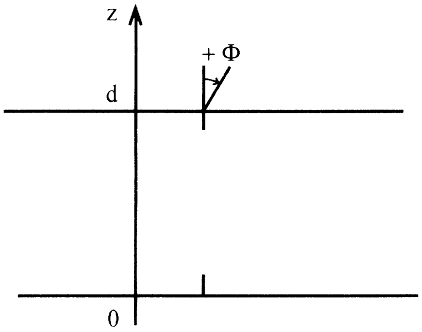

FIG. 3. Nematic liquid crystal slab, characterized by homeotropic and tilted easy axes.

By minimizing the total free energy one again obtains Eq. (2.5), whose solution is now odd in z: $\phi(z)=-\phi(-z)$. By solving Eq. (2.5) for the case under consideration, we obtain

$$\phi(z)=-\Phi+\phi_b' J\left(-\frac{d}{2},z\right), \quad z\in\left[-\frac{d}{2},-\frac{d}{2}+\rho\right],$$
$$\phi(z)=\phi_b' z, \quad z\in\left[-\frac{d}{2}+\rho,0\right]. \tag{2.31}$$

By imposing the usual conditions of continuity and taking into account (2.30), we have

$$\phi\left(-\frac{d}{2}+\rho\right)=-\frac{-\frac{d}{2}+\rho}{-\frac{d}{2}+\rho-J\left(-\frac{d}{2},-\frac{d}{2}+\rho\right)}\Phi \tag{2.32}$$

and

$$\phi_b'=-\frac{\Phi}{-\frac{d}{2}+\rho-J\left(-\frac{d}{2},-\frac{d}{2}+\rho\right)}. \tag{2.33}$$

The extrapolated value of the tilt angle is then

$$\phi_{\text{ex}}\left(-\frac{d}{2}\right)=\phi_b'\left(-\frac{d}{2}\right)=\frac{\frac{d}{2}}{-\frac{d}{2}+\rho-J\left(-\frac{d}{2},-\frac{d}{2}+\rho\right)}\Phi. \tag{2.34}$$

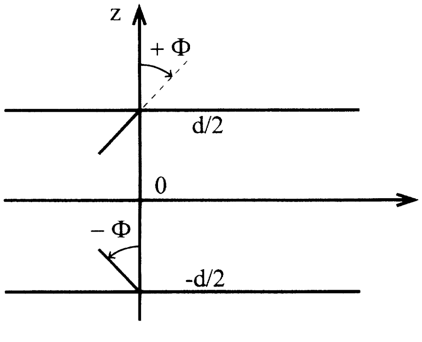

FIG. 4. Nematic liquid crystal slab, characterized by opposite easy axes.

In order to find the equivalent anchoring energy we now have to identify $\phi_{\text{ex}}(-d/2)$ with the surface tilt angle obtained by minimizing the quantity

$$F=\int_{-d/2}^{d/2}\frac{k_b}{2}\phi'^2 dz+\frac{w}{2}\left[\phi\left(-\frac{d}{2}\right)+\Phi\right]^2+\frac{w}{2}\left[\phi\left(\frac{d}{2}\right)-\Phi\right]^2. \tag{2.35}$$

Expression (2.35) refers to a NLC sample for which it is possible to assume $k(z)=k_b$, but characterized by finite anchoring energies w, and easy directions $\pm\Phi$, due to short-range surface forces. Simple calculations give

$$\phi\left(-\frac{d}{2}\right)=-\frac{\frac{d}{2}}{\frac{d}{2}+L}\Phi, \tag{2.36}$$

where $L=k/w$. By comparing (2.36) with (2.34), we obtain

$$L=J\left(-\frac{d}{2},-\frac{d}{2}+\rho\right)-\rho$$
$$=\int_{-d/2}^{-d/2+\rho}\frac{k_b-k(z)}{k(z)}=\rho\left\langle\frac{k_b-k(z)}{k(z)}\right\rangle, \tag{2.37}$$

coinciding with (2.29).

The case considered now is important because it gives us the opportunity to analyze the situation in which the elastic constants are position dependent and, at the same time, the anchoring energy is finite. In this manner we can show that the effective surface energy has an intrinsic part and a part coming from the spatial variation of k. To show this, let us consider the situation in which the total free energy is given by

$$F=\int_{-d/2}^{d/2}\frac{k(z)}{2}\phi'^2 dz+\frac{w_i}{2}\left[\phi\left(-\frac{d}{2}\right)+\Phi\right]^2+\frac{w_i}{2}\left[\phi\left(\frac{d}{2}\right)-\Phi\right]^2, \tag{2.38}$$

instead of (2.2). In (2.38), w_i is the intrinsic anchoring energy where, as before, the surface contributions are supposed connected to the NLC-substrate interactions of very short range. In the event in which surface long-range interactions contribute to the free energy, the analysis has to be modified, as will be discussed at the end of this section.

Let us now neglect these long-range contributions. By minimizing (2.38), we again obtain Eq. (2.5), whose solution is odd in z, and the boundary condition

$$-k\left[-\frac{d}{2}\right]\phi'\left[-\frac{d}{2}\right]+w_i\left[\phi\left[-\frac{d}{2}\right]+\Phi\right]=0\ , \qquad (2.39)$$

at $z=-d/2$. By using Eqs. (2.5) and (2.39) we obtain

$$\phi\left[-\frac{d}{2}\right]=\frac{k_i}{w_i}\phi'_b-\Phi \qquad (2.40)$$

for the surface tilt angle, and

$$\begin{gathered}\phi(z)=\phi\left[-\frac{d}{2}\right]+\phi'_b J\left[-\frac{d}{2},z\right]\ ,\\ z\in\left[-\frac{d}{2},-\frac{d}{2}+\rho\right]\ ,\\ \phi(z)=\phi'_b z,\quad z\in\left[-\frac{d}{2}+\rho,0\right]\end{gathered} \qquad (2.41)$$

for the $\phi(z)$ profile near the wall and in the bulk.

By using (2.41) and (2.40), for the extrapolated value of ϕ we obtain the expression

$$\phi_{\text{ex}}=\phi'_b\left[-\frac{d}{2}\right]=\frac{\frac{d}{2}}{-\frac{d}{2}+\rho-J\left[-\frac{d}{2},-\frac{d}{2}+\rho\right]-\frac{k_b}{w_i}}\Phi\ . \qquad (2.42)$$

Comparing (2.42) with (2.36), we have

$$L=J\left[-\frac{d}{2},-\frac{d}{2}+\rho\right]-\rho+\frac{k_b}{w_i} \qquad (2.43)$$

for the effective extrapolation length. Equation (2.43) may be rewritten as

$$L=\rho\left\langle\frac{k_b-k(z)}{k(z)}\right\rangle+\frac{k_b}{w_i}\ , \qquad (2.44)$$

showing that L has an intrinsic part, k_b/w_i, and a part connected to the spatial variation of k. The effective anchoring energy is then found to be

$$\frac{1}{w}=\rho\left\langle\frac{k_b-k(z)}{k_b k(z)}\right\rangle+\frac{1}{w_i}\ . \qquad (2.45)$$

From (2.45) we may conclude that a spatial variation of the elastic constant is equivalent to a finite anchoring energy. The effective anchoring energy can be separated into intrinsic and extrinsic parts.

The analysis reported after Eq. (2.38) holds in the case in which the surface contributions are connected only to short-range interactions. In the event in which long-range contributions play an important role, the total free energy to be minimized is

$$\begin{aligned}F=&\int_{-d/2}^{d/2}\left[\frac{k(z)}{2}\phi'^2+\tfrac{1}{2}u(z)\phi^2\right]dz\\ &+\frac{w_i}{2}\left[\phi\left[-\frac{d}{2}\right]+\Phi\right]^2+\frac{w_i}{2}\left[\phi\left[\frac{d}{2}\right]-\Phi\right]^2\ ,\end{aligned} \qquad (2.46)$$

instead of (2.38). In (2.46), $\frac{1}{2}u(z)\phi^2$ is the anisotropic contribution to the bulk energy connected with the long-range contributions of the NLC-substrate interaction, in the limit of small tilt angle ϕ. A problem of this kind was considered, in a different context, by Dubois-Violette and de Gennes [11].

$u(z)$ is different from zero only in two surface layers of thickness r, i.e.,

$$\begin{aligned}&u(z)\neq 0\ \text{ for }\ z\in\left[-\left[\frac{d}{2}\right],-\left[\frac{d}{2}\right]+r\right]\ \text{ and }\ z\in\left[\left[\frac{d}{2}\right]-r,\left[\frac{d}{2}\right]\right]\ ,\\ &u(z)=0\ \text{ for }\ z\in\left[-\left[\frac{d}{2}\right]+r,\left[\frac{d}{2}\right]-r\right]\ .\end{aligned} \qquad (2.47)$$

A simple analysis of (2.46) shows that for $r \ll \rho$, the long-range term renormalizes the short-range ones. In this framework (2.46) is equivalent to

$$\begin{aligned}F=&\int_{-d/2}^{d/2}\frac{k(z)}{2}\phi'^2 dz\\ &+\tfrac{1}{2}(w_i+A)\left[\phi\left[-\frac{d}{2}\right]+\frac{w_i}{w_i+A}\Phi\right]^2\\ &+\tfrac{1}{2}(w_i+A)\left[\phi\left[\frac{d}{2}\right]-\frac{w_i}{w_i+A}\Phi\right]^2+\text{const}\ ,\end{aligned} \qquad (2.48)$$

where

$$A=\int_{d/2}^{-(d/2)+r}u(z)dz=r\langle u(z)\rangle\ . \qquad (2.49)$$

Hence, in this case ($r \ll \rho$) the previous analysis works well. In particular, Eq. (2.44) remains valid if w_i is changed in w_i+A and Φ in $[w_i/(w_i+A)]\Phi$. However, the situation $r \ll \rho$ is not very interesting because it is equivalent to supposing again that the surface forces are short ranged. The most important situation is the one in which $r \simeq \rho$. From the physical point of view this means that the interaction of the NLC molecules with the substrate molecules has a short-range contribution due to steric effects (responsible for w_i), and a long-range contribution, connected, for instance, to the anisotropic van der Waals interactions, of the same kind as those responsible for the NLC phase.

In this case, by minimizing (2.46) we obtain

$$\frac{d}{dz}[k(z)\phi'(z)]-u(z)\phi(z)=0, \quad z\in\left[-\frac{d}{2},\frac{d}{2}\right], \tag{2.50}$$

for the bulk equation, and again the boundary condition (2.39). The solution of (2.50) depends, obviously, on the z dependence of $k(z)$ and $u(z)$. However, it is important to stress that in this case it is no longer possible to separate the $k(z)$ effect from the $u(z)$ effect. Consequently an expression of the kind of (2.45), in which the apparent surface free energy is written as the sum of an elastic contribution and an intrinsic contribution, does not exist. This means that our analysis works well only in the case in which only short-range forces due to NLC-substrate interactions are important.

III. GENERALIZED SURFACE ANCHORING ENERGY

The first attempt to take into account the spatial variation of the elastic constant has been carried out by Mada [8]. We observe that $k(z)$ may be written in the form

$$k(z)=k_b+\Delta k(z), \tag{3.1}$$

where k_b is its bulk value, and $\Delta k(z)$ its variation due to the presence of the surface. Consequently the elastic energy connected with $k(z)$ is

$$F=\int_{-d/2}^{d/2}\tfrac{1}{2}k(z)\phi'^2dz =\int_{-d/2}^{d/2}\tfrac{1}{2}k_b\phi'^2dz+\int_{-d/2}^{d/2}\tfrac{1}{2}\Delta k(z)\phi'^2dz . \tag{3.2}$$

Since $\Delta k(z)\neq 0$ only in two boundary layers of thickness ρ, the last term in (3.2) is equivalent to

$$\int_{-d/2}^{d/2}\tfrac{1}{2}\Delta k(z)\phi'^2dz =\int_{-d/2}^{-d/2+\rho}\tfrac{1}{2}\Delta k(z)\phi'^2dz+\int_{d/2-\rho}^{d/2}\tfrac{1}{2}\Delta k(z)\phi'^2dz, \tag{3.3}$$

where ρ is a quasimicroscopic length. In the framework of the continuum theory, $\phi(z)$ is expected to change over a macroscopic length. Hence (3.3) may be rewritten as

$$\int_{-d/2}^{d/2}\tfrac{1}{2}\Delta k(z)\phi'^2dz =\tfrac{1}{2}\rho\langle\Delta k\rangle_-\phi'^2(z_-^*)+\tfrac{1}{2}\rho\langle\Delta k\rangle_+\phi'^2(z_+^*), \tag{3.4}$$

where

$$\langle\Delta k\rangle_-=\frac{1}{\rho}\int_{-d/2}^{-d/2+\rho}\Delta k(z)dz \tag{3.5}$$

is the mean value of the $\Delta k(z)$ function evaluated in the surface layer near the lower surface, and

$$-\frac{d}{2}<z_-^*<-\frac{d}{2}+\rho .$$

$\langle\Delta k\rangle_+$ and z_+^* have analogous meanings. According to Mada [8], it is possible to identify $\phi'(z_\pm^*)$ with $\phi'(\pm d/2)$, the surface gradients of the tilt angle, and rewrite (3.4) as a true surface term in the form

$$\int_{-d/2}^{d/2}\tfrac{1}{2}\Delta k(z)\phi'^2dz=\tfrac{1}{2}\tilde{w}\phi'^2\left[-\frac{d}{2}\right]+\tfrac{1}{2}\tilde{w}\phi'^2\left[\frac{d}{2}\right], \tag{3.6}$$

where

$$\tilde{w}=\rho\langle\Delta k\rangle \tag{3.7}$$

is an anchoring energy strength connected to the z dependence of the elastic constant. According to Mada, Eq. (3.2) has to be rewritten as

$$F=\int_{-d/2}^{d/2}\tfrac{1}{2}k_b\phi'^2dz+\tfrac{1}{2}\tilde{w}\phi'^2\left[-\frac{d}{2}\right]+\tfrac{1}{2}\tilde{w}\phi'^2\left[\frac{d}{2}\right], \tag{3.8}$$

in the strong anchoring case. The $\phi(z)$ profile is then obtained by minimizing (3.8), with the boundary conditions

$$\phi\left[\pm\frac{d}{2}\right]=\pm\Phi \tag{3.9}$$

if the antisymmetrical case considered at the end of Sec. II has to be solved. The idea of Mada has a physical meaning, but his theoretical analysis is not correct [9,10]. In fact, as is well known, the function minimizing (3.8) is not of the C_1 class [12], but it generally presents a surface discontinuity [13,14]. As we have shown long ago [15,16], it is possible to consider surface energies depending on ϕ and ϕ' and have a well-posed variational problem only by generalizing the bulk elastic energy density. To be more precise, it is possible to consider surface free energies of the kind $\psi=\psi(\phi,\phi')$ only if $f=f(\phi,\phi',\phi'')$. A simple generalization for f is

$$f=\tfrac{1}{2}k_b\phi'^2+\tfrac{1}{2}k^*\phi''^2, \tag{3.10}$$

which was proposed to analyze the influence of the k_{13} elastic constant on the $\phi(z)$ profile [15,16].

In the following we want to connect the effective anchoring energy with the $\tilde{w}$ parameter introduced above. In this manner we will be able to recover, in some special cases, the results obtained in Sec. II. However, we will generalize the results obtained there, in the framework of the second-order elasticity.

Let us consider a NLC slab of thickness d characterized by two opposite easy directions, as done in the last part of Sec. II. The surface free energy densities are supposed to be of the kind

$$\begin{aligned}\psi_1&=\frac{w_1}{2}(\phi_1+\Phi)^2+k_{13}\phi_1\phi_1'+\frac{\tilde{w}_1}{2}\phi_1'^2,\\ \psi_2&=\frac{w_2}{2}(\phi_2-\Phi)^2-k_{13}\phi_2\phi_2'+\frac{\tilde{w}_2}{2}\phi_2'^2,\end{aligned} \tag{3.11}$$

which generalize the ones proposed in [15,16]. In Eq. (3.11) the meaning of the subscripts 1 and 2 is $z=-d/2$ and $+d/2$, respectively. In Eq. (3.11), k_{13} is the splay-bend surfacelike elastic constant [17–19].

Let us now suppose that the surfaces are equal, and hence $w_1=w_2=w$ and $\tilde{w}_1=\tilde{w}_2=\tilde{w}$, implying $\phi(z)=-\phi(-z)$. The total free energy of the NLC slab is given by

$$F=\int_{-d/2}^{d/2}(\tfrac{1}{2}k_b\phi'^2+\tfrac{1}{2}k^*\phi''^2)dz+\psi_1+\psi_2 . \tag{3.12}$$

As usual the $\phi(z)$ profile is obtained by minimizing

(3.12). Simple calculations give

$$b^2\phi'''' - \phi'' = 0, \quad \forall z \in \left[-\frac{d}{2}, \frac{d}{2} \right], \tag{3.13}$$

and the boundary conditions

$$\begin{gathered} (1-R)\phi_2' - b^2\phi_2''' + \frac{1}{L_i}(\phi_2 - \Phi) = 0 , \\ b^2\phi_2'' + R\phi_2 + \tilde{L}\phi_2' = 0 , \end{gathered} \tag{3.14}$$

where

$$b^2 = \frac{k^*}{k}, \quad R = \frac{k_{13}}{k}, \quad L_i = \frac{k}{w}, \quad \tilde{L} = \frac{\tilde{w}}{k} . \tag{3.15}$$

b is a semimicroscopic length, R gives an idea about the importance of the k_{13} elastic term with respect to the usual elastic term, and L_i is the intrinsic extrapolation length connected with the anchoring energy originated by the z dependence of the elastic constants. The solution of (3.13), which is odd with respect to z, is

$$\phi(z) = \alpha \left[\frac{z}{b} \right] + \beta \sin \left[\frac{z}{b} \right] , \tag{3.16}$$

where α and β have to be determined by means of Eq. (3.14). Simple calculations give

$$\alpha = \frac{b}{L_i} \Phi \frac{1 - R + \dfrac{\tilde{L}}{b}}{(1-R)^2 + \tilde{L}\left[\dfrac{1}{b} - \dfrac{1}{L_i} \right] + \dfrac{d}{2L} \left[1 + \dfrac{\tilde{L}}{b} - R^2 \dfrac{L_i}{b} \right]} , \tag{3.17}$$

and

$$\beta = \frac{1}{L_i} \Phi \frac{1}{\sinh X} \frac{R\dfrac{d}{2} - \tilde{L}}{(1-R)^2 + \tilde{L}\left[\dfrac{1}{b} - \dfrac{1}{L_i} \right] + \dfrac{d}{2L_i} \left[1 + \dfrac{\tilde{L}}{b} - R^2 \dfrac{L_i}{b} \right]} , \tag{3.18}$$

where $X = (d/2L) \gg 1$ and hence tgh$X \approx$ ctgh$X = 1$. Since X is very large, it follows that $\phi(z)$ differs from $\alpha(z/b)$ only in the layers near the surfaces at $z = \pm d/2$. Consequently the extrapolated value of the surface tilt angle is found to be

$$\begin{aligned} \phi_{\text{ex}} &= \alpha \left[-\frac{d}{2b} \right] \\ &= -\Phi \frac{\dfrac{d}{2}}{\dfrac{1 + \dfrac{\tilde{L}}{b} - R^2 \dfrac{L_i}{b}}{1 - R + \dfrac{\tilde{L}}{b}} \dfrac{d}{2} + \dfrac{(1-R)^2 + \tilde{L}\left[\dfrac{1}{b} - \dfrac{1}{L_i} \right]}{1 - R + \dfrac{\tilde{L}}{b}} + L_i} . \end{aligned} \tag{3.19}$$

By comparing (3.19) with expression (2.36), it is possible to obtain an expression for the effective surface energy in terms of R, L_i, b, and $\tilde{L}$. Simple calculations for the effective extrapolation length give

$$L = \frac{R - R^2 \dfrac{L_i}{b}}{1 - R + \dfrac{\tilde{L}}{b}} \frac{d}{2} + \frac{(1-R)^2 + \tilde{L}\left[\dfrac{1}{b} - \dfrac{1}{L_i} \right]}{1 - R + \dfrac{\tilde{L}}{b}} L_i . \tag{3.20}$$

L is found to be thickness dependent. This is not surprising because the surface energy density (3.11) is a nonlocal quantity. In the case in which $L_i \to 0$ (strong anchoring) and $R \to 0$ (i.e., by neglecting the k_{13} elastic term), Eq. (3.20) writes

$$L = -\frac{\tilde{L}}{1 + \dfrac{\tilde{L}}{b}} = -\frac{\dfrac{\tilde{w}}{k_b}}{1 + \dfrac{\tilde{w}}{k_b b}} . \tag{3.21}$$

By taking into account that $\tilde{w} = \rho\langle \Delta k(z) \rangle = \rho\langle k_b - k(z) \rangle = -\rho\langle k(z) - k_b \rangle$, it follows from (3.4) and (3.1) that expression (3.21) may be rewritten as

$$L = \frac{\rho \left\langle \dfrac{k(z) - k_b}{k_b} \right\rangle}{1 - \left\langle \dfrac{k(z) - k_b}{k_b} \right\rangle \dfrac{\rho}{b}} . \tag{3.22}$$

Comparing (3.22) with (2.37), we deduce that the two approaches are equivalent only if

$$\left\langle \frac{k(z)-k_b}{k_b} \right\rangle \frac{\rho}{b} \ll 1 \ . \tag{3.23}$$

Otherwise the analysis presented in Sec. II has to be considered a first approximation. In fact, in Sec. II the deformed state of the NLC material is characterized only by the first derivative of the tilt angle ϕ. For this reason the elastic energy density is written in the form (2.1), i.e., in the harmonic approximation. This approach is correct only if $k(z)$ changes slowly and hence $k(z)-k_b$ is very small. In the opposite case, in which $k(z)$ changes very much over ρ, the usual elastic description in term of ϕ' may only be a very rough approximation. To improve the elastic description it is necessary, in this case, to take into account other derivatives of $\phi(z)$ and therefore at least its second derivative. In order to have a well-posed variational problem, the bulk term has to be quadratic in ϕ''. From the above discussion we derive that, in the case in which $\langle k(z)-k_b \rangle$ is not negligible with respect to k_b, the approach presented in this section is expected to work better than the one presented in Sec. II.

In the case in which $R=0$ but $L_i \neq 0$, Eq. (3.20) gives

$$L = \frac{1+\tilde{L}\left[\frac{1}{b}-\frac{1}{L_i}\right]}{1+\frac{\tilde{L}}{b}} L_i \ , \tag{3.24}$$

from which the effective anchoring energy is found to be

$$\frac{1}{w} = \frac{\frac{1}{w_i}+\rho\left\langle \frac{k(z)-k_b}{k_b^2} \right\rangle - \frac{\rho}{b}\left\langle \frac{k(z)-k_b}{k_b} \right\rangle \frac{1}{w_i}}{1-\frac{\rho}{b}\left\langle \frac{k(z)-k_b}{k_b} \right\rangle} \ , \tag{3.25}$$

which generalizes the previous formula (2.45). As before, if (3.23) holds, (3.25) reduces to (2.45).

In the general case in which R and L_i are different from zero, Eq. (3.20) shows that L changes sign when d has the critical value given by

$$d_c = \frac{(1-R)^2+\tilde{L}\left[\frac{1}{b}-\frac{1}{L_i}\right]}{R-R^2\frac{L_i}{b}} L_i \ , \tag{3.26}$$

that in the case of $L_i=0$ reduces to

$$d_c = -2\rho \frac{\langle k(z)-k_b \rangle}{k_{13}} \ . \tag{3.27}$$

Equation (3.27) has a meaning only if $d_c>0$, which implies $\langle [k(z)-k_b]/k_{13} \rangle < 0$, i.e., $k(z) \le k_b$ and $k_{13}>0$, or $k(z) \ge k_b$ and $k_{13}<0$.

IV. FRÉEDERICKSZ TRANSITION

Now let us consider the Fréedericksz transition induced by an electric field on a NLC slab homeotropically oriented by the surface treatments. In our analysis we will assume that the surface energy density has the form (3.1) and that the electric field is perpendicular to the z axis and $\varepsilon_a>0$, or parallel to the z axis and $\varepsilon_a<0$. ε_a is the dielectric anisotropy defined as $\varepsilon_a=\varepsilon_\parallel-\varepsilon_\perp$, where $||$ and $\perp$ refer to the nematic director **n**. In the framework of the second-order elasticity the thermodynamical potential to be minimized is

$$F=2\left\{\int_{-d/2}^{0}\left(\tfrac{1}{2}k\phi'^2+\tfrac{1}{2}k^*\phi''^2-\tfrac{1}{2}\varepsilon_a E^2\phi^2\right)dz+\psi_1\right\} \ . \tag{4.1}$$

Equation (4.1) holds under the hypothesis that the two surfaces are exactly the same, and hence $\phi(z)=\phi(-z)$. Furthermore, F is written in the limit of small tilt angles. By minimizing (4.1), it follows that

$$b^2\phi''''-\phi''-\frac{1}{\xi^2}\phi=0, \quad \forall z \in \left[-\frac{d}{2},\frac{d}{2}\right] \ , \tag{4.2}$$

with the boundary conditions

$$\begin{aligned} &-(1-R)\phi_1'+b^2\phi_1'''+\frac{1}{L}\phi_1=0 \ , \\ &-b^2\phi_1''+R\phi_1+\tilde{L}\phi_1'=0 \ , \end{aligned} \tag{4.3}$$

where $\phi_1=\phi(-d/2)$, $\xi^{-2}=\varepsilon_a E^2/k$ is the electric coherence length, and the other symbols have the usual meaning. The solution of (4.2), even in z, is of the kind

$$\phi(z)=A_1\cos(\eta_1 z)+A_2\cosh(\eta_2 z) \ , \tag{4.4}$$

where A_1 and A_2 are the amplitudes of the deformation, and η_1 and η_2 are given by

$$\eta_1=\left[-\frac{1}{2b^2}+\left[\frac{1}{(2b)^2}+\frac{1}{b^2\xi^2}\right]^{1/2}\right]^{1/2} \tag{4.5}$$

and

$$\eta_2=\left[\frac{1}{2b^2}+\left[\frac{1}{(2b)^2}+\frac{1}{b^2\xi^2}\right]^{1/2}\right]^{1/2} \ . \tag{4.6}$$

We stress that in the $b \to 0$ limit, η_1 and η_2 tend to

$$\eta_1 \to \frac{1}{\xi} \quad \text{and} \quad \eta_2 \to \frac{1}{b} \ . \tag{4.7}$$

By substituting (4.4) into (4.3), we obtain

$$\begin{aligned} &\left\{\frac{1}{L}\cos\left[\eta_1\frac{d}{2}\right]-[b^2\eta_1^2+(1-R)]\eta_1\sin\left[\eta_1\frac{d}{2}\right]\right\}A_1+\left\{\frac{1}{L}\cosh\left[\eta_2\frac{d}{2}\right]-[b^2\eta_2^2-(1-R)]\eta_2\sinh\left[\eta_2\frac{d}{2}\right]\right\}A_2=0 \ , \\ &\left\{\tilde{L}\eta_1\sin\left[\eta_1\frac{d}{2}\right]+(R-b^2\eta_1^2)\cos\left[\eta_1\frac{d}{2}\right]\right\}A_1+\left\{-\tilde{L}\eta_2\sinh\left[\eta_2\frac{d}{2}\right]+(R-b^2\eta_2^2)\cosh\left[\eta_2\frac{d}{2}\right]\right\}A_2=0 \ . \end{aligned} \tag{4.8}$$

System (4.8) is homogeneous. It has a solution different from the trivial one only if the determinant of the coefficients vanishes. This condition gives the threshold field. Since ξ is expected to be of the order of the thickness of the sample d, whereas $b \ll d$, it is possible for η_1 and η_2 to use the values (4.7). In this case the threshold condition is

$$\frac{1}{\xi} tg\left[\frac{d}{2\xi}\right] = \frac{\frac{1}{L_i} - \frac{R^2}{b} + \frac{\tilde{L}}{bL_i}}{(1-R)\left[1-R+\frac{\tilde{L}}{b}\right] - \left[\frac{1}{L_i} - \frac{R}{b}\right]\tilde{L}} . \tag{4.9}$$

Equation (4.9), in which $\tilde{L}=0$ (i.e., the elastic constant is position independent), gives

$$\frac{1}{\xi} tg\left[\frac{d}{2\xi}\right] = \frac{1}{(1-R)^2}\left[\frac{1}{L_i} - \frac{R^2}{b}\right] , \tag{4.10}$$

which coincides with a result obtained a few years ago [15]. It is important to stress that the R term reduces the effective anchoring energy. In fact, by comparing (4.10) with the Rapini-Papoular expression [20]

$$\frac{1}{\xi} tg\left[\frac{d}{2\xi}\right] = \frac{1}{L} , \tag{4.11}$$

we derive that the effective anchoring energy is

$$w = \frac{1}{(1-R)^2}\left[w_i - k_b\frac{R^2}{b}\right] . \tag{4.12}$$

This equation shows that w is reduced of a quantity equal to $k_b R^2/b$, in addition to the renormalization factor $(1-R)^{-2}$.

In the general case, for the effective extrapolation length Eq. (4.9) gives

$$\frac{1}{L} = \frac{\frac{1}{L_i}\left[1+\frac{\tilde{L}}{b}\right] - \frac{R^2}{b}}{(1-R)^2 + \tilde{L}\left[\frac{1}{b} - \frac{1}{L_i}\right]} , \tag{4.13}$$

from which results the effective anchoring energy that we are looking for:

$$w = \frac{w_i\left[1+\frac{\tilde{L}}{b}\right] - \frac{k_b R^2}{b}}{(1-R)^2 + \frac{\tilde{L}}{b}\left[1 - \frac{b}{L_i}\right]} . \tag{4.14}$$

In the limit of $L_i \rightarrow 0$, (4.14) gives

$$\frac{1}{L} = -\frac{1+\frac{\tilde{L}}{b}}{\tilde{L}} , \tag{4.15}$$

i.e., we recover Eq. (3.21). However, Eq. (4.14) generalizes Eq. (4.12) in the case in which the elastic constants of the nematic are position dependent, and $\Delta k(z)$ is not negligible with respect to k_b.

V. CONCLUSIONS

The surface properties of nematic liquid crystals have been analyzed. We have shown that the separation of the total energy into bulk and surface contributions is arbitrary. In particular, the contribution to the usual surface free energy, coming from the spatial variation of the elastic constants, is evaluated in the framework of first- and second-order elasticity theories. The main conclusion is that in the event in which the spatial variation of the elastic constants is very small with respect to the bulk elastic constants, the following hold.

(i) The equivalent surface energy is proportional to the average value of the difference between the actual value of the elastic constants and the bulk ones.

(ii) The extrapolation length connected to this surface energy is of the order of the interaction range of the intermolecular forces giving rise to the nematic phase.

On the contrary, in the case in which the spatial variation of the elastic constants is large with respect to the bulk elastic constants, we have shown that analysis has to be performed in the framework of second-order elasticity. The results obtained in this case generalize results published by other groups.

ACKNOWLEDGMENT

Many thanks are due to Professor P. P. Delsanto for useful discussions.

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