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G. Barbero[a]; L. R. Evangelista[b]
[a] Dipartimento di Fisica del Politecnico and I. N. F. M., Corso Duca degli Abruzzi, 24 - 10129 Torino, Italy, [b] Departamento de Física, Universidade Estadual de Maringá, Avenida Colombo, 5790 - 87020-900 Maringá, Paraná, Brazil,

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Role of the linear elastic term in the spatial derivatives of the nematic director in a 1D geometry

G. BARBERO† and L. R. EVANGELISTA*†‡

†Dipartimento di Fisica del Politecnico and I. N. F. M., Corso Duca degli Abruzzi, 24 - 10129 Torino, Italy

‡Departamento de Física, Universidade Estadual de Maringá, Avenida Colombo, 5790 - 87020-900 Maringá, Paraná, Brazil

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The role of the linear elastic term in the spatial derivatives of the nematic director on the director field is analysed. We consider a nematic sample in the shape of a slab, confined by two surfaces treated to induce homeotropic alignment. It is shown that this term can be responsible for spontaneous Fréedericksz transitions. The connection between the linear term and the flexoelectric contribution, associated with a surface field, to the bulk energy density, is discussed. The importance of dielectric anisotropy on the spontaneous Fréedericksz transition is also investigated.

1. Introduction

The elastic theory for nematic liquid crystals was proposed many years ago by Frank [1], Ericksen [2] and Leslie [3]. In this theory, the nematic medium is described by the director, **n**, which coincides with the symmetry axis of a uniaxial crystal. The elastic energy density is written as a quadratic form of the spatial derivatives of **n**. Linear terms are omitted, because the ground state is assumed to be undistorted [4]. The elastic theory for nematic media has been modified to describe the elastic behaviour of smectic liquid crystals [5] or of lamellar systems, such as Langmuir–Blodgett films [6]. Recently, modulated structures in media having directional order have been investigated by several groups. Selinger and Schnur proposed a continuum theory for the self-assembly of cylindrical tubules from chiral lipid bilayers in any tilted fluid phase [7]. Selinger and Selinger developed an elastic theory for chiral defects in Langmuir monolayers [8]. Periodic modulations of the director inside smectic layers have been observed and theoretically described by Gorecka *et al.* [9]. Modulated structures in Langmuir monolayers and in smectic films are also described by Ohyama *et al.* [10]. More recently, Tabe *et al.* [11] carried out the first quantitative measurements of the correlated modulation of molecular tilt and azimuthal angles in two dimensions and in smectic C Langmuir monolayers. The authors explain these results using an extended Landau theory for tilted smectics. A similar theoretical description has been used by Bogdanov and Rößler [12] to describe the breaking of chiral symmetry in magnetic nanostructures.

In all these theoretical analyses to describe the appearance of modulated structures, linear terms in the spatial derivatives of the director have been introduced. Terms of this kind are well known in the continuum description of magnetic materials, and are called Lifchitz invariants [13]. Until now the influence of these terms in one-dimensional problems has not been described in detail. The aim of our paper is to analyse the influence of the linear term in the spatial derivatives of the director, allowed by the nematic symmetry, on the stable nematic orientation.

This paper is organized as follows. Section 2 is devoted to the general case in which the nematic liquid crystal is characterized by a planar splay–bend deformation. The general form, allowed by the symmetry of the problem, for the linear term in the spatial nematic director derivatives is obtained, and its origin discussed. The connection between this term and the flexoelectric term is also analysed. Section 3 is devoted to the analysis of a nematic sample confined by two identical substrates. In this situation the elastic constant relevant to the linear elastic term is expected to be position-dependent. The condition for which the initial home-otopic orientation, induced by the surface treatment, is no longer stable is deduced by means of different degrees of approximation in §4, 5, 6. The influence of the dielectric anisotropy on the stable orientation is

*Author for correspondence;
e-mail: lre@dfi.uem.br

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discussed in §7. In §8 the possibility of a spontaneous Fréedericksz transition induced by the thickness of the sample is investigated.

2. General case

Let us consider the situation in which a splay–bend distortion is present in the system. The elastic energy density compatible with the symmetry requirements (**n** equivalent to $-\mathbf{n}$) of the nematic phase is $f=f_2+f_1$, where

$$f_2=\frac{1}{2}K_{11}(\nabla\cdot\mathbf{n})^2+\frac{1}{2}K_{33}(\mathbf{n}\times\nabla\times\mathbf{n})^2 \qquad (1)$$

is the usual Frank term, and

$$f_1=\lambda_1(\mathbf{n}\cdot\mathbf{k})(\nabla\cdot\mathbf{n})+\lambda_3\mathbf{k}\cdot(\mathbf{n}\times\nabla\times\mathbf{n}) \qquad (2)$$

is a linear term in the spatial derivatives of the nematic director.

In our analysis we consider a sample in the shape of a slab of thickness d, with the z axis normal to the confining walls. The director **n** is defined by the tilt angle $\theta(z)=\cos^{-1}(\mathbf{n}\cdot\mathbf{k})$, where **k** is the normal to the confining surfaces, at $z=\pm d/2$. More precisely, $\mathbf{n}=(\sin\theta,\ 0,\ \cos\theta)$. In this case f_1 is

$$f_1=\frac{1}{2}\lambda\sin(2\theta)\theta' \qquad (3)$$

where $\lambda=\lambda_3-\lambda_1$ and $\theta'=\mathrm{d}\theta/\mathrm{d}z$.

The contribution of f_1 to f exists only if it is possible to choose the direction of **k**, which represents the symmetry breaking variable. It is similar to the term describing the coupling between the flexoelectric polarization, $\mathbf{P}_\mathrm{f}$, and an external d.c. field, **E** [4]. This term is of the kind $-\mathbf{P}_\mathrm{f}\cdot\mathbf{E}=-(e_{11}\mathbf{n}\nabla\cdot\mathbf{n}-e_{33}\mathbf{n}\times\nabla\times\mathrm{n})\cdot\mathbf{E}$. If $\mathbf{E}=E\mathbf{k}$, it coincides with the term described above by putting $\lambda_1=-e_{11}E$ and $\lambda_3=e_{33}E$. An electric field associated with the presence of the limiting surfaces may be due, for example, to selective ion adsorption, as discussed elsewhere [14]. If the surfaces are assumed to be identical, this electric field is position dependent, $E(z)=-E(-z)$, and the elastic constant of the linear term, λ, is a local property. It depends on the properties of the liquid crystal, via the flexoelectric coefficients, and on the properties of the substrate and of the liquid crystal, via the electric field.

In our analysis we use the analogy with the flexoelectric term [4]. However, an elastic term linear in the spatial derivatives of the nematic director may be associated with phenomena other than that of ion-adsorption. For example, let us consider a nematic liquid crystal formed by conical molecules. In the bulk, the two orientations of a given molecule are equally probable. In the proximity of a limiting surface, if the two extremities of the molecule have different chemical affinities with the substrate, a polar order exists. Even in this case λ depends on the liquid crystal and on the surface. It is different from zero only in the surface layers where the bulk symmetry is broken. The elastic constant λ will be indicated by $eE(z)$, where e is a property of the nematic liquid crystal, and $E(z)$ a property of the liquid crystal and of the substrate.

3. Basic equations of the problem

The linear term, according to equation (3), is $f_1=(1/2)eE(z)\sin(2\theta)\theta'$, where $E(z)$ is not constant across the sample. In the limit of small deformations, close to the homeotropic configuration, the total bulk energy density, in the one-constant approximation ($K_{11}=K_{33}=K$), reads

$$f=\frac{1}{2}K\theta'^2+eE(z)\theta\theta'. \qquad (4)$$

In this case the bulk differential equilibrium equation is

$$\theta''+\frac{e}{K}E'(z)\theta=0. \qquad (5)$$

In our analysis the surfaces are assumed identical. Consequently $E(z)=-E(-z)$, and hence $E'(z)=E'(-z)$. In particular $E(-d/2)=-E(d/2)=\mathsf{E}$. Furthermore, we suppose that the surface treatments are such as to induce homeotropic alignment on both surfaces, and that the anisotropic part of the surface tension is described by the Rapini–Papoular form [4]. Within this framework, equation (5) has to be solved with the boundary conditions

$$\theta'\mp\frac{w-e\mathsf{E}}{K}\theta=0 \qquad (6)$$

for $z=-d/2$ and $z=d/2$. The solution of equation (5) with the boundary conditions (6) can be written in the form

$$\theta(z)=\alpha_\mathrm{e}\theta_\mathrm{e}(z)+\alpha_\mathrm{o}\theta_\mathrm{o}(z) \qquad (7)$$

where α_e and α_o are two constants, and $\theta_\mathrm{e}(z)=\theta_\mathrm{e}(-z)$, and $\theta_\mathrm{o}(z)=-\theta_\mathrm{o}(-z)$ are the even and odd solutions of the differential equation (5) and of the boundary condition

$$\theta'_i-\frac{w-e\mathsf{E}}{K}\theta_i=0 \qquad (8)$$

where $i=\mathrm{o,\ e}$, at $z=-d/2$.

We note that the differential equation (5), with the boundary conditions (6), always has the trivial solution $\theta(z)=0$, for $-d/2\le z\le d/2$, which corresponds to the homeotropic alignment. However, for particular values of E, this problem also provides solutions differing from the trivial one. The procedure used to obtain the eigenvalue is the conventional one. If $\theta(\mathsf{E},z)$ is a solution of equation (5), with a well defined parity, the boundary conditions (6) give the relation

$$\frac{w}{K}=\frac{e}{K}\mathsf{E}+\left\{\frac{\theta'(\mathsf{E},z)}{\theta(\mathsf{E},z)}\right\}_{z=-d/2} \tag{9}$$

which defines the critical values of the surface field E to have the instability.

To analyse the stability of the deformed structure it is necessary to evaluate the total energy, per unit surface, of the sample for a defined θ-profile, solution of equation (5). For the problem under consideration, the bulk energy density is given by equation (4). Since

$$\theta'^2=\frac{\mathrm{d}}{\mathrm{d}z}(\theta\theta')-\theta\theta'' \tag{10}$$

and by taking into account that $\theta''=-(eE'/K)\theta$, because of the hypothesis that θ is a solution of equation (5), we obtain

$$\theta'^2=\frac{\mathrm{d}}{\mathrm{d}z}(\theta\theta')+\frac{eE'}{K}\theta^2. \tag{11}$$

It follows that the bulk energy density can be rewritten as

$$f=\frac{1}{2}\theta'^2+\frac{eE}{K}\theta\theta'=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left\{\theta\theta'+\frac{eE}{K}\theta^2\right\}. \tag{12}$$

The total energy per unit surface is given by

$$F=\int_{-d/2}^{d/2} f\,\mathrm{d}z+\frac{1}{2}w_1\theta_1^2+\frac{1}{2}w_2\theta_2^2 \tag{13}$$

if the sample is a slab of thickness d. By substituting equation (12) into (13) we get

$$F=\frac{1}{2}K\left\{\theta_2\theta'_2-\theta_1\theta'_1+\frac{e}{K}\left(E_2\theta_2^2-E_1\theta_1^2\right)\right\}+\frac{1}{2}w_1\theta_1^2+\frac{1}{2}w_2\theta_2^2 \tag{14}$$

where $E_2=E(d/2)$ and $E_1=E(-d/2)$, w_1 and θ_1 refer to the lower surface at $z=-d/2$, and w_2 and θ_2 refer to the upper surface, located at $z=d/2$. Since the surfaces are assumed identical, $w_1=w_2=w$ and $E(z)=-E(-z)$, from which we obtain $E_2=-E_1=-\mathsf{E}$. In this case the solutions of (5) are even or odd in z. If $\theta(z)$ is even in z, $\theta(z)=\theta(-z)$, and $\theta'(z)=-\theta'(-z)$. In particular $\theta_2=\theta_1$, $\theta'_2=-\theta'_1$. In this case from equation (14) we obtain

$$F=\left[w-\left(e\mathsf{E}+K\frac{\theta'_1}{\theta_1}\right)\right]\theta_1^2. \tag{15}$$

If $\theta(z)$ is odd in z, $\theta(z)=-\theta(-z)$, and $\theta'(z)=\theta'(-z)$. In particular $\theta_2=-\theta_1$, $\theta'_2=\theta'_1$. In this case from equation (14) we again obtain (15).

Equation (15) shows that the presence of the linear term in θ' in the elastic energy density renormalizes the anchoring energy strength. In fact, from (15) it is clear that the total energy of the nematic sample reduces to a surface contribution. Since the two surfaces are assumed to be identical, each of them contributes to the total energy with one half of (15). The effective anchoring energy is then

$$w_{\mathrm{eff}}=w-\left(e\mathsf{E}+K\frac{\theta'_1}{\theta_1}\right). \tag{16}$$

Expression (16) shows that the the renormalization of the anchoring energy is not simply $-e\mathsf{E}$. It also contains a term connected with the elastic properties of the nematic liquid crystal.

Expression (15) for F is useful for analysing the stability of the deformed state. In fact, in a linear analysis, $\theta(z)=\alpha\theta_i(z)$, where $\theta_i(z)$ is a solution of the differential equation (5) of a given symmetry, and α an integration constant. Within this framework, F is a quadratic function of α of the kind $F=a\alpha^2$, where, according to (15)

$$a=\left[w-\left(e\mathsf{E}+K\frac{\theta'_{i1}}{\theta_{i1}}\right)\right]\theta'^2_{i1}. \tag{17}$$

From equation (17) one obtains the critical line (9). If E is smaller than value defined by equation (9), $a>0$, and F is minimized for $\alpha=0$. This means that the stable state is the non-deformed one. By contrast, if E is larger than defined by (9), $a<0$ and F has a maximum for $\alpha=0$. This means that the stable state is the deformed one. From the point of view of phase transitions, the critical curve $w=w(\mathsf{E})$ divides the (w, E)-plane into two regions. The area below the curve corresponds to deformed configurations, while above the curve corresponds to the homeotropic configuration.

If the sample is halved the total energy per unit surface is given by

$$F=\int_0^\infty f\,\mathrm{d}z+\frac{1}{2}w_1\theta_1^2. \tag{18}$$

In this case, by using equation (14) and taking into account that $\lim_{z\to\infty}E(z)=0$, and $\lim_{z\to\infty}\theta'=0$, we re-obtain for F expression (15).

In the following, we will consider differing approximations of the problem.

4. First approximation

Let us assume that the field $E(z)$, due to the confining surfaces, can be approximated by the function

$$E(z)=\begin{cases}-(\mathsf{E}/b)(z+z^*)\\ 0\\ -(\mathsf{E}/b)(z-z^*)\end{cases} \tag{19}$$

for $-d/2\le z\le -z^*$, $-z^*\le z\le z^*$, and $z^*\le z\le d/2$, respectively. In (19) $z^*=d/2-b$, and b is a typical length associated with the penetration of the surface field into the bulk. In this approximation $E'(z)=-(\mathsf{E}/b)$ in the surface layers, and $E'(z)=0$ in the bulk.

First we assume that $eE>0$. Within this framework the bulk differential equations of the problem are

$$\begin{aligned} \theta'' - \mu^2\theta = 0, \\ \theta'' = 0, \end{aligned} \tag{20}$$

in the surface layers $-d/2 \le z \le -z^*$, $z^* \le z \le d/2$, and in the bulk $-z^* \le z \le z^*$, respectively. In equation (20) we put

$$\mu = \left(\frac{e\mathsf{E}}{Kb}\right)^{\frac{1}{2}}. \tag{21}$$

We are looking for a function θ which has to satisfy the boundary conditions (6), and to be continuous with its first derivative at $z = \pm z^*$.

The function $\theta_e(z)$ for the present problem is

$$\theta_e(z) = \begin{cases} \alpha_e \exp(-\mu z)\{1 + \exp[2\mu(z + z^*)]\} \\ 2\alpha_e \exp(\mu z^*) \\ \alpha_e \exp(\mu z)\{1 + \exp[-2\mu(z - z^*)]\} \end{cases} \tag{22}$$

for $-d/2 \le z \le -z^*$, $-z^* \le z \le z^*$, and $z^* \le z \le d/2$, respectively. The equation determining the eigenvalue of the problem is governed by the condition (9), which yields

$$\frac{w_e}{K} = \frac{e}{K}\mathsf{E} - \left(\frac{e\mathsf{E}}{Kb}\right)^{\frac{1}{2}} \tanh\left(\frac{e\mathsf{E}}{K}b\right)^{\frac{1}{2}}. \tag{23}$$

Note that from equation (23) it follows that $w_e < e\mathsf{E}$. Consequently the critical field to have the instability is larger than the one to have the surface instability, given by $w = e\mathsf{E}$. In fact, if $E(z)$ is assumed position-independent, the effect of the linear term is just to renormalize the surface anchoring energy, whereas in the present case it also has a stabilizing effect on the homeotropic orientation of the bulk.

The function $\theta_o(z)$ for the same problem is

$$\theta_o(z) = \begin{cases} \alpha_o \exp(-\mu z)\left\{1 - \frac{1-\mu z^*}{1+\mu z^*} \exp[2\mu(z + z^*)]\right\} \\ -\mu\alpha_o \exp(\mu z^*) \frac{2z}{1+\mu z^*} \\ -\alpha_o \exp(\mu z)\left\{1 - \frac{1-\mu z^*}{1+\mu z^*} \exp[-2\mu(z - z^*)]\right\} \end{cases} \tag{24}$$

for $-d/2 \le z \le -z^*$, $-z^* \le z \le z^*$, and $z^* \le z \le d/2$, respectively. The equation determining the eigenvalue of the problem is now

$$\frac{w_o}{K} = \frac{e}{K}\mathsf{E} - \left(\frac{e\mathsf{E}}{Kb}\right)^{\frac{1}{2}} \frac{1 + (e\mathsf{E}b/K)^{\frac{1}{2}}[(d/2b) - 1] \tanh(e\mathsf{E}b/K)^{\frac{1}{2}}}{(e\mathsf{E}b/K)^{\frac{1}{2}}[(d/2b) - 1] + \tanh(e\mathsf{E}b/K)^{\frac{1}{2}}}. \tag{25}$$

Also in this case $w_o < e\mathsf{E}$, because the bulk contribution to the energy density is such as to stabilize the homeotropic orientation.

To obtain a numerical estimation of the critical anchoring energies we use the analogy between the linear term and flexoelectric coupling, and assume $|e| \sim 10^{-11}\,\mathrm{C\,m^{-1}}$ [15,16], $K \sim 10^{-11}\,\mathrm{N}$ [5], $\varepsilon \sim 10\varepsilon_0$ [5], and $b \sim 10^{-7}\,\mathrm{m}$. The parameter b has been assumed to be of the order of the Debye screening length for commercial liquid crystals [17]. For the density of surface adsorbed charges we use the value estimated by Thurston *et al.* [17], $\sigma \sim 10^{-4}\,\mathrm{C\,m^{-2}}$. With the values reported above, $\mathsf{E} \sim \sigma/\varepsilon \sim 10^6\,\mathrm{V m^{-1}}$, and $e\mathsf{E} \sim 10^{-5}\,\mathrm{J\,m^{-2}}$. Hence, the phenomenon described by us is important whenever the extrapolation length $L = K/w$ is on the micron scale.

In figure 1 we show the critical curves $w_e = w_e(\mathsf{E})$, and $w_o = w_o(\mathsf{E})$ obtained using equations (23) and (25), respectively. In the limit of large d they are practically coincident, as expected. In fact in this limit the deformation is localized in the surface layers of thickness b, and the bulk is homeotropically oriented. However, it is observed that $E_e < \mathsf{E}_o$. This implies that for a given anchoring energy strength, the deformation characterized by a tilt angle which is an even function of z costs less energy than the one odd in z.

By means of the linearized analysis presented above it is not possible to obtain the full profile $\theta_e(z)$. But simple considerations show that the deformation is mainly localized in the surface layers. In fact, since $w < e\mathsf{E}$, it follows that $\theta'_e(-d/2) = [(w - e\mathsf{E})/K]\theta(-d/2) < 0$. Furthermore, from equation (20) we have $\theta''_e(z) = \mu\theta_e(z) > 0$ for $-d/2 \le z \le d/2$. Consequently, the tilt angle is larger in the surface layers than in the bulk.

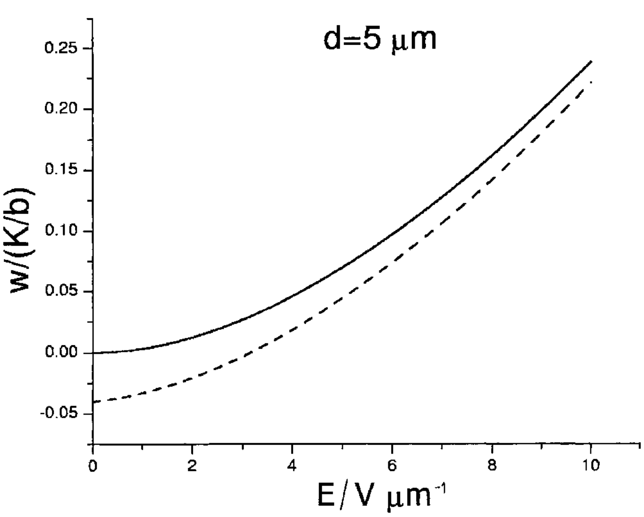

Figure 1. Critical lines $w_e/(K/b)$ (solid) and $w_o/(K/b)$ (dashed) for deformations even and odd in z obtained from the simple analysis reported in §4. For large E the curves are practically coincident. For a given anchoring energy w the critical value of the surface field for the even deformation in z is smaller than the one for the odd deformation. Hence, the actual deformation induced by the surface field is the even one. The curves are drawn for the case $e\mathsf{E} > 0$, using the parameters $e = 1 \times 10^{-11}\,\mathrm{C\,m^{-1}}$, $K = 10^{-11}\,\mathrm{N}$, $b = 0.1\,\mu\mathrm{m}$ and $0 < \mathsf{E} < 10^7\,\mathrm{V\,m^{-1}}$.

Let us consider now the case $e\mathsf{E}<0$. Within this framework the bulk differential equation is

$$\theta''(z)+\frac{|e\mathsf{E}|}{Kb}\theta(z)=0. \quad (26)$$

The relevant boundary conditions are

$$\theta'\mp\frac{w+|e\mathsf{E}|}{K}\theta=0 \quad (27)$$

for $z=-d/2$ and $z=d/2$, respectively. In this case the presence of the surface field reinforces the anchoring energy strength, because w is substituted by $w+|e\mathsf{E}|$. Furthermore, it destabilizes the bulk, as follows from equation (26).

A calculation similar to the one reported above shows that the eigenvalue for the even deformation is

$$\frac{w_{\mathrm{e}}}{K}=-\frac{|e\mathsf{E}|}{K}+\left(\frac{|e\mathsf{E}|}{Kb}\right)^{\frac{1}{2}}\tan\left(\frac{|e\mathsf{E}|b}{K}\right)^{\frac{1}{2}} \quad (28)$$

whereas the eigenvalue for the odd deformation is given by

$$\frac{w_{\mathrm{o}}}{K}=-\frac{|e\mathsf{E}|}{K}+\left(\frac{|e\mathsf{E}|}{Kb}\right)^{\frac{1}{2}}\frac{(|e\mathsf{E}|b/K)^{\frac{1}{2}}[(d/2b)-1]\tan(|e\mathsf{E}|b/K)^{\frac{1}{2}}-1}{(|e\mathsf{E}|b/K)^{\frac{1}{2}}[(d/2b)-1]+\tan(|e\mathsf{E}|b/K)^{\frac{1}{2}}}. \quad (29)$$

The critical curves $w_{\mathrm{e}}=w_{\mathrm{e}}(\mathsf{E})$ and $w_{\mathrm{o}}=w_{\mathrm{o}}(\mathsf{E})$ are shown in figure 2. From this figure it follows that the deformation even in z is favoured. It can take place also in the case of strong anchoring, where $w\to\infty$. The

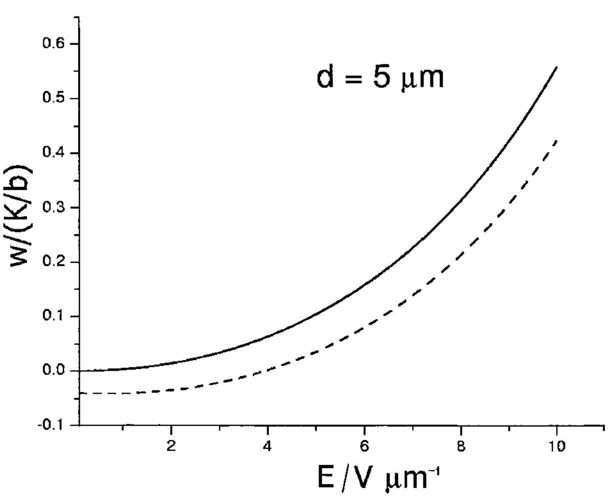

Figure 2. As in figure 1 with $e\mathsf{E}<0$. In this case the flexoelectric contribution reinforces the anchoring energy, changing w in $w+|e\mathsf{E}|$, and destabilizes the homeotropic orientation in the bulk. Now, even in the strong anchoring situation, the bulk can be distorted by the surface field. As in the previous case the even deformation is favoured. Parameters as in figure 1, with $e=-1\times10^{-11}\,\mathrm{C\,m^{-1}}$.

relevant critical field is found to be

$$\mathsf{E}=\left(\frac{\pi}{2}\right)^2\frac{K}{|e|b}. \quad (30)$$

Since in the case under consideration $\theta'(-d/2)=[(w+|e\mathsf{E}|/K]\theta(-d/2)>0$, and $\theta''(z)=-((|e\mathsf{E}|/Kb))^{\frac{1}{2}}\theta(z)<0$ for $-d/2\le z\le d/2$, the deformation is larger in the bulk than in the surface layers.

5. Half-space approximation

The analysis presented in the previous section is very simple, and allows us to obtain explicit expressions for the surface fields inducing the instability due to the presence of the linear elastic term in the spatial derivative of the nematic director. However it is connected with a very special z-dependence of the surface field. It is possible to generalize the previous analysis if $d\gg b$. In this case the sample can be considered, as for as the surface field is concerned as being formed by two halves. In each half the field can be assumed to decrease exponentially with a typical length b. We limit our investigation to the half $z\ge0$, and assume that the surface field is

$$E(z)=\mathsf{E}\exp(-z/b) \quad (31)$$

By substituting equation (31) into (5) we have that the bulk differential equation is now

$$\theta''(z)-\frac{e\mathsf{E}}{Kb}\exp(-z/b)\theta(z)=0 \quad (32)$$

that has to be solved with the boundary condition

$$\theta'-\frac{w-e\mathsf{E}}{K}\theta=0 \quad (33)$$

at $z=0$, and

$$\lim_{z\to\infty}\theta'(z)=0. \quad (34)$$

Let us suppose first $e\mathsf{E}>0$. In this case the solution of equation (32), which remains finite for $z=0$, and whose first z derivative tends to zero for $z\to\infty$ is

$$\theta(\mathsf{E},z)=\beta I_0\left[2\left(\frac{e\mathsf{E}b}{K}\right)^{\frac{1}{2}}\exp(-z/2b)\right] \quad (35)$$

where I_0 is the modified Bessel function of order zero, and β is a constant. By means of equation (35) the critical field is found to satisfy

$$\frac{w}{K}=\frac{e\mathsf{E}}{K}+\left\{\frac{\theta'(\mathsf{E},z)}{\theta(\mathsf{E},z)}\right\}_{z=0}. \quad (36)$$

In figure 3 we show the critical line obtained by means of equation (36) and the one given by (23). As it is evident from the figure, (23) is a good approximation of (36), and the agreement increases with d. Also in the

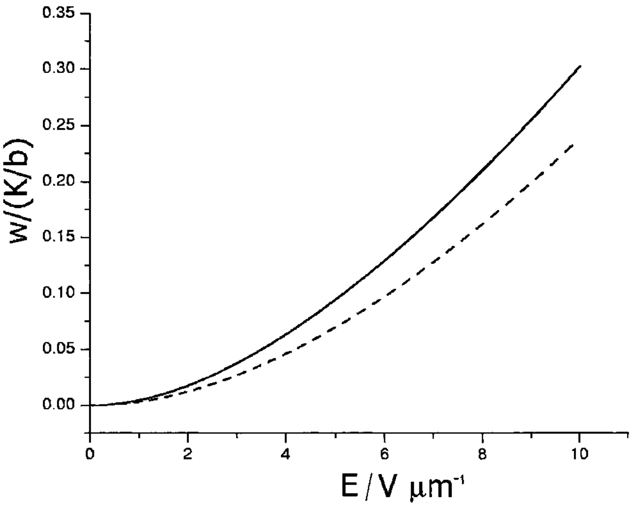

Figure 3. Critical line $w/(K/b)$ (solid) obtained by means of the model reported in §5, where the surface field is assumed to be exponentially decreasing with a typical length b. Case $e\mathsf{E} > 0$. The dashed line is the approximated curve $w_e/(K/b)$ obtained in §4. Physical parameters as in figure 1.

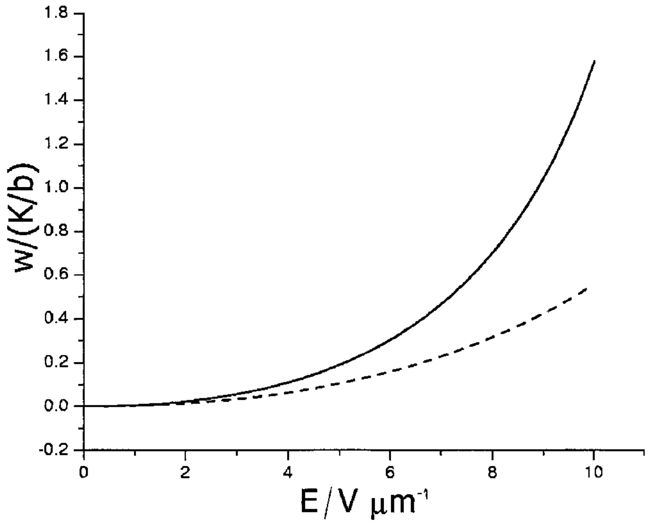

Figure 4. As in figure 3 with $e\mathsf{E}<0$. The dashed line is the approximated curve $w_e/(K/b)$ obtained in §4. Physical parameters as in figure 2.

case considered now, $w<e\mathsf{E}$. Consequently $\theta'(0)<0$. Since $\theta''(z)>0$ for $0\leq z<\infty$, we deduce that $\theta(0)>\theta(\infty)$.

Let us suppose now that $e\mathsf{E}<0$. In this case the solution of the problem under consideration is

$$\theta(z)=\beta J_0\left[-2\left(\frac{|e\mathsf{E}|b}{K}\right)^{\frac{1}{2}}\exp\left(-z/2b\right)\right] \tag{37}$$

where J_0 is the Bessel function of order zero, and β is a constant. By substituting equation (37) into (36) we obtain the critical field for the instability. Note that even in the case of strong anchoring the instability exists and its critical field is given by

$$J_0\left[-2\left(\frac{|e\mathsf{E}|b}{K}\right)^{\frac{1}{2}}\right]=0 \tag{38}$$

from which we obtain

$$E^*=\left(\frac{j_0}{2}\right)^2\frac{K}{|e|b} \tag{39}$$

where $j_0=2.4048$ is the first zero of the Bessel function $J_0(x)$. In figure 4 we show the critical line obtained with the present analysis with the one given by equation (28).

6. Finite sample confined by two identical surfaces

If d is comparable to b the half space approximation no longer applies. In this case the field due to the continuing surfaces, supposed to be identical, can be approximated by

$$E(z)=-\mathsf{E}\frac{\sinh\left(z/b\right)}{\sinh\left(d/2b\right)}. \tag{40}$$

From equation (40) $E(-d/2)=-E(d/2)=\mathsf{E}$, and the surface field is localized in surface layers of thickness of the order of b. If $d\gg b$ from (40) we re-obtain the half-space approximation discussed in the previous section. By substituting equation (40) into (5) we obtain the bulk differential equation for the present problem in the form

$$\theta''-\frac{e\mathsf{E}}{Kb}\frac{\cosh\left(z/b\right)}{\sinh\left(d/2b\right)}\theta=0 \tag{41}$$

which has to be solved with the boundary conditions (6). The even solution of equation (41) is

$$\theta_e(z)=\alpha_e\Psi_e(\mathsf{E},z) \tag{42}$$

and the odd solution of the same equation is

$$\theta_o(z)=\alpha_o\Psi_o(\mathsf{E},z) \tag{43}$$

where $\Psi_e(\mathsf{E},z)$ and $\Psi_o(\mathsf{E},z)$ are the modified Mathieu's function, usually indicated by [18]

$$\Psi_e(\mathsf{E},z)=\mathcal{C}\left(0,-2\frac{e\mathsf{E}b}{K\sinh\left(d/2b\right)},-\mathrm{i}\frac{z}{2b}\right)$$

$$\Psi_o(\mathsf{E},z)=\mathcal{S}\left(0,-2\frac{e\mathsf{E}b}{K\sinh\left(d/2b\right)},-\mathrm{i}\frac{z}{2b}\right). \tag{44}$$

Repeating step by step the previous calculations, we obtain that the critical surface field to induce an even or odd deformation is given by

$$\frac{w_i}{K}=\frac{e\mathsf{E}}{K}+\left\{\frac{\Psi'_i(\mathsf{E},z)}{\Psi_i(\mathsf{E},z)}\right\}_{z=-d/2} \tag{45}$$

where $i=$e, o.

If $e\mathsf{E}>0$ the behaviour of w_e and w_o is that shown in figure 5. As before, the actual deformation is θ_e, because

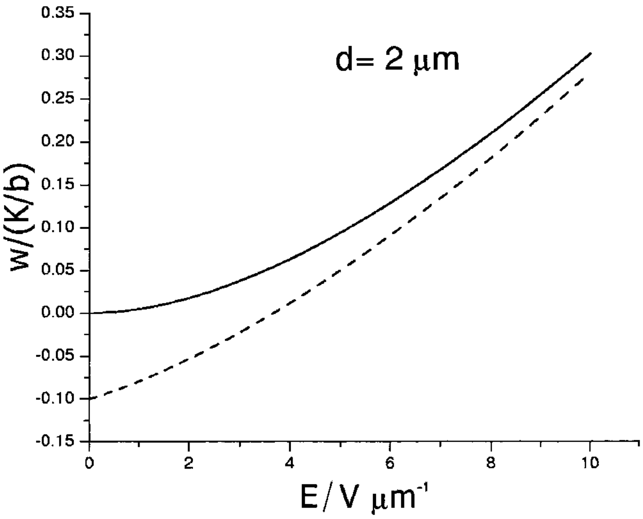

Figure 5. Critical lines $w_e/(K/b)$ (solid) and $w_o/(K/b)$ (dashed) obtained from the analysis reported in §6. Physical parameters as in figure 3.

the relevant critical field is smaller than the one connected to θ_o. In the opposite case, $e\mathsf{E}<0$, the critical lines are shown in figure 6. As already stressed, in this case the instability is possible even in the case of strong anchoring. The relevant threshold field is obtained by the condition

$$\Psi_e(\mathsf{E},-d/2)=\mathcal{C}\left(0,-2\frac{e\mathsf{E}b}{K\sinh(d/2b)},\mathrm{i}\frac{d}{4b}\right)=0. \quad (46)$$

In figure 7 we show the ratio between the critical field given by equation (46) and E^* obtained by means of (39) vs. the thickness of the sample. As expected, if

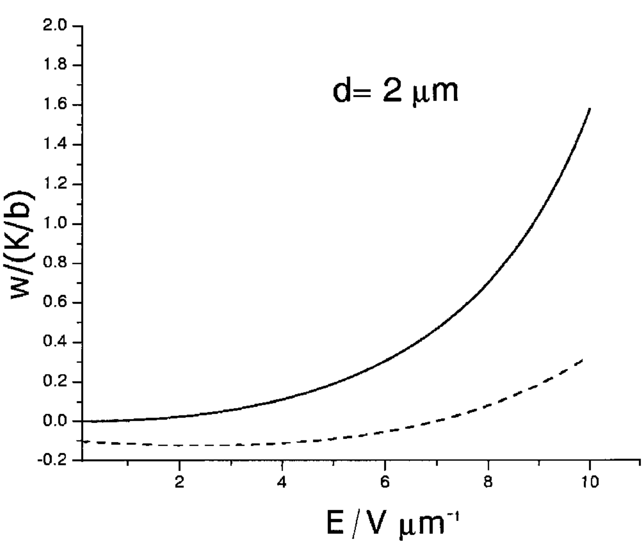

Figure 6. Critical lines $w_e/(K/b)$ (solid) and $w_o/(K/b)$ (dashed) obtained from the analysis reported in §6. Physical parameters as in Figure 4.

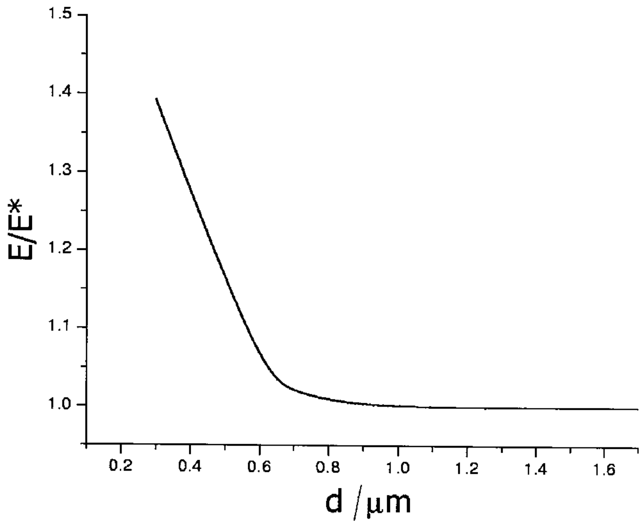

Figure 7. Reduced critical field E/E^*, where E^* is the critical field in the half-space appoximation, as defined in Equation (39), having a surface instability in a sample of finite thickness d, vs. d. Physical parameters as in figure 1.

$d\gg b$, $\mathsf{E}\to\mathsf{E}^*$. The agreement is already very good for $d\sim 10b$.

7. Influence of the dielectric anisotropy on the instability

Up to now we have described the effect of the linear term in the spatial derivatives of the nematic director on the stable orientation as the coupling of an intrinsic electric field with the flexoelectric polarization, because the contributions to the energy density are of the same functional type. However, if the linear term is really connected to the coupling of a surface electric field due to the adsorption phenomenon, our analysis also has to take into account the electric term connected with the dielectric anisotropy [19, 20].

Let us consider a nematic sample confined by two identical substrates, where the surface electric field is such that $E(z)=-E(-z)$. For this case we have obtained different approximate solutions of the problem. As is evident from figures 5 and 6 the agreement between the half-space approximation and the case where d is of the same order of magnitude of b is already very good for $d=10b$. Since $b\sim 0.1\,\mu$m for usual nematic samples used in experiments, our half-space approximation works very well. In this approximation we can investigate the influence of the dielectric anisotropy $\varepsilon_a=\varepsilon_{||}-\varepsilon_{\perp}$ (where $||$ and $\perp$ refer to the directions parallel and perpendicular to the director $\mathbf{n}$, respectively) on the phenomenon under consideration. If $\varepsilon_a\neq 0$ the bulk energy density of the nematic liquid crystal submitted to an electric field is, in the limit of $\theta \to 0$

$$f = \frac{1}{2}K\theta'^2 + \frac{1}{2}\varepsilon_a E^2(z)\theta^2 + eE(z)\theta\theta'. \qquad (47)$$

The bulk equilibrium equation of the problem is, in the exponential approximation for the electric field,

$$K\theta'' - \left[\varepsilon_a \mathsf{E}^2 \exp(-2z/b) + \frac{e\mathsf{E}}{b}\exp(-z/b)\right]\theta = 0 \qquad (48)$$

which has to be solved with the boundary conditions (33) and (34), where E is assumed to be positive. If $e=0$, equation (48) becomes

$$K\theta'' - \varepsilon_a \mathsf{E}^2 \exp(-2z/b)\theta = 0 \qquad (49)$$

whose solution is

$$\theta(z) = \alpha I_0\left[-\left(\frac{\varepsilon_a}{K}\right)^{\frac{1}{2}}\mathsf{E}b\exp(-2z/b)\right] \qquad (50)$$

where α is an integration constant. In this case the surface instability exists only if $\varepsilon_a < 0$, and the corresponding critical field is

$$\mathsf{E} = \frac{j_0}{b}\left(\frac{K}{|\varepsilon_a|}\right)^{\frac{1}{2}}. \qquad (51)$$

The term connected with the dielectric anisotropy, and the one connected with the flexoelectric polarization for the values of the physical parameters used above, are comparable for $z=0$, if $\varepsilon_a \sim \varepsilon_0$. In this situation, the dielectric anisotropy can play an important role in the instability we are analysing.

The solution of equation (48), with the boundary conditions (33) and (34) is

$$\theta = \alpha\exp\left[-\mathrm{sign}(e)\left(\frac{\varepsilon_a}{K}\right)^{\frac{1}{2}}\mathsf{E}b\exp(-z/b)\right]\mathcal{F}(\mathsf{E},z) \qquad (52)$$

where $\mathcal{F}(\mathsf{E},z)$ is the hypergeometric function [18]

$$\mathcal{F}(E,z) = F_1\left\{\frac{1}{2}\left[1+\left(\frac{e^2}{K\varepsilon_a}\right)^{\frac{1}{2}}\right], 1, 2\mathrm{sign}(e) \times \left(\frac{\varepsilon_a}{K}\right)^{\frac{1}{2}}\mathsf{E}b\right\}\exp(-z/b) \qquad (53)$$

The eigenvalues for the present problem are obtained by substituting (52) into equation (36). In figure 8 we show the critical curves relevant to the present case, for different values of the dielectric anisotropy. For small ε_a the influence of the dielectric term is negligible. However, for $\varepsilon_a \sim \varepsilon_0$, the dielectric contribution is such that the homeotropic configuration is stable for all surface fields, for reasonable values of the flexoelectric coefficient. By contrast for $\varepsilon_a \sim -\varepsilon_0$ the value of the surface field giving rise to the instability is strongly reduced due to the destabilizing effect of the dielectric term.

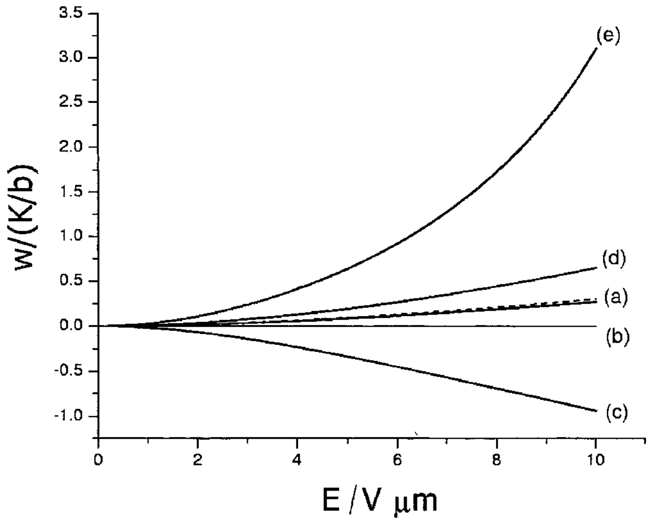

Figure 8. Critical line $w/(K/b)$ obtained using the analysis reported in §7. The dashed line is the critical curve obtained in §5, where the dielectric anisotropy is neglected. Physical parameters as in figure 3, with $\varepsilon_a/\varepsilon_0 = .1$(a), 1(b), 5(c), -1(d), and -5(e).

As before, the critical field to have the instability in the case of strong anchoring is obtained by the condition

$$\mathcal{F}(\mathsf{E},0) = F_1\left\{\frac{1}{2}\left[1+\left(\frac{e^2}{K\varepsilon_a}\right)^{\frac{1}{2}}\right], 1, 2\mathrm{sign}(e)\left(\frac{\varepsilon_a}{K}\right)^{\frac{1}{2}}\mathsf{E}b\right\} = 0. \quad (54)$$

In figure 9 we show the critical field for the instability vs. the dielectric anisotropy, for $e = \pm 1$. As expected, if $e > 0$, which means that the flexoelectric term stabilizes the homeotropic orientation in the bulk, the surface instability is possible only for $\varepsilon_a < 0$. By contrast, if $e < 0$, the instability can occur even with positive dielectric anisotropy. In this case, from equation (54), the maximum value of the dielectric anisotropy to have the instability is $\varepsilon_a < e^2/K$.

8. Spontaneous Fréedericksz transition

In this paper we have discussed the possibility of observing spontaneous Fréedericksz transition induced by the surface field. This instability is, actually, a flexoelectric instability induced by the electric field due to the adsorption phenomenon. Our analysis was devoted to the case in which the electric field is thickness independent [21]. However the analysis can be easily extended to take into account its thickness dependence by means of the results reported in [14]. To a first approximation, it is possible to assume, in the limit of large adsorption energies, that the surface field involved

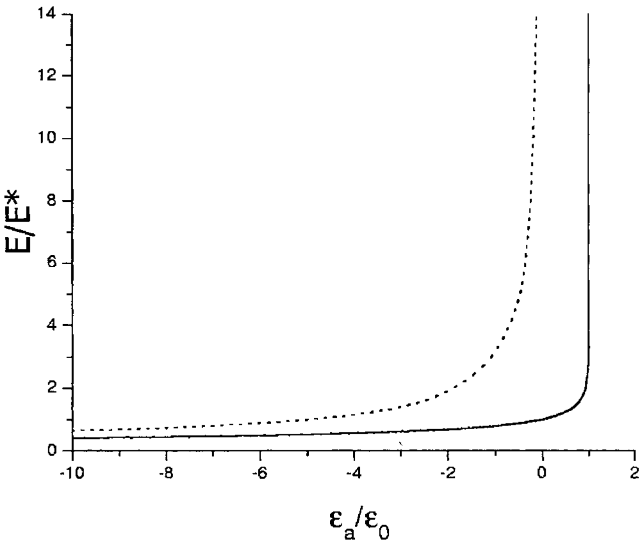

Figure 9. Reduced critical field E/E^*, where E^* is the critical field in the half-space approximation, defined by equation (39) for a compensated nematic liquid crystal ($\varepsilon_a = 0$), to have a surface instability vs. ε_a. $e = 1 \times 10^{-11}\,\mathrm{C\,m^{-1}}$, dotted line, $e = -1 \times 10^{-11}\,\mathrm{C\,m^{-1}}$, solid line. Other physical parameters as in figure 1.

in the phenomenon is given by

$$E = \frac{\Sigma}{\varepsilon} \tanh\left(\frac{n_0 d}{\Sigma}\right). \quad (55)$$

In equation (55), Σ is the saturation surface density of adsorbed charges, which depends on the adsorption energies, and n_0 is the bulk density of ions, in equilibrium conditions (sample of infinite thickness, without surface adsorption). Since E is an increasing function of d, the phase diagrams (w, E) reported in figures 1–7 are, actually, phase diagrams (w, d).

Chuvyrov *et al.* [22, 23] and Blinov and Sonin [24] have observed that thick samples undergo spontaneous tilt transitions above a critical thickness $d = d_c$. This phenomenon was termed a spontaneous Fréedericksz transition, and related to the existence of surface electric polarization [25–27]. According to the theory proposed in [26, 27], the uniform homeotropic configuration becomes unstable because the electrostatic contribution, connected with the surface polarization, destabilizes the surface treatment imposing the initial homeotropic orientation. It overcomes the bare anchoring strength for $d > d_c$. This view has been discussed in detail in [28]. However, from the discussion reported above, another possible mechanism explaining the experimental data by [22–24] could be connected to the existence of the elastic constants associated with the linear term in the elastic energy density. Of course, to observe the predicted instability in this case it is necessary that $w < |eE|$.

9. Conclusion

We have considered the influence of the elastic term, linear in the spatial director derivatives, on the nematic orientation. The analysis has been performed by assuming that the nematic sample is of slab shape, and the surfaces are treated in such a manner as to induce homeotropic orientation. We have shown that the linear term can induce, in particular cases, a spontaneous Fréedericksz transition, where the control parameter is the thickness of the sample.

References

[1] Frank, F. C., 1958, *Discuss. Faraday Soc.*, **25**, 19.
[2] Ericksen, J. L., 1960, *Arch. Ration. Mech. Analysis*, **40**, 231; 1962; **10**, 189; 1966, **23**, 266.
[3] Leslie, F. M., 1966, *Quart. J. Mech. appl. Math.*, **19**, 357.
[4] Barbero, G., and Evangelista, L. R., 2000, *An Elementary Course on the Continuum Theory for Nematic Liquid Crystals* (Singapore: World Scientific).
[5] Vertogen, G., and De Jeu, W. H., 1988, *Thermotropic Liquid Crystals, Fundamentals* (Berlin: Springer-Verlag).
[6] De gennes, P. G., and Prost, J., 1994, *The Physics of Liquid Crystals* (Oxford: Clarendon Press).
[7] Selinger, J. V., and Schnur, J. M., 1993, *Phys. Rev. Lett.*, **71**, 4091.
[8] Selinger, J. V., and Selinger, R. L. B., 1995, *Phys. Rev. E*, **51**, R860.
[9] Gorecka, E., Glogarova, M., Lejeck, L., and Sverenyak, H., 1995, *Phys. Rev. Lett.*, **75**, 4047.
[10] Ohyama, T., Jacobs, A. E., and Mukamel, D., 1996, *Phys. Rev. E*, **53**, 2595.
[11] Tabe, Y., Shen, N., Mazur, E., and Yokoyama, H., 1999, *Phys. Rev. Lett.*, **85**, 759.
[12] Bogdanov, A. N., and Rößler, U. K., 2001, *Phys. Rev. Lett.*, **87**, 037203.
[13] Indenbom, V. L., Pikin, V. L., and Loginov, E. B., 1976, *Kristallografiya*, **21**, 1093.
[14] Barbero, G., Evangelista, L. R., and Zvezdin, A. K., 1999, *Phys. Rev. E*, **59**, 1846.
[15] Maheswara Murthy, P. R., Raghunatan, V. A., and Madhusudana, N. V., 1993, *Liq. Cryst.*, **14**, 483.
[16] Blinov, L. M., Barnik, M. I., Ozaki, M., Shtykov, N. M., and Yoshino, K., 2000, *Phys. Rev. E*, **62**, 8091.
[17] Thurston, R. N., Cheng, J., Meyer, R. B., and Boyd, G. D., 1984, *J. appl. Phys.*, **56**, 263.
[18] Gradshtein, I. S., and Ryzhik, I. M., 1980, *Table of Integrals, Series and Products*, (San Diego: Academic Press).
[19] Barbero, G., Evangelista, L. R., and Madhusudana, N. V., 1998, *Eur. Phys. J. B*, **1**, 337.
[20] Pereira, H. A., and Evangelista, L. R., 2000, *Eur. Phys. J. E*, **3**, 123.
[21] Meister, R., and Jerome, B., 1999, *J. appl. Phys.*, **86**, 2473.
[22] Chuvyrov, A. N., and Lachirov, A. V., 1978, *Sov. Phys. JETP*, **47**, 749.

[23] CHUVYROV, A. N., 1980, *Sov, Phys. Crystallog.*, **25**, 188.

[24] BLINOV, L. M., and SONIN, A. A., 1984, *Sov. Phys. JETP*, **60**, 272.

[25] CHUVYROV, A. N., SONIN, A. S., and ZAKIROV, A. D., 1976, *Sov. Phys. Solid State*, **18**, 1797.

[26] KAZNACHEEV, A. V., and SONIN, A. S., 1983, *Sov. Phys. Solid State*, **25**, 528.

[27] SONIN, A. A., and KAZNACHEEV, A. V., 1984, *Sov. Phys. Solid State*, **26**, 486.

[28] BARBERO, G., and DURAND, G., 1987, *Liq. Crvst.*, **2**, 401.