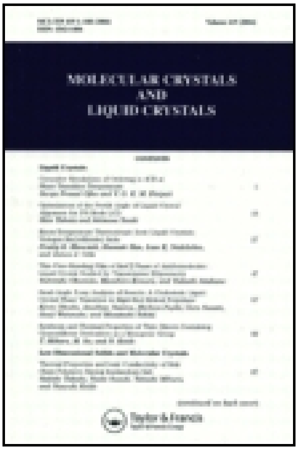

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Tilt Angle Profiles for Splay-Bend Deformations in a Nematic Sample Submitted to an External Field

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The exact tilt angle profiles for splay-bend deformations, in nematic liquid crystal samples limited by inhomogeneous surfaces, are determined in the one-constant approximation. The boundary value problem, concerning the situation of strong anchoring at the surfaces of a sample in the shape of a slab of thickness d (Dirichlet's problem) in the presence of an external uniform field, is analytically solved. The solutions are given in closed general forms, written in terms of propagators. This general formalism is applied to two representative examples to obtain the explicit expressions for the tilt angles and to determine analytically the optical path differences.

Keywords: external field effects; liquid crystals; nematics; splay-bend deformations

Pacs: 61.30.-v 61.30.Gd 61.30.Cz

I. INTRODUCTION

The intermolecular interaction energy, responsible for the nematic liquid crystal (NLC) phase, tends to align the long molecular axes parallel to a common direction **n**. This field gives the local average molecular long axis direction, and in particular situations, it can be written in terms of the tilt angle [1,2]. The determination of the equilibrium profile for the tilt angle is made in the framework of the elastic

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continuum theory [3–6]. In the absence of external fields, the director **n** can be non-uniform in view of the surface treatment. According to the treatment it is possible to characterize surface inhomogeneities influencing the NLC orientation [7]. Alignment of NLC by spatially inhomogeneous surfaces has been analyzed since the pioneer work of Berreman [8], who investigated the anchoring effect of a periodically undulating surface where the surface anchoring is locally strong. Since them, the influence of inhomogeneous surfaces on the molecular orientation of an NLC sample has been analyzed by several authors in the framework of the Frank-Oseen elasticity [7,9–16].

In the last few years, it has been recognized the importance of a complete understanding of the alignment of NLC with patterned isotropic surfaces for practical applications [17]. Of particular interest is the investigation of multiple stable orientations of NLC for the reduction of power consumption in devices [18]. In general, control the surface treatment is crucial for the performance of NLC devices and for the understanding of the molecular orientation in NLC samples [19–21].

Some years ago, a complete analytical model for the determination of the profile of the tilt angle was proposed [15] in the strong- and weak-anchoring hypothesis. The analysis was motivated by the necessity to improve the definition of the surface energy [14] in a continuum description, and in order to connect the anchoring energy experimentally detected with the random distribution of the easy axes. The same analysis [15] was extended in order to describe walls of orientation induced by sharp variations of the surface treatment [16]. In these works, the solution for the tilt angle distribution was obtained in analytical manner for the case of strong anchoring at the surfaces, in the absence of external field, for a general easy axes distribution. Likewise, the situation of weak anchoring was analyzed and the formal solution of the problem was explicitly given in terms of two coupled integral equations. Very recently, the situation of weak anchoring was analyzed in an alternative manner and exact solutions for the mixed (or intermediate) problem were obtained [22].

In this article, we determine the exact profiles of the tilt angle for splay-bend geometry in a sample of NLC in the shape of a slab of thickness d for the case of strong anchoring, in the one-constant approximation, under the action of an uniform external electric field, for the cases in which the surface treatment ensures a distribution of easy axes depending on one-coordinate. The general solutions are given in terms of Green's functions. These exact solutions can be directly employed to establish, in closed forms, the thickness dependence as well as applied field dependence of the optical path difference in real samples.

II. MATHEMATICAL PROBLEM FOR A SLAB

We consider a nematic slab of thickness d. The Cartesian reference frame is chosen with the z axis normal to the surfaces, placed at $z = \pm d/2$. The x axis is parallel to the direction along which the surface tilt angle is expected to change, and the tilt angle, θ, made by the nematic director with the z axis, is supposed y independent and such that $n_x = \sin\theta(x,z)$, $n_y = 0$ and $n_z = \cos\theta(x,z)$. In the one constant approximation, $K_{11} = K_{33} = K$, the bulk free energy density due to elastic distortions is given by [1]:

$$f_b = \frac{1}{2}K(\vec{\nabla}\theta)^2 \tag{1}$$

where $\vec{\nabla}\theta = \mathrm{i}(\partial\theta/\partial x) + \mathrm{k}(\partial\theta/\partial z)$, whilst $\mathbf{i}$ and $\mathbf{k}$ are the unit vectors parallel to the x and z axes, respectively. The general situation can be analyzed by taking into account the existence of a finite surface energy which we will assume to be of the kind proposed by Rapini and Papoular [23], but in the parabolic approximation, i.e., $f_s = W/2(\theta - \Theta)^2$, where W is the anchoring strength. The strong anchoring case corresponds to the limit $W \to \infty$. The total elastic free energy of the nematic sample, per unit length along the y axis, is given by

$$F[\theta(x,z)] = \int_{-\infty}^{\infty} dx \int_{-d/2}^{d/2} dz \frac{1}{2}K(\vec{\nabla}\theta)^2 + \frac{1}{2}\int_{-\infty}^{\infty} dx \times \left\{ W_-[\theta_-(x) - \Theta_-(x)]^2 + W_+[\theta_+(x) - \Theta_+(x)]^2 \right\} \tag{2}$$

where $\theta_\pm(x)$ are the actual values of the surface tilt angle, W_- and W_+ refer to the low and upper surface respectively. Hereafter, for simplicity, we will assume that $W_- = W_+ = W$. The principle of the continuum theory states that the actual director profile, or $\theta(x,z)$, is deduced by minimizing the total free energy given by (2). Usual calculations give

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial z^2} = 0, \quad -\infty < x < \infty, \quad -\frac{d}{2} \le z \le \frac{d}{2} \tag{3}$$

The solution is a harmonic function $\theta(x,z)$ which needs to satisfy appropriated boundary conditions. In the general case of weak anchoring the boundary conditions are [24]:

$$\pm L\left[\frac{\partial\theta}{\partial z}\right]_{z=\pm d/2} + \theta_\pm(x) - \Theta_\pm(x) = 0. \tag{4}$$

In Eq. (4), $L = K/W$ is the extrapolation length [9], and $\Theta_\pm(x)$ account for the surface orientation imposed by the surface treatment, i.e., the easy axes on the upper and lower surfaces, respectively. It is possible to show that the general solution of Eq. (3), satisfying boundary conditions (4), can be expressed in terms of propagators as [15,16]:

$$\theta_W(x,z) = \int_{-\infty}^{\infty} dx'[G_+(x'-x,z)\theta_+(x') + G_-(x'-x,z)\theta_-(x')] \tag{5}$$

where

$$G(x'-x,z) = \frac{1}{2d}\frac{\cos(\pi z/d)}{\cosh[\pi(x'-x)/d] \mp \sin(\pi z/d)}. \tag{6}$$

By substituting the general solution into the boundary conditions Eq. (4), one obtains

$$\theta_\pm(x,z) = \Theta_\pm \pm L\int_{-\infty}^{\infty} dx'[h_+(x-x',z)\theta_+(x') + h_-(x-x',z)\theta_-(x')]\Big|_{z=\pm d/2}, \tag{7}$$

where $h_\pm(x-x',z) = \partial G_\pm(x-x',z)/\partial z$. Therefore, to solve the boundary value problem relative to the weak anchoring situation, one has to solve the set of two coupled Fredholm integral equations of second kind, Eq. (7), in order to obtain the tilt angle at the surfaces $\theta_\pm(x)$. Once a solution is obtained, Eq. (5) can be used to give the tilt angle profile. An alternative approach for discussing the general situation of weak anchoring - which in the present context represents the mixed (or intermediate) boundary value problem - was considered in detail in Ref. [22]. Here, instead, we focus our attention on the effect of an external field in the determination of the exact tilt angle profile for planar deformations in NLC. For this reason, we restrict the analysis to the strong anchoring case.

III. EXTERNAL FIELD EFFECT: STRONG-ANCHORING CASE

We consider the simpler case of strong anchoring, which corresponds to the limit $L \rightarrow 0$. In this case, (7) reduces to

$$\theta\left(x, \pm\frac{d}{2}\right) = \Theta_\pm(x) \tag{8}$$

and the exact solution is simply written as

$$\theta_S(x,z) = \int_{-\infty}^{\infty} dx'[G_+(x'-x,z)\Theta_+(x') + G_-(x'-x,z)\Theta_-(x')] \tag{9}$$

Equations (6) and (9) give the complete solution of the problem in the strong-anchoring hypothesis and have been discussed in details in Refs. [15,16].

When the NLC is submitted to an electric field, E, parallel to z, the total energy per unit length along y may be written as

$$F[\theta(x,z)] = \int_{-\infty}^{\infty} dx \int_{-d/2}^{d/2} dz \left[\frac{1}{2}K(\vec{\nabla}\theta)^2 + \frac{\varepsilon_a}{2}E^2\theta^2\right] \tag{10}$$

in the limit of small θ. This approximation can be valid for a sample in which the applied field is lower than or in the order of the Fréedericksz threshold field to induce deformations in the nematic structure. In this manner, the deformations can be always considered as small. For this reason, we can consider that the field inside the sample, in a first approximation, is homogeneous. This implies also that we neglect the effect of ion adsorption on the electric field distribution in the sample. In (10), $\varepsilon_a = \varepsilon_\parallel - \varepsilon_\perp$ ($\parallel$ and $\perp$ refer to the direction of $\mathbf{n}$) is the dielectric anisotropy. By minimizing Eq. (10) we obtain

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial z^2} = \alpha^2\theta \tag{11}$$

where $\alpha^2 = (\varepsilon_a/K)E^2$. In order to obtain the solution for this equation, we start by considering the Fourier transform of Eq. (11) on the x variable, which yields:

$$-k^2\theta(k,z) + \frac{d^2}{dz^2}\theta(k,z) = \alpha^2\theta(k,z). \tag{12}$$

By solving the above equation, we obtain in the k-space the solution

$$\theta(k,z) = g_+(k,z)\Theta_+(k) + g_-(k,z)\Theta_-(k) \tag{13}$$

with

$$g_\pm(k,z) = \frac{\sinh[\sqrt{k^2+\alpha^2}(d/2 \pm z)]}{\sinh[\sqrt{k^2+\alpha^2}d]} \tag{14}$$

Now, by using the inverse Fourier transform, taking the convolution theorem into account, we obtain that

$$\theta(x,z) = \int_{-\infty}^{\infty} dx'[g_+(x-x',z)\Theta_+(x') + g_-(x-x',z)\Theta_-(x')] \tag{15}$$

where

$$g_{\pm}(x,z) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{n\pi}{d} \frac{\sin[n\pi/d(d/2 \pm z)]}{\sqrt{(n\pi)^2 + (\alpha d)^2}} e^{-\sqrt{(n\pi/d)^2+(\alpha)^2}|x|} \tag{16}$$

Note that Eq. (16) recovers Eq. (6) for $\alpha = 0$, i.e., by removing the electric field from the system we consistently obtain the situation described by Eq. (6).

IV. ILLUSTRATIVE EXAMPLES

In order to show the generality of the solution represented by Eq. (15), we first consider, for illustrative purposes, a simple problem dealing with the presence of a pretilt. We consider a sample in the shape of a slab such that

$$\Theta_+(x) = \Theta_0 \quad \text{and} \quad \Theta_-(x) = -\Theta_0 \tag{17}$$

where $|\Theta_0| \ll 1$ is a uniform angle characterizing the pretilt at the surfaces. In this simple, but representative, case the general solution (15) is written as

$$\begin{aligned} \theta(x,z) &= \Theta_0 \int_{-\infty}^{\infty} dx'[g_+(x-x',z) - g_-(x-x',z)] \\ &= \Theta_0 \sum_{n=1}^{\infty} (-1)^{n+1} \frac{2n\pi \cos(n\pi/2) \sin(n\pi z/d)}{(n\pi)^2 + (\alpha d)^2} \\ &= \Theta_0 \frac{\sinh(2\alpha z)}{\sinh(\alpha d)} \end{aligned} \tag{18}$$

as can be easily verified by expanding $\sinh(2\alpha z)$ in Fourier Series in the interval $-d/2 \leq z \leq d/2$. Notice that $\theta(x,z)$ is, in fact, independent of x, as expected, because this kind of boundary conditions imply that the orientation at the surface is uniform.

The second illustrative case to be considered now is the one in which the surface treatment insures an easy axes distribution that is inhomogeneous on one surface, while on the other one the alignment is uniform. Specifically, consider that

$$\Theta_+(x) = \Theta_0 \quad \text{and} \quad \Theta_-(x) = \Theta_1 \sin(qx) \tag{19}$$

where $q = 2\pi/\lambda$, with λ being the spatial periodicity in the easy axes distribution over the lower surface of the slab. In this case the general solution (15) is written as

$$\begin{aligned}\theta(x,z) &= \int_{-\infty}^{\infty} dx'[g_+(x-x',z)\Theta_0 + g_-(x-x',z)\Theta_1\sin(qx')] \\ &= 2\Theta_0\sum_{n=1}^{\infty}(-1)^{n+1}\frac{n\pi\sin[n\pi/d(d/2+z)]}{(n\pi)^2+(\alpha d)^2} \\ &\quad + 2\Theta_1\sin(qx)\sum_{n=1}^{\infty}(-1)^{n+1}\frac{n\pi\sin[n\pi/d(d/2-z)]}{(n\pi)^2+(\alpha d)^2+(qd)^2} \end{aligned} \tag{20}$$

Notice that this solution is valid always the condition $|\theta(x,z) << 1|$ is satisfied because we are working in the limit of small θ. When $\theta(x,z)$ is known, the physical properties of the NLC sample can be explored. For instance, in the case in which a linear polarized beam impinges normally on the nematic sample, the optical path difference Δl, between the ordinary and the extraordinary ray is given by

$$\Delta l = \frac{1}{\Lambda}\int_{-\Lambda/2}^{\Lambda/2} dx \int_{-d/2}^{d/2} dz \Delta n(\theta) = \frac{1}{2} n_0 R d\langle\theta^2\rangle, \tag{21}$$

where

$$\langle\theta^2\rangle = \frac{1}{d\Lambda}\int_{-\Lambda/2}^{\Lambda/2} dx \int_{-d/2}^{d/2} dz \theta^2(x,z) \tag{22}$$

is the average square tilt angle, evaluated over a typical length Λ, connected with the diameter of the light beam. Furthermore, $R = 1-(n_0/n_e)^2$, and n_0 and n_e are, respectively, the ordinary and extraordinary refractive indices.

For the examples mentioned above it is possible to obtain closed analytic expression for Δl. For the solution (18) we easily obtain

$$\begin{aligned}\Delta l &= \frac{n_0 R\Theta_0^2}{8\alpha d}\frac{\sinh(2\alpha d)-2\alpha d}{\sinh^2(\alpha d)} \\ &= \frac{n_0 R\Theta_0^2}{8\pi h}\frac{\sinh(2\pi h)-2\pi h}{\sinh^2(\pi h)}\end{aligned} \tag{23}$$

where we have introduced the quantity

$$\alpha d = \frac{\pi E}{E_c} = \pi h \tag{24}$$

where $E_c = \pi/d\sqrt{K/\varepsilon_a}$ is the usual Fréedericksz threshold for the order phase transition in a sample of thickness d, and will be used here as a reference value to define the reduced field as $h = E/E_c$ [24].

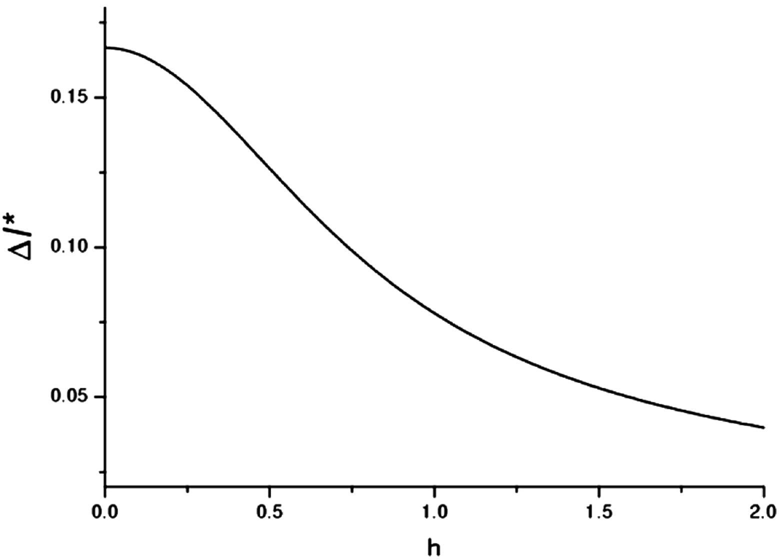

FIGURE 1 Reduced optical path difference $\Delta l^* = \Delta l \Theta_0^2 / n_0 R$ versus the reduced field h. The sample, with antisymmetric boundary conditions, is distorted for all the values of the external field.

In Figure 1, the trend of $\Delta l^* = \Delta l \Theta_0^2 / n_0 R$ versus h is shown. One observes that $\Delta l \neq 0$ everywhere. This is an expected result since the boundary conditions (17) imply that the sample is always distorted.

For the solution (20) the calculations, even if straightforward, are lengthy. One obtains

$$\begin{aligned}\langle \theta^2(x,z) \rangle = & 4\Theta_0^2 \sum_{n,m=1}^{\infty} (-1)^{n+m} \frac{nm\pi^2}{[(n\pi)^2 + (\alpha d)^2][(m\pi)^2 + (\alpha d)^2]} I_1 \\ & + 4\Theta_1^2 \sum_{n,m=1}^{\infty} (-1)^{n+m} \frac{nm\pi^2}{[(n\pi)^2 + (\alpha d)^2 + (qd)^2][(m\pi)^2 + (\alpha d)^2 + (qd)^2]} I_3 \end{aligned} \quad (25)$$

where the integrals I_1 and I_3 are, respectively, given by

$$I_1 = \begin{cases} \dfrac{n\cos(n\pi)\sin(m\pi) - m\cos(m\pi)\sin(n\pi)}{(m^2 - n^2)\pi}, & m \neq n \\ \dfrac{1}{2}\left(1 - \dfrac{\sin(2n\pi)}{2n\pi}\right), & m = n \end{cases} \quad (26)$$

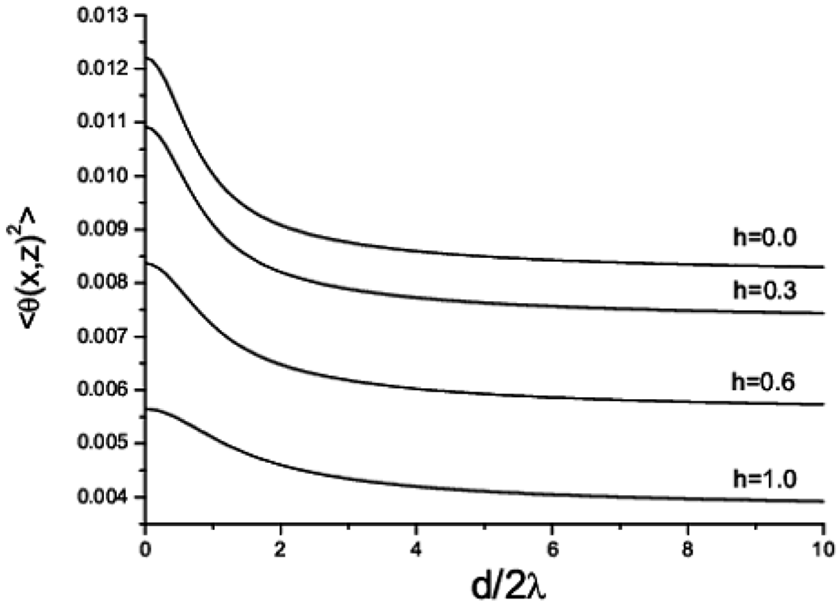

FIGURE 2 $\langle \theta(x,z)^2 \rangle$ versus the reduced thickness of the sample $d/2\lambda$. The calculations were made for $q\Lambda = 2\pi\Lambda/\lambda = 10$ and for $\Theta_0 = \Theta_1 = \pi/20$ and several small values for the reduced field.

and

$$I_3 = \frac{1}{2}\left(1 - \frac{\sin(q\Lambda)}{q\Lambda}\right) I_1 \tag{27}$$

In Figure 2, Δl^* is shown as a function of the reduced thickness of the sample, $d/2\lambda$ for four different values of the reduced field. The behavior is similar to the one reported in Figure 1 because, even in the present case, the orientation is always distorted in view of the strong anchoring at the surfaces. As expected, the optical path difference decreases in magnitude with increasing h, because in the center of the sample the molecular orientation tends to follow the applied field, while on the surface, due to the strong anchoring, the orientation follows the easy directions imposed by the surface treatment.

V. CONCLUDING REMARKS

Exact tilt angle profiles have been determined for a nematic liquid crystals sample of thickness d, when only splay-bend deformations are allowed in the system. Different situations of surface inhomogeneities have been considered in the case of strong anchoring in the presence of an external uniform applied field. The general results, given in terms of propagators, have been applied to a two illustrative cases. In particular, the case in which at one of the surfaces the easy axis distribution is periodic whereas in the other one it is uniform was discussed. For this representative case, the optical path difference was calculated as a function of the reduced thickness of the sample, for representative values of the reduced field $h = E/E_c$ indicating that the molecular orientation is never uniform, even for arbitrary values of the applied field. The calculations may be relevant for a sample in which the zapplied field is lower than or in the order of the Fréedericksz threshold, with permits us to treat small deformations and to consider, in a first approximation, that the electric field inside the sample is homogeneous.

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