Reorientation of the director field in nematic liquid crystals in weak anchoring situation

N. Sodré, R.S. Zola, E.K. Lenzi, and L.R. Evangelista
Departamento de Física, Universidade Estadual de Maringá Avenida Colombo, 5790-87020-900 Maringá (PR), Brazil.

L.R. da Silva
Departamento de Física, Universidade Federal do Rio Grande do Norte, 59078-970 Natal-RN, Brazil.

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The behavior of the nematic director field under the action of an external time dependent field is theoretically investigated in the situation of weak anchoring. By considering the one-constant approximation and a parabolic approximation for the surface energy, the initial conditions and boundary-value problem for the profile of the tilt angle in a sample of slab shape of thickness \( d \), limited by inhomogeneous surfaces, is analytically solved. The results are valid for small deformations in the sample and can be relevant for investigating the phase shift in a nematic cell subjected to a small external voltage.

Keywords: Liquid crystal; nematic; director field; weak anchoring.

Se investiga teóricamente el comportamiento del campo director de un nemático bajo la acción de un campo externo dependiente del tiempo cuando el anclaje es débil. Bajo la aproximación de constantes elásticas iguales y la aproximación parabólica para la superficie de energía, se resuelve analíticamente el problema de condiciones iniciales y de condiciones de frontera para el perfil del ángulo de orientación en una muestra de grosor \( d \) y limitada por superficies inhomogéneas. Los resultados son válidos para deformaciones pequeñas de la muestra y pueden ser relevantes para investigar el corrimiento de fase en una celda nemática sometida a un voltaje externo pequeño.

Descriptores: Cristales líquidos; nemático; campo director; anclaje débil.

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When subjected to the influence of external fields, nematic liquid crystals (NLC) exhibit a rich variety of dynamical behavior [1]. The most common phenomenon is probably the field-induced distortion known as the Fréedericksz transition, in which the initial uniform configuration changes beyond a critical value of the applied field [2]. The effects of external applied fields are also crucial in the performance of electro-optical devices based on liquid crystalline materials [3]. A large class of problems, dealing with the equilibrium orientational states of NLC, can be faced in the framework of the elastic continuum theory for liquid crystalline materials [4–12] and, from the mathematical point of view, can be formulated as boundary value problems. Recently, the influence of the inhomogeneity in the distribution of easy directions at the surfaces on the bulk molecular orientation in a nematic cell has been considered in two typical situations: the Dirichlet’s problem and the mixed Dirichlet - Neumann problem [13–18]. The former problem refers to the situation of strong anchoring in the presence of static deformations in a typical NLC cell. The latter problem is the general one and deals with the situation of weak anchoring at the surfaces. Despite the importance of these problems, both theoretically and experimentally, closed solutions to them can be obtained only for simplified or specific models [19].

In this paper, we establish the exact dynamical behavior of the tilt angle for splay-bend geometry in a sample of NLC in the shape of a slab of thickness \( d \) for the cases of weak anchoring at the surfaces. The profile of the tilt angle is determined when the sample is subjected to the action of a time-dependent applied electric field, when the surfaces are characterized by a spatially-dependent distribution of easy axes. We present the complete analytical solution for the problem in the framework of the elastic continuum theory, in the one-constant approximation, by taking into account the viscous torque. The surface energy, for simplicity, is assumed to be of the kind proposed by Rapini-Papoular, but in the parabolic approximation [20], i.e. valid for small deviations from the easy direction. This implies that the general results can be relevant to 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, because the present approach considers only small deformations. We are therefore assuming that the electric field is homogeneous across the sample, and effects like the selective adsorption of ions are not considered in a first approximation [21]. We assume, furthermore, that in the vicinity of the Fréedericksz transition, the backflow effects can be ignored. Since the general solution is presented in closed analytical form, it can be used to calculate relevant experimental quantities, like the optical path difference.

We consider a nematic slab of thickness \( d \). The geometry is the same as that considered previously in the problem of strong anchoring [22]. The Cartesian reference frame is chosen with the \( z \)-axis normal to the surfaces, located at
z = ±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(x, z), made by the nematic director with the z-axis, is assumed to be y independent and such that \( \mathbf{n} = \sin \theta(x, z) \mathbf{i} + \cos \theta(x, z) \mathbf{k} \), where \( \mathbf{i} \) and \( \mathbf{k} \) are the unit vectors parallel to the x- and z-axes, respectively. In the one-constant approximation, \( K_{11} = K_{22} = K_{33} = K \), the bulk free energy density due to elastic distortions in the presence of a time-dependent external field \( \mathbf{E} = E(t) \mathbf{k} \) is given by [11]

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

where \( \theta_\pm(x) \) is the actual value of the surface tilt angle, and \( W_- \) and \( W_+ \) refer to the low and upper surface respectively. We consider the case in which \( W_- = W_+ = W \). Note also that Eq. (1) is obtained in the limit of small \( \theta \). This approximation is justified if we limit our analysis to the cases in which the applied field is of the order of the Frédéricksz transition [23]. In Eq. (1), \( \epsilon_a = \epsilon_\parallel - \epsilon_\perp \) (\( \parallel \) and \( \perp \) refer to the direction of \( \mathbf{n} \)) is the dielectric anisotropy. When the sample is submitted to an electric field, the electric torque can destabilize the initial homeotropic orientation if \( \epsilon_a < 0 \), and tends to reinforce the homeotropic pattern if \( \epsilon_a > 0 \), since we are not taking into account the flexoelectric contribution to the free energy [24].

To analyze the dynamics of the orientation induced by the field, we need to consider also a viscous torque. By minimizing Eq. (1), taking into account the viscous torque, we find that the dynamical evolution of the system is governed by the equation

\[
\frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \zeta^2} = \alpha^2(t) \theta + \frac{\partial \theta}{\partial t},
\]

written in a non-dimensional form by introducing reduced coordinates \( \xi \rightarrow x/d \), and \( \zeta \rightarrow z/d \) and a reduced time \( t \rightarrow t/\tau_v \), where \( \tau_v = \lambda d^2/K \) is the viscous relaxation time and \( \lambda \) is an effective viscosity coefficient of the liquid crystal [25]. In this manner,

\[
\alpha^2(t) = \pi^2 \left( \frac{E(t)}{E_c} \right)^2,
\]

where \( E_c^2 = \pi^2 K/\epsilon_a \) is the threshold field for the Frédéricksz transition in strong anchoring [11].

The solution to Eq. (2) is the function \( \theta(\xi, \zeta, t) \), subjected to an initial condition and satisfying appropriate boundary conditions. The case of strong anchoring was recently considered and the problem was analytically solved [22]. In that case, one has to solve Eq. (2) subject to the boundary conditions

\[
\theta(\xi, \zeta, t)|_{\zeta=\pm1/2} = \Theta_\pm(\xi),
\]

For the more general case, characterized by the weak anchoring on both surfaces, the boundary conditions must be [11]:

\[
\pm L \frac{\partial}{\partial \zeta} \theta(\xi, \zeta, t) + \theta(\xi, \zeta, t)|_{\zeta=\pm1/2} = \Theta_\pm(\xi),
\]

where \( L = b/d \) (\( b = K/W \) is the extrapolation length [26]), and \( \Theta_\pm(x) \) accounts for the surface orientation imposed by the surface treatment, i.e. the easy axes on the upper (+) and lower (−) surfaces, respectively. In the limit in which \( b \rightarrow 0 \), which corresponds to the strong anchoring case, the boundary conditions reduce to (3). Therefore, the problem considered in the present approach is the more general one, and the situation treated in Ref. 22 can be considered as a particular case. The initial condition, for simplicity, is assumed as \( \theta(\xi, \zeta, 0) = \theta_0(\xi, \zeta) \). Thus, we characterize the initial state of the system, i.e. how the system was initially prepared, by \( \theta_0(\xi, \zeta) \). In order to solve Eq. (2), we consider that the solution has the form

\[
\theta(\xi, \zeta, t) = \theta_S(\xi, \zeta, t) + \tilde{\theta}(\xi, \zeta, t),
\]

where \( \theta_S(\xi, \zeta) \) is the stationary solution obtained from Laplace equation

\[
\nabla^2 \theta_S = 0,
\]

taking the boundary condition

\[
\pm L \frac{\partial}{\partial \zeta} \theta(\xi, \zeta) + \theta(\xi, \zeta)|_{\zeta=\pm1/2} = \Theta_\pm(\xi)
\]

into account. In particular, the solution for \( \theta_S(\xi, \zeta) \) is given by [16–18]

\[
\theta_S(\xi, \zeta) = \sum_{i=+, -} \int_{-\infty}^{\infty} d\xi' G_{S, i}(\xi - \xi', \zeta) \Theta_i(\xi'),
\]

where

\[
G_{S, \pm}(\xi, \zeta) = \sum_{n=1}^{\infty} \frac{\sin \left[ k_n (1/2 \pm \zeta) \right] + k_n L \cos \left[ k_n (1/2 \pm \zeta) \right]}{2k_n L (L + 1) \sin (k_n) - \left[ 1 - (k_n L)^2 \right] + 2L \cos (k_n)} e^{-k_n |\xi|},
\]

with the values of $k_n$ obtained from equation $2k_n L \cos (k_n) + [1 - (k_n L)^2] \sin (k_n) = 0$. By substituting Eq. (5) in Eq. (2) and Eq. (4), we obtain

$$\frac{\partial^2}{\partial \xi^2} \tilde{\theta}(\xi, \zeta, t) + \frac{\partial^2}{\partial \zeta^2} \tilde{\theta}(\xi, \zeta, t) - \alpha^2(t) \left[ \tilde{\theta}(\xi, \zeta, t) + \theta_S(\xi, \zeta) \right] = \frac{\partial}{\partial t} \tilde{\theta}(\xi, \zeta, t)$$

(9)

subject to the initial condition $\tilde{\theta}(\xi, \zeta, 0) = \theta_0(\xi, \zeta) - \theta_S(\xi, \zeta)$ and to the boundary condition

$$\pm L \frac{\partial}{\partial \zeta} \tilde{\theta}(\xi, \zeta, t) + \tilde{\theta}(\xi, \zeta, t) \bigg|_{\zeta = \pm 1/2} = 0.$$ 

(10)

By applying the Fourier transform on the spatial variable $\xi$ and using

$$\tilde{\theta}(k, z, t) = e^{-k^2 t - \int_0^t \alpha^2(\tau) d\tau} \tilde{\theta}(k, z, t),$$

we may simplify Eq. (9) to

$$\frac{\partial^2}{\partial \zeta^2} \tilde{\theta}(k, \zeta, t) - \alpha^2(t) e^{k^2 t + \int_0^t \alpha^2(\tau) d\tau} \theta_S(k, \zeta) = \frac{\partial}{\partial t} \tilde{\theta}(k, \zeta, t).$$

(11)

In order to find the solution to Eq. (11) subject to appropriate boundary and initial conditions, we employ the Green’s function approach. Thus, after these considerations it is possible to show that the solution to Eq. (11) is given by

$$\tilde{\theta}(k, \zeta, t) = \int_0^{1/2} d\zeta' \int_0^t dt' \mathcal{G}(\zeta, \zeta', t-t') \alpha^2(t') \theta_S(k, \zeta') e^{k^2 t' + \int_0^{t'} \alpha^2(\tau) d\tau}$$

$$- \int_{-1/2}^{1/2} d\zeta' \mathcal{G}(\zeta, \zeta', t) \tilde{\theta}(k, \zeta', 0),$$

(12)

where $\tilde{\theta}(\xi, \zeta, 0) = \theta_0(\xi, \zeta) - \theta_S(\xi, \zeta)$ and Green’s function $\mathcal{G}(\zeta, \zeta', t)$ is defined as follow:

$$\mathcal{G}(\zeta, \zeta', t) = -\sum_{n=1}^{\infty} \frac{\sin \left( k_n \left( \zeta + \frac{1}{2} \right) \right) + k_n L \cos \left( k_n \left( \zeta + \frac{1}{2} \right) \right)}{L (L+1) k_n \sin (k_n) - (1 - L^2 k_n^2 / 2 + L) \cos (k_n)}$$

$$\times \left[ \sin \left( k_n \left( \frac{1}{2} - \zeta' \right) \right) + k_n L \cos \left( k_n \left( \frac{1}{2} - \zeta' \right) \right) \right],$$

(13)

for $-1/2 \leq \zeta < \zeta'$ and

$$\mathcal{G}(\zeta, \zeta', t) = -\sum_{n=1}^{\infty} \frac{\sin \left( k_n \left( \zeta + \frac{1}{2} \right) \right) + k_n L \cos \left( k_n \left( \zeta + \frac{1}{2} \right) \right)}{L (L+1) k_n \sin (k_n) - (1 - L^2 k_n^2 / 2 + L) \cos (k_n)}$$

$$\times \left[ \sin \left( k_n \left( \frac{1}{2} - \zeta \right) \right) + k_n L \cos \left( k_n \left( \frac{1}{2} - \zeta \right) \right) \right],$$

(14)

for $\zeta' < \zeta \leq 1/2$, where $k_n$ are the roots of the equation $2k_n L \cos (k_n) + [1 - (k_n L)^2] \sin (k_n) = 0$, as before.

By using the above results, we may obtain $\theta(\xi, \zeta, t)$ and consequently $\theta(\xi, \zeta, t)$. Thus, after some calculations, we can show that

$$\theta(\xi, \zeta, t) = \theta_S(\xi, \zeta) + \int_{-1/2}^{1/2} d\zeta' \int_0^t dt' \mathcal{G}(\zeta, \zeta', t-t') \alpha^2(t') e^{k^2 t' + \int_0^{t'} \alpha^2(\tau) d\tau}$$

$$\times \int_{-\infty}^{\infty} d\zeta' \theta_S(\zeta', \zeta') \mathcal{G}^{(2)}(\xi - \zeta', t-t')$$

$$- \int_{-1/2}^{1/2} d\zeta' \mathcal{G}(\zeta, \zeta', t) \tilde{\theta}(\zeta', \zeta', 0),$$

(15)
dependent external field, when the distribution of easy axes is inhomogeneous. In the limit of strong anchoring, i.e. $L \to 0 (b \to 0)$, we recover the general results reported in Ref. 22, as expected. From the above expression, 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 $\Delta l$, between the ordinary and the extraordinary ray, is given by \[ \Delta l = \frac{1}{2} n_o R d (\theta^2), \] where $n_o$ and $n_e$ are the ordinary and extraordinary refractive indices, respectively.

To sum up, a general theoretical framework for investigating the dynamics of the director reorientation in a nematic liquid crystal sample, under the action of an external time-dependent field, in the case in which deformations of the splay-bend type are present, has been proposed. The calculations assume that only small deviations from the easy direction at the surfaces are allowed. Furthermore, backflow effects are not taken into account and we consider that the field distribution across the sample is homogeneous. In this framework, which is the usual one for investigating the reorientation process governed by external fields near the Fréedericksz threshold, the results have been obtained in an exact manner for the general case of weak anchoring at the surfaces, in the case in which these surfaces are characterized by a homogeneous distribution of easy directions.

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