Dynamical behavior of the director field for splay-bend deformations in nematic liquid crystals

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The exact dynamical evolution of the director field for splay-bend deformations, in nematic liquid crystal samples limited by inhomogeneous surfaces, is determined in the one-constant approximation. The initial conditions and boundary-value problem concerning the situation of strong anchoring at the surfaces of a sample of slab shape of thickness d is analytically solved in the presence of a time dependent external electric field, and taking into account the viscous torque. The results are used to analytically obtain the time dependence of the phase shift between the two components of a linearly polarized beam impinging perpendicularly on the sample. The analysis can be relevant to investigate the phase retardation of a nematic cell submitted to an external voltage which is lower than or in the order of the Féedericksz threshold to induce deformations in the sample.

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The evaluation of the director field **n**, or the determination of the profile of the tilt angle of a nematic liquid crystal (NLC) sample, is performed in the framework of the elastic continuum theory [1–6]. In the absence of external fields, the director **n** depends on the surface treatment. The influence of inhomogeneous surfaces on the molecular orientation of a NLC sample has been analyzed by several authors in the framework of the Frank-Oseen elasticity [7–22]. On the other hand, the effects of external applied fields are crucial in the performance of electro-optical devices based on liquid crystalline materials [23]. As is well known, when submitted to the influence of external fields NLCs exhibit a large variety of dynamical behavior [24]. The most common phenomenon is the field-induced distortion known as the Fréedericksz transition [25], which is usually treated as a second order phase transition, except near the inversion point of main anisotropy [26] or when feedback effects are taken into account [27], when it can be first order. To face these complex phenomena from the theoretical side is a hard task and only simplified or specific models can be treated in an analytical way [28].

In this Brief Report, 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 strong anchoring under the action of a time-dependent applied electric field, when the surfaces are characterized by a spatially dependent distribution of the easy axes. We present the complete analytical solution for the profile of the tilt angle in the framework of the elastic continuum theory, in the one-constant approximation, by taking into account the viscous torque. The 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, i.e., we are considering 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 [29]. 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, one illustrative example of a time-dependent electric field is discussed in detail. We consider the typical case in which the applied field is represented by a square-wave signal, but as will be clearer below, other general forms of time variation of the applied field can be considered.

We consider a nematic slab of thickness d. The Cartesian reference frame is chosen with the z axis normal to the bounding plates, located 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, $\theta(x,z)$, made by the nematic director with the z axis, is supposed 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 [30]

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

in the limit of small θ. This approximation is justified if we limit our analysis to the cases in which the applied field is of the order of the Fréedericksz threshold [31]. In Eq. (1) $\epsilon_a=\epsilon_\parallel-\epsilon_\perp$ ($\parallel$ and $\perp$ refer to the direction of **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 [32].

To analyze the dynamics of the orientation induced by the field we have 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

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

written in a nondimensional form by introducing reduced coordinates $\xi\to x/d$, and $\zeta\to z/d$ and a reduced time $t\to t/\tau_v$, where $\tau_v=\lambda d^2/K$ is the viscous relaxation time and λ is an effective viscosity coefficient of the liquid crystal [2].

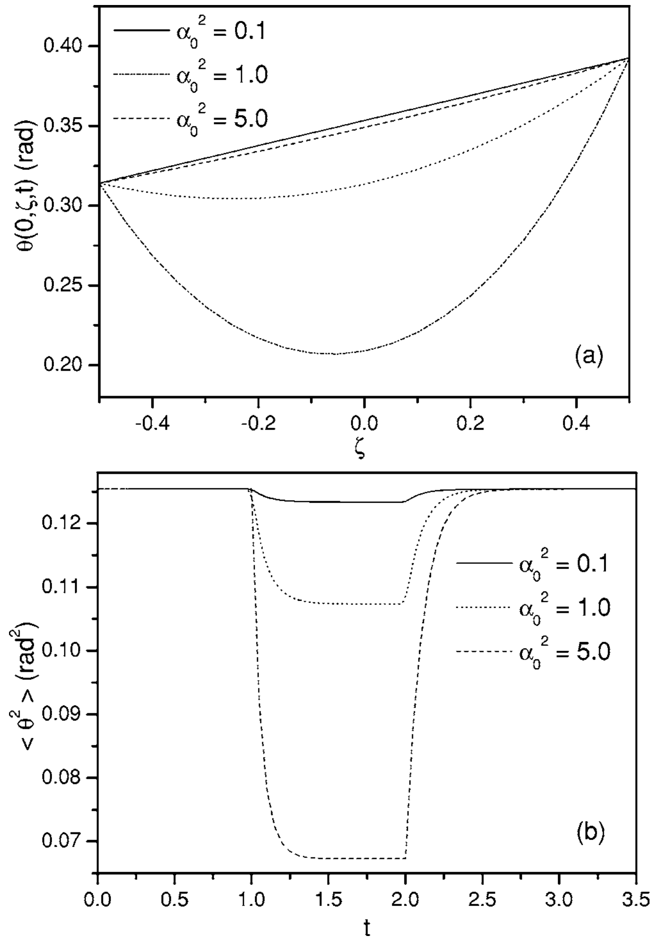

FIG. 1. (a) Profile of the tilt angle $\theta(0,\zeta,t)$ versus ζ for different amplitudes of the step-like applied field. Solid line for $t=0$ and the other lines for $t=1.5$. (b) $\langle\theta^2\rangle$ versus dimensionless time t for different strengths of the step-like applied field.

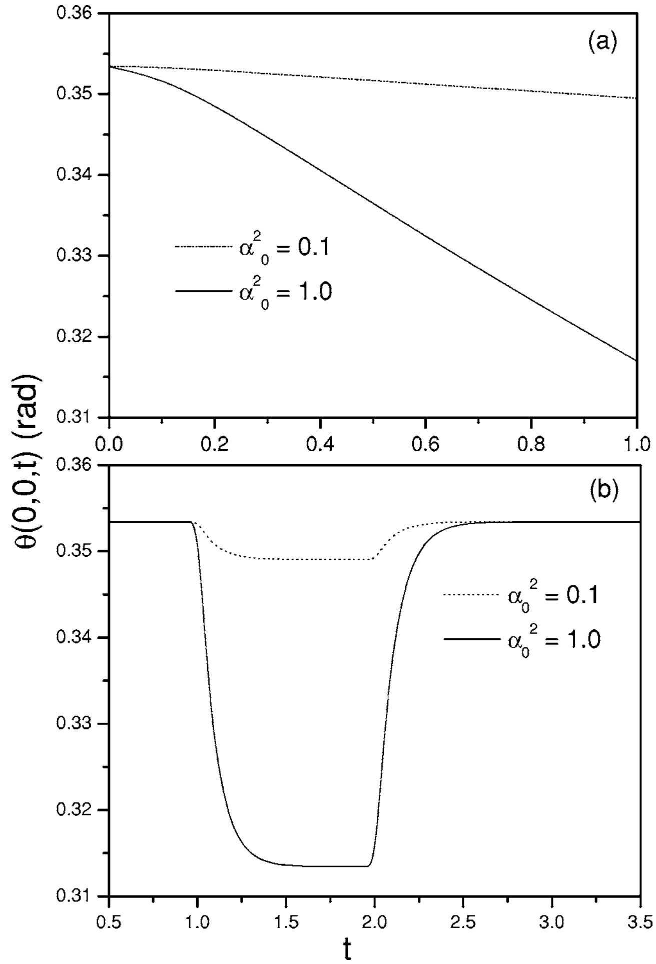

FIG. 2. Time dependence of the exact profile of the tilt angle in the center of the sample $\theta(0,0,t)$ for different strengths of the applied field. In (a) the field has the form $\alpha^2(t)=\alpha_0^2 t$ and in (b) $\alpha(t)$ has the step-like profile of (12).

In this manner, $\alpha^2(t)=\pi^2(E(t)/E_c)^2$, where $E_c^2=\pi^2K/\epsilon_a$ is the threshold field for the Fréedericksz transition in strong anchoring [30]. As will be shown below, for $\epsilon_a>0$ increasing the strength of the applied field will produce a decrease in the optical path difference, because, as pointed out above, the field tends to stabilize the uniform orientation. The solution of Eq. (2) is the function $\theta(\xi,\zeta,t)$ subjected to an initial condition and satisfying appropriated boundary conditions. For the case characterized by the strong anchoring on both surfaces the boundary conditions are [30]

$$\theta(\xi,\zeta,t)\big|_{\zeta=\pm 1/2}=\Theta_\pm(\xi). \tag{3}$$

In Eq. (3), $\Theta_\pm(\xi)$ accounts for the surface orientation imposed by the surface treatment, i.e., the easy axes on the upper (+) and lower (−) surfaces, respectively. 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

$$\theta(\xi,\zeta,t)=\theta_S(\xi,\zeta)+\tilde{\theta}(\xi,\zeta,t), \tag{4}$$

where $\theta_S(\xi,\zeta)$ is the stationary solution obtained from the Laplace equation $\nabla^2\theta_S=0$ taking the boundary condition $\theta_S(\xi,\zeta)\big|_{\zeta=\pm 1/2}=\Theta_\pm(\xi)$ into account. In particular, the solution for $\theta_S(\xi,\zeta)$ is given by [15–17]

$$\theta_S(\xi,\zeta)=\sum_{i=+,-}\int_{-\infty}^{\infty} d\xi'\,\mathcal{G}_i(\xi-\xi',\zeta)\Theta_i(\xi') \tag{5}$$

with

$$\mathcal{G}_\pm(\xi,\zeta)=\frac{1}{2}\frac{\cos(\pi\zeta)}{\cosh(\pi\xi)\mp\sin(\pi\zeta)}. \tag{6}$$

By substituting Eq. (4) in Eq. (2) and Eq. (3), we obtain

$$\frac{\partial^2}{\partial\xi^2}\tilde{\theta}(\xi,\zeta,t)+\frac{\partial^2}{\partial\zeta^2}\tilde{\theta}(\xi,\zeta,t)-\alpha^2(t)[\tilde{\theta}(\xi,\zeta,t)+\theta_S(\xi,\zeta)]$$
$$=\frac{\partial}{\partial t}\tilde{\theta}(\xi,\zeta,t) \tag{7}$$

subjected to the initial condition $\tilde{\theta}(\xi,\zeta,0)=\theta_0(\xi,\zeta)-\theta_S(\xi,\zeta)$ and the boundary condition $\tilde{\theta}(\xi,\zeta=\pm 1/2,t)=0$. The solution for Eq. (7) is given by

$$\widetilde{\theta}(\xi,\zeta,t)=\sum_{n=1}^{\infty}\{\mathcal{A}_n(\xi,t)\cos[(2n-1)\pi\zeta]+\mathcal{B}_n(\xi,t)\sin(2n\pi\zeta)\} \tag{8}$$

where $\mathcal{A}_n(\xi,t)$ and $\mathcal{B}_n(\xi,t)$ are coefficients to be determined. In particular, these coefficients can be obtained by substituting Eq. (8) in Eq. (7), employing the Fourier transform on ξ and using the orthogonality of the $\cos(nx)$ and $\sin(nx)$ functions. Thus, after some calculations it is possible to show that the coefficients present in Eq. (8) are given by

$$\begin{aligned}\mathcal{A}_n(\xi,t)=&\int_{-1/2}^{1/2}ds\,\cos[(2n-1)\pi s]\int_{-\infty}^{\infty}d\xi'\frac{e^{-(\xi-\xi')^2/4t}}{\sqrt{4\pi t}}\\&\times[\theta_0(\xi',s)-\theta_S(\xi',s)]\\&\times e^{-[(2n-1)\pi]^2t}e^{-\int_0^t dt'\,\alpha^2(t')}\\&-2\int_{-1/2}^{1/2}ds\,\cos[(2n-1)\pi s]\int_0^t dt'\,\alpha^2(t')\\&\times\int_{-\infty}^{\infty}d\xi'\frac{e^{-(\xi-\xi')^2/4(t-t')}}{\sqrt{4\pi(t-t')}}\theta_S(\xi',s)\\&\times e^{-[(2n-1)\pi]^2(t-t')}e^{-\int_0^t d\bar{t}\alpha^2(\bar{t})+\int_0^{t'}d\bar{t}\alpha^2(\bar{t})}\end{aligned} \tag{9}$$

and

$$\begin{aligned}\mathcal{B}_n(\xi,t)=&\int_{-1/2}^{1/2}ds\,\sin(2n\pi s)\int_{-\infty}^{\infty}d\xi'\frac{e^{-(\xi-\xi')^2/4t}}{\sqrt{4\pi t}}\\&\times[\theta_0(\xi',s)-\theta_S(\xi',s)]e^{-(2n\pi)^2t}e^{-\int_0^t dt'\,\alpha^2(t')}\\&-2\int_{-1/2}^{1/2}ds\,\sin(2n\pi s)\int_0^t dt'\,\alpha^2(t')\int_{-\infty}^{\infty}\\&\times d\xi'\frac{e^{-(\xi-\xi')^2/4(t-t')}}{\sqrt{4\pi(t-t')}}\theta_S(\xi',s)\\&\times e^{-(2n\pi)^2(t-t')}e^{-\int_0^t d\bar{t}\alpha^2(\bar{t})+\int_0^{t'}d\bar{t}\alpha^2(\bar{t})}.\end{aligned} \tag{10}$$

When $\theta(\xi,\zeta)$ 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 [30] $\Delta l=1/2n_oRd\langle\theta^2\rangle$, where

$$\langle\theta^2\rangle=\frac{d}{\Lambda}\int_{-\Lambda/2d}^{\Lambda/2d}\int_{-1/2}^{1/2}\theta(\xi,\zeta)^2d\xi d\zeta, \tag{11}$$

is the average square tilt angle, evaluated over a typical length Λ, connected with the diameter of the light beam. Furthermore, $R=1-(n_o/n_e)^2$, and n_o and n_e are, respectively, the ordinary and extraordinary refractive indices. Thus, to illustrate the effect produced by a time dependent electric field applied to the system we use the previous results found for $\theta(\xi,\zeta,t)$ in Eq. (11).

For simplicity, we consider a pretilted cell characterized by the boundary condition $\theta|_{\zeta=1/2}=\pi/8$, $\theta|_{\zeta=-1/2}=\pi/10$, such that we can assure the limit of small distortions. Furthermore, we assume for the electric field part the form

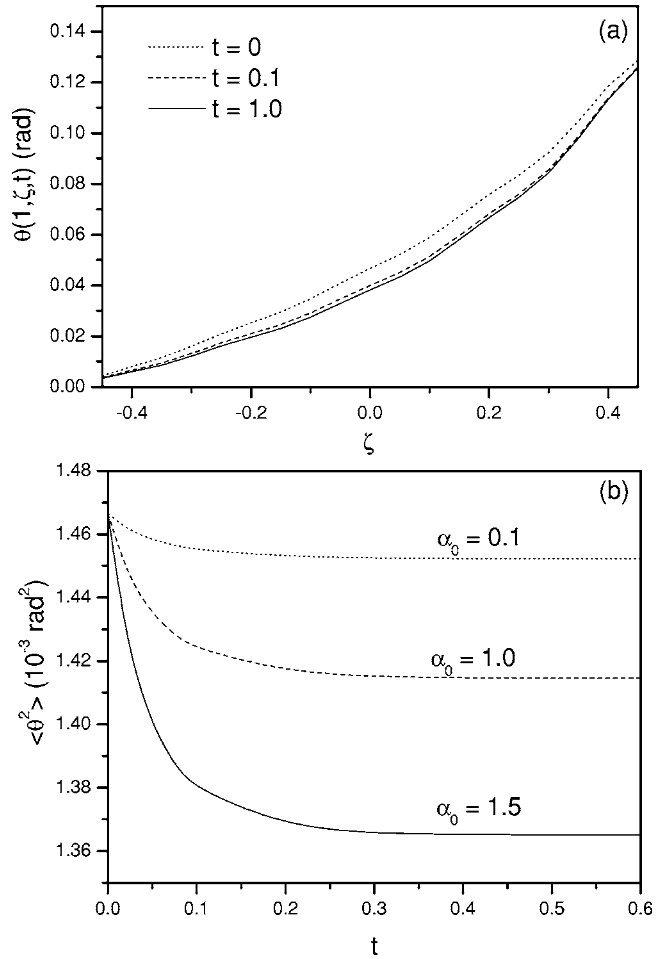

FIG. 3. (a) Profile of the tilt angle $\theta(1,\zeta,t)$ for three different values of the dimensionless time t. (b) $\langle\theta^2\rangle$ versus t for different strengths of the constant applied field. The curves were depicted for $\lambda/d=\pi$.

$$\alpha^2(t)=\alpha_0^2[H(t-1)-H(t-2)], \tag{12}$$

where $H(\xi)$ is the Heaviside step function. The initial condition is such that $\theta(\xi,\zeta,0)=\theta_S(\xi,\zeta)$, i.e., corresponding to the stationary solution given by Eq. (5) for the boundary conditions given above. In Fig. 1(a), four instantaneous profiles of the tilt angle are shown in the position $\xi=0$, as a function of the distance from the surface in the case in which the applied field has the form (12). The solid line refers to the situation before the application of the field at $t=0$, whereas the other curves were depicted for the particular time $t=1.5$, which corresponds precisely to the middle of the time interval during which the field, of different amplitudes α_0, is applied. From this figure we observe that, depending on the strength of the applied field, we may have a small or relatively large deformation of the director field in a particular point of the sample. In Fig. 1(b), the average of the square of the tilt angle, $\langle\theta^2\rangle$, which is proportional to the optical path difference and is given by Eq. (11), is shown as a function of time.

The step-like form of the applied field governs the response of the orientation of the sample, whose reorientation dynamics is explicitly determined.

In Fig. 2 the time dependence of the exact profile of the tilt angle in the center of the sample is shown for two different distributions of the applied field. In Fig. 2(a), we consider an applied field in the form $\alpha^2(t)=\alpha_0^2 t$, whereas in Fig. 2(b) the field has the step-like profile (12).

The response in Fig. 2(a) is slightly nonlinear for very small times, due to the viscous torque, and becomes practically linear for long times, because the field increases for increasing time. The common features of these illustrative figures are the possibility of determining the exact response, and consequently the precise characteristic times of these responses, to applied fields in the sample. Another common feature is that in these cases involving uniform easy directions the profile of the tilt angle is independent of ξ. An illustrative example involving nonhomogenous distribution of the easy direction could be the case represented by the boundary conditions (similar to the ones considered by Berreman [7])

$$\theta(\xi,-1/2,t)=0 \text{ and } \theta(\xi,1/2,t)=\Theta_0 \sin(q\xi), \qquad (13)$$

where $q=2\pi d/\lambda$, with λ representing the spatial periodicity of the distribution. For simplicity, we assume furthermore a constant electric field, such that $\alpha(t)^2=\alpha_0$. In Fig. 3(a) a typical z-dependence of the tilt angle is shown in the position $\xi=x/d=1$ for three different times. In Fig. 3(b) $\langle\theta^2\rangle$ is shown versus t for different strengths of the constant applied field. As expected, for $\epsilon_a>0$ (as is the case considered here) the increase of the strength of the applied field is accompanied by a decrease in the optical path difference, because the field tends to favor the (uniform) homeotropic orientation in the sample despite the periodic distribution of the easy axis on the upper surface. Anyway, due to the strong anchoring conditions the optical path difference indicates that the sample is always distorted.

In conclusion, we have presented a theoretical framework to investigate 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. We work on the hypothesis that only small deformations are allowed. Furthermore, backflow effects are not taken into account and we consider that the field distribution across the sample is homogenous. In this framework, which is the usual one to investigate the reorientation process governed by external fields near the Fréedericksz threshold, the results can be obtained in an exact manner for a large class of external field profiles.

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