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Exact dynamical reorientation in nematic liquid crystals: Green's function approach

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Abstract

The exact dynamical behavior of the nematic director field in a cell limited by two planar surfaces, having inhomogeneous distribution of easy axes, is theoretically investigated within the Green's function approach. The equilibrium configurations are determined for splay-bend deformations in the framework of Frank elasticity, in the one-constant approximation. Both, the strong anchoring (Dirichlet's problem) and the weak anchoring cases (mixed Dirichlet–Neumann problem) are solved in the presence of an external time dependent field. The general solutions for both problems are obtained for the more general case in which the boundary conditions are position and time dependent.

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1. Introduction

A significant number of problems, dealing with the equilibrium orientational states of nematic liquid crystals (NLC), can be faced in the framework of the elastic continuum theory for liquid crystalline materials [1–11] and, from the mathematical point of view, can be formulated as boundary value problems. The basic principle involved in the application of the continuum theory to the solution of relevant problems is that the equilibrium state of the director **n** is always given by the configuration that minimizes the total elastic energy of the system [10,11]. 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 [12–17]. The first problem refers to the situation of strong anchoring in the presence of static deformations in a typical NLC cell. The second 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 [18].

In this work, we consider splay-bend deformations in an NLC cell limited by two planar treated surfaces having inhomogeneous distribution of easy axes. We present the complete analytical solution for the initial conditions and boundary-value problem concerning the situation of weak anchoring at the surfaces in the presence of a time dependent external electric field, taking into account the viscous torque, when the surfaces are characterized by a space–time dependent distribution of easy axes. The general solution is given in terms of Green's function. In this manner, the exact dynamical evolution of the director field is established in closed form. The results are relevant to a cell in which the applied field is of the order of the Fréedericksz threshold field [19] to induce small deformations in the nematic structure. We suppose that the electric field is homogeneous across the sample and effects like the selective adsorption of ions are not considered [20]. We assume, furthermore, that in the vicinity of the Fréedericksz transition the backflow effects can be ignored. The situation in which the easy axis changes direction continuously with time, embodied by the general solution we find, is relevant to investigate systems whose surfaces are covered with photopolymeric films [21,22]. In these sys-

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tems, the orientational changes of the photochromic molecules promoted by incident light lead to remarkable changes in the orientation direction of the liquid crystal molecules.

2. Statement of the problem

The elastic energy density of an NLC cell is given by the Frank elastic energy density [10,11,23,24]

$$f = \frac{1}{2}\left\{K_{11}(\nabla\cdot\mathbf{n})^2 + K_{22}\left[\mathbf{n}\cdot(\nabla\times\mathbf{n})\right]^2 + K_{33}\left[\mathbf{n}\times(\nabla\times\mathbf{n})\right]^2\right\} - (K_{22}+K_{24})\nabla\cdot\left[\mathbf{n}\nabla\cdot\mathbf{n}+\mathbf{n}\times(\nabla\times\mathbf{n})\right], \tag{1}$$

in which $\mathbf{n}$ is a unit vector representing the average molecular orientation of the nematic phase. Furthermore, $K_{ii} > 0$, with $i = 1, 2, 3$ are, respectively, the bulk elastic constants of splay, twist, and bend, whereas K_{24} is the saddle-splay elastic constant, associated to a surface-like term. If this term is absent, as will be considered here, the elastic energy density reduces to a positive definite quadratic form in the distortions. When the sample is submitted to an external electric field $\mathbf{E}$, another contribution, having the form

$$f_E = -\frac{1}{2}\epsilon_a(\mathbf{n}\cdot\mathbf{E})^2, \tag{2}$$

has to be added to f to complete the bulk elastic energy density [10]. In (2), $\epsilon_a = \epsilon_\parallel - \epsilon_\perp$ ($\parallel$ and $\perp$ refer to the direction of $\mathbf{n}$) is the dielectric anisotropy. 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 [25]. For simplicity, we particularize the analysis to the case in which the total energy density can be written in terms of one angle only, i.e., the tilt angle θ, made by $\mathbf{n}$ with the normal to the surfaces. To do this, we consider a cell in the shape of a slab of thickness d, bounded by two flat surfaces as in Fig. 1, and limit the analysis to the case of splay-bend distortions. In this situation, the director is everywhere parallel to the (x–z) plane. The Cartesian reference frame is chosen with the z axis normal to the surfaces, 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 is 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. The surface energy is assumed as the one proposed by Rapini–Papoular [26], written here as

$$f_S = \frac{1}{2}W_\pm \sin^2(\theta_\pm - \Theta_\pm), \tag{3}$$

where $W_\pm$ are known as the anchoring strengths connected to the surfaces located at $z = \pm d/2$, $\Theta_\pm(x)$ characterize the easy axes, that is, the surface-tilt angles for which the surface energy f_S is minimum, and $\theta_\pm(x)$ are the actual values of the tilt angle at the surface. In the parabolic approximation, i.e., when the actual values of the tilt angle at the surface are close to the angles defining the easy directions, $f_S = 1/2 W_\pm(\theta_\pm - \Theta_\pm)^2$.

The total energy of the cell, per unit length along y, is given by

$$F = \int_{-\infty}^{\infty} dx \left\{ \int_{-d/2}^{d/2} \left[f\left(\frac{\partial\theta}{\partial x}, \frac{\partial\theta}{\partial z}\right) + f_E(\theta)\right] dz + f_S(\theta_+) + f_S(\theta_-)\right\}. \tag{4}$$

In the one-constant approximation, $K_{11} = K_{22} = K_{33} = K$, and in the presence of a time dependent external field $\mathbf{E} = E(t)\mathbf{k}$, expression (4) reduces to

$$F\left[\theta(x,z)\right] = \int_{-\infty}^{\infty} dx \int_{-d/2}^{d/2} dz \left[\frac{1}{2}K(\vec{\nabla}\theta)^2 + \frac{\epsilon_a}{2}E^2(t)\theta^2\right] + \int_{-\infty}^{\infty} dx\, \frac{1}{2}\left[W_-\left[\theta_-(x) - \Theta_-(x)\right]^2 + W_+\left[\theta_+(x) - \Theta_+(x)\right]^2\right], \tag{5}$$

where $\vec{\nabla}\theta = (\partial\theta/\partial x)\mathbf{i} + (\partial\theta/\partial z)\mathbf{k}$. We consider the case in which $W_- = W_+ = W$. Note also that Eq. (5) is obtained in the limit of small θ. As pointed out before, this approximation is justified if we limit our analysis to the cases in which the applied field is in the order of the Fréedericksz threshold [27].

To analyze the dynamics of the orientation induced by the field we have to consider also a viscous torque [28]. By minimizing Eq. (5), taking into account the viscous torque, we find that the dynamical evolution of the system is governed by the equation

$$\frac{\partial^2\theta}{\partial\xi^2} + \frac{\partial^2\theta}{\partial\zeta^2} = \alpha^2(t)\theta + \frac{\partial\theta}{\partial t}, \tag{6}$$

written in a non-dimensional 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 [28]. In this manner,

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

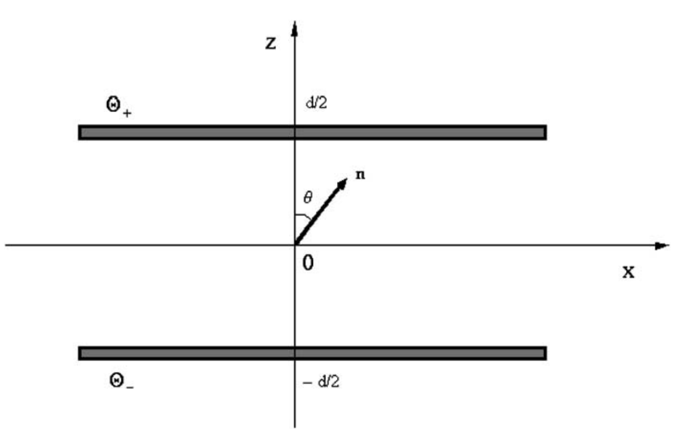

Fig. 1. Cell of thickness d filled with nematic liquid crystals.

where $E_c^2 = \pi^2 K/\epsilon_a$ is the threshold field for the Fréedericksz transition in strong anchoring [10]. The solution of Eq. (6) is the function $\theta(\xi,\zeta,t)$ subjected to an initial condition and satisfying appropriated boundary conditions.

3. Strong and weak anchoring

Let us start our discussion concerning the solutions of Eq. (6) by considering the case characterized by the strong anchoring. For this case, we have a Dirichlet boundary value problem, i.e., the boundary condition is given by $\theta(\xi,\zeta,t)|_{\zeta=\pm 1/2} = \Theta_\pm(\xi,t)$. $\Theta_\pm(\xi,t)$ is the surface orientation imposed by the surface treatment, i.e., the easy axes on the upper $(+)$ and lower $(-)$ surfaces, respectively. Note that, in contrast with the situation recently worked out in [17], this boundary condition is also time dependent. This time dependence can be useful, for instance, to describe systems whose surface is prepared with photopolymeric films. 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. (6) taking these considerations into account, we use the Fourier transform and the Green's function approach. After some calculations, it is possible to show that Eq. (6) can be reduced to

$$\frac{\partial^2}{\partial\zeta^2}\bar\theta(k,\zeta,t) = \frac{\partial}{\partial t}\bar\theta(k,\zeta,t) \tag{7}$$

by using the Fourier transform and

$$\theta(k,\zeta,t) = e^{-k^2 t - \int_0^t d\bar t\,\alpha^2(\bar t)}\bar\theta(k,\zeta,t) \tag{8}$$

where $\theta(k,\zeta,t) = \mathcal{F}\{\bar\theta(\xi,\zeta,t)\}$ ($\mathcal{F}\{\cdots\} = \int_{-\infty}^{\infty} d\xi\, e^{-ik\xi}\cdots$ and $\mathcal{F}^{-1}\{\cdots\} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik\xi}\cdots$). By incorporating these changes in the boundary and initial condition, we obtain that $\bar\theta(k,\zeta,t)|_{\zeta=\pm 1/2} = e^{k^2 t + \int_0^t d\bar t\,\alpha^2(\bar t)}\Theta_\pm(k,t)$ and $\bar\theta(k,\zeta,0) = \theta(k,\zeta,0) = \theta_0(\xi,\zeta)$. Now, by using the Green's function approach [29] with appropriated boundary conditions, it is possible to find the solution for Eq. (7). It is given by

$$\bar\theta(k,\zeta,t) - \int_{-1/2}^{1/2} d\zeta'\,\theta_0(\xi,\zeta)\mathcal{G}^{(s)}(\zeta,\zeta',t) + \int_0^t d\bar t \sum_{i=-,+}\mathcal{G}_i^{(s)}(\zeta,t-\bar t)\Theta_i(k,\bar t)e^{k^2\bar t + \int_0^{\bar t} d\tilde t\,\alpha^2(\tilde t)}, \tag{9}$$

where the Green's function $\mathcal{G}^{(s)}(\zeta,\zeta',t)$ is given by

$$\begin{aligned}\mathcal{G}^{(s)}(\zeta,\zeta',t) &= 2\sum_{n=1}^{\infty}(-1)^n e^{-(n\pi)^2 t} \\ &\quad\times\begin{cases}\sin\left(n\pi\left(\zeta+\frac12\right)\right)\sin\left(n\pi\left(\frac12-\zeta'\right)\right), & -\frac12 \leqslant \zeta < \zeta', \\ \sin\left(n\pi\left(\zeta'+\frac12\right)\right)\sin\left(n\pi\left(\frac12-\zeta\right)\right), & \zeta' < \zeta \leqslant \frac12\end{cases}\end{aligned} \tag{10}$$

and

$$\begin{aligned}\mathcal{G}_\pm^{(s)}(\zeta,t) &= \pm\frac{d}{dz}\mathcal{G}^{(s)}(\zeta,\zeta',t)\bigg|_{\zeta=\pm\frac12,\zeta'=\zeta} \\ &= 2\sum_{n=1}^{\infty}(-1)^{n+1} n\pi\sin\left(n\pi\left(\frac12\pm\zeta\right)\right)e^{-(n\pi)^2 t}.\end{aligned} \tag{11}$$

The first term of Eq. (9) is due to the initial condition and the second term explicitly depends on the surface treatment, i.e., how the surfaces of the sample were prepared. By substituting Eq. (9) in Eq. (8) and inverting the Fourier transform, we obtain the tilt angle, for the strong anchoring case, as follows:

$$\begin{aligned}\theta(\xi,\zeta,t) = &-\int_{-1/2}^{1/2} d\zeta' \int_{-\infty}^{\infty} d\bar\xi\,\mathcal{G}^{(s)}(\zeta,\zeta',t)\mathcal{G}(\xi-\bar\xi,t)\theta_0(\bar\xi,\zeta') \\ &\times e^{-\int_0^t d\bar t\,\alpha^2(\bar t)} \\ &+ \int_{-\infty}^{\infty} d\bar\xi \int_0^t d\bar t\,\mathcal{G}(\xi-\bar\xi,t-\bar t) \\ &\times e^{-\int_0^t d\bar t\,\alpha^2(\bar t) + \int_0^{\bar t} d\tilde t\,\alpha^2(\tilde t)} \\ &\times \sum_{i=-,+}\mathcal{G}_i^{(s)}(\zeta,t-\bar t)\Theta_i(k,\bar t)\end{aligned} \tag{12}$$

with $\mathcal{G}(\xi,t) = e^{-\xi^2/(4t)}/\sqrt{4\pi t}$ (see Fig. 2).

We may extend the previous situation by considering the weak anchoring on both surfaces. For this case the boundary conditions on the surfaces are given by

$$\pm L\frac{\partial}{\partial\zeta}\theta(\xi,\zeta,t) + \theta(\xi,\zeta,t)\bigg|_{\zeta=\pm 1/2} = \Theta_\pm(\xi,t), \tag{13}$$

where $L = b/d$ ($b = K/W$ is the extrapolation length [30]). Note that for this case we also incorporated a time dependence in the surface orientation as the previous case characterized by the strong anchoring, and the limit $L\to 0$ ($b\to 0$) corresponds to the strong anchoring case. The situation has some similarity with the problem of surface friction, if the anchoring is not strong [31]. By employing the above procedure for this case it is possible to show that the solution for Eq. (6) subjected to the boundary condition given by Eq. (13) is

$$\begin{aligned}\theta(\xi,\zeta,t) \\ = &-\int_{-1/2}^{1/2} d\zeta' \int_{-\infty}^{\infty} d\bar\xi\,\mathcal{G}^{(w)}(\zeta,\zeta',t)\mathcal{G}(\xi-\bar\xi,t)\theta(\bar\xi,\zeta',0) \\ &\times e^{-\int_0^{\bar t} d\tilde t\,\alpha^2(\tilde t)} \\ &- \frac{1}{L}\int_0^t d\bar t \int_{-\infty}^{\infty} d\bar\xi\left[\mathcal{G}^{(w)}\left(\frac12,\zeta,t-\bar t\right)\Theta_+(\bar\xi,\bar t)\right. \\ &\left. + \mathcal{G}^{(w)}\left(-\frac12,\zeta,t-\bar t\right)\Theta_-(\bar\xi,\bar t)\right] \\ &\times \mathcal{G}(\xi-\bar\xi,t-\bar t)e^{-\int_0^t d\bar t\,\alpha^2(\bar t) + \int_0^{\bar t} d\tilde t\,\alpha^2(\tilde t)},\end{aligned} \tag{14}$$

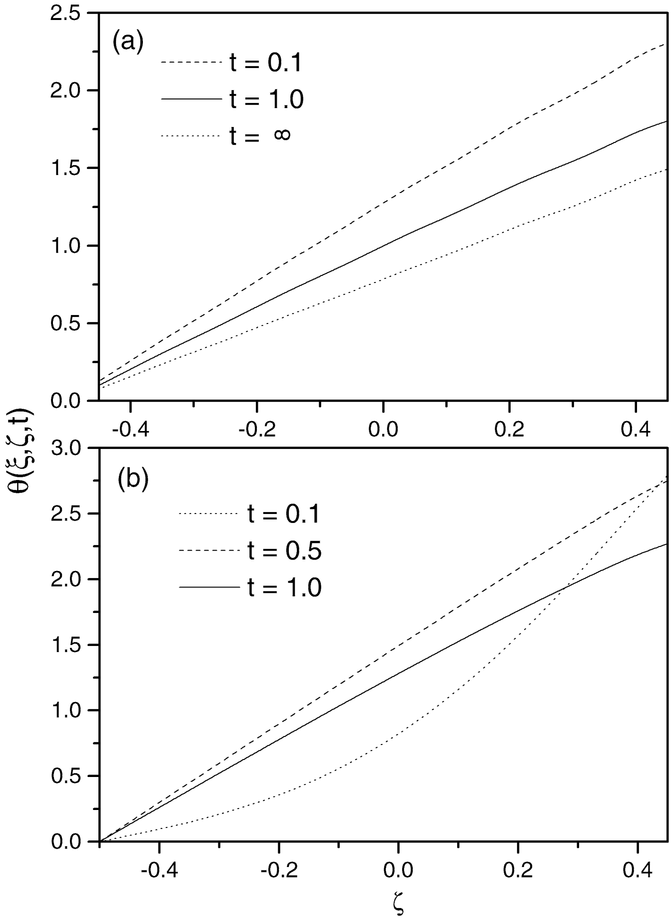

Fig. 2. Behavior of $\theta(\xi,\zeta,t)$ versus ζ is illustrated for the strong anchoring in figures (a) and (b) in the absence of external field with $\theta_0(\xi,\zeta)=0$. Figure (a) shows the behavior of the tilt angle for the case $\Theta_-(\xi,t)=0$ and $\Theta_+(\xi,t)=\Theta(1+e^{-t}\cos(t))$. Note that for long time this case recovers the stationary solution found in [15]. Figure (b) shows the behavior of the tilt angle for the case $\Theta_-(\xi,t)=0$ and $\Theta_+(\xi,t)=\Theta(1+\cos(t))$. This case, in contrast to the case of the figure (a), does not have a stationary solution and the tilt angle oscillates with the time. In both cases, we consider $\xi=1$ and $\Theta=\pi/2$.

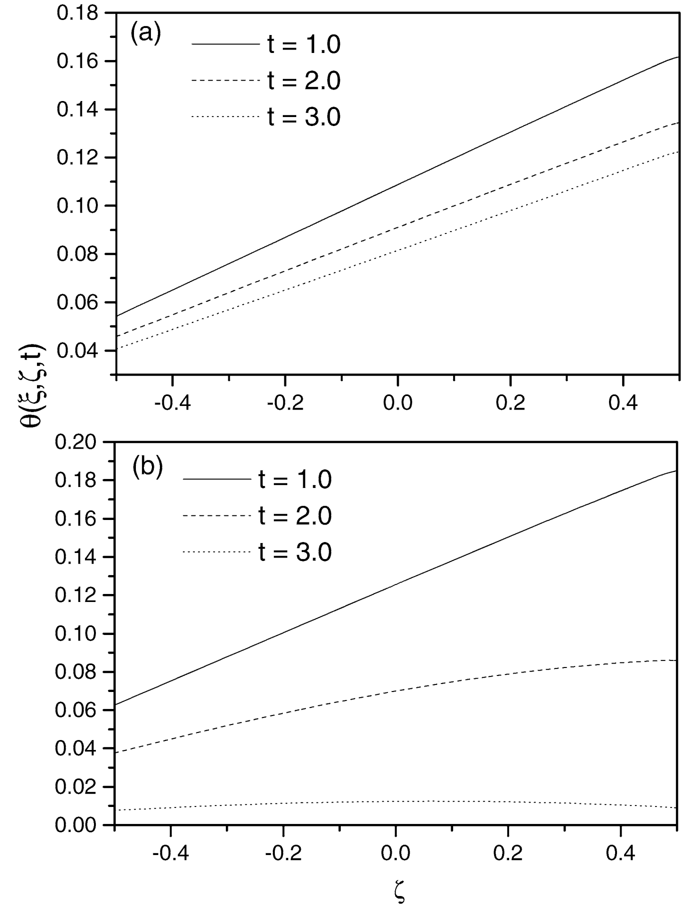

Fig. 3. Behavior of $\theta(\xi,\zeta,t)$ versus ζ is illustrated by considering a constant external field, i.e., $\alpha^2(t)=\alpha^2$ with $\alpha^2=0.1$. Figure (a) corresponds to the case $\Theta_-(\xi,t)=0$ and $\Theta_+(\xi,t)=\Theta(1+e^{-t})$. Figure (b) represents the case $\Theta_-(\xi,t)=0$ and $\Theta_+(\xi,t)=\Theta(1+\cos(t))$. In both cases, we consider $\theta_0(\xi,\zeta)=0$, $\xi=1$, $L=0.5$ and $\Theta=\pi/20$.

where Green's function $\mathcal{G}^{(w)}(\zeta,\zeta',t)$ for this case is given by

$$\mathcal{G}^{(w)}(\zeta,\zeta',t) = -\sum_{n=1}^{\infty}\frac{[\sin(k_n(\zeta+\frac{1}{2}))+k_nL\cos(k_n(\zeta+\frac{1}{2}))]e^{-k_n^2t}}{L(L+1)k_n\sin(k_n)-[(1-L^2k_n^2)/2+L]\cos(k_n)} \times\left[\sin\left(k_n\left(\frac{1}{2}-\zeta'\right)\right)+k_nL\cos\left(k_n\left(\frac{1}{2}-\zeta'\right)\right)\right] \tag{15}$$

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

$$\mathcal{G}^{(w)}(\zeta,\zeta',t) = -\sum_{n=1}^{\infty}\frac{[\sin(k_n(\zeta'+\frac{1}{2}))+k_nL\cos(k_n(\zeta'+\frac{1}{2}))]e^{-k_n^2t}}{L(L+1)k_n\sin(k_n)-[(1-L^2k_n^2)/2+L]\cos(k_n)} \times\left[\sin\left(k_n\left(\frac{1}{2}-\zeta\right)\right)+k_nL\cos\left(k_n\left(\frac{1}{2}-\zeta\right)\right)\right] \tag{16}$$

for $\zeta'<\zeta\leqslant 1/2$ with the k_n determined by the equation $2k_nL\cos(k_n)+[1-(k_nL)^2]\sin(k_n)=0$ (see Figs. 3 and 4). Similarly to the strong anchoring case, the second term of Eq. (14) is due to the condition employed on the surface.

The expression (14) represents the complete analytical solution of the mixed Dirichlet–Neumann problem relative to the weak anchoring in the cell, i.e., it is the solution of Eq. (6) satisfying the boundary conditions Eq. (13). It gives the time dependent profile of the tilt angle in the presence of a time dependent external field, when the distribution of easy axes on the surfaces is inhomogeneous. In the limit of strong anchoring, i.e., $L\to 0$, we recover, as expected, the results previously presented and we extend the results reported in Ref. [17]. 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 Δl, between the ordinary and the extraordinary ray, is given by [10] $\Delta l=1/2n_oRd\langle\theta^2\rangle$, where

$$\langle\theta^2\rangle=\frac{d}{\Lambda}\int_{-\Lambda/2d}^{\Lambda/2d}\int_{-1/2}^{1/2}\theta(\xi,\zeta)^2\,d\xi\,d\zeta, \tag{17}$$

is the average square tilt angle, evaluated over a typical length Λ, connected with the diameter of the light beam. Fur-

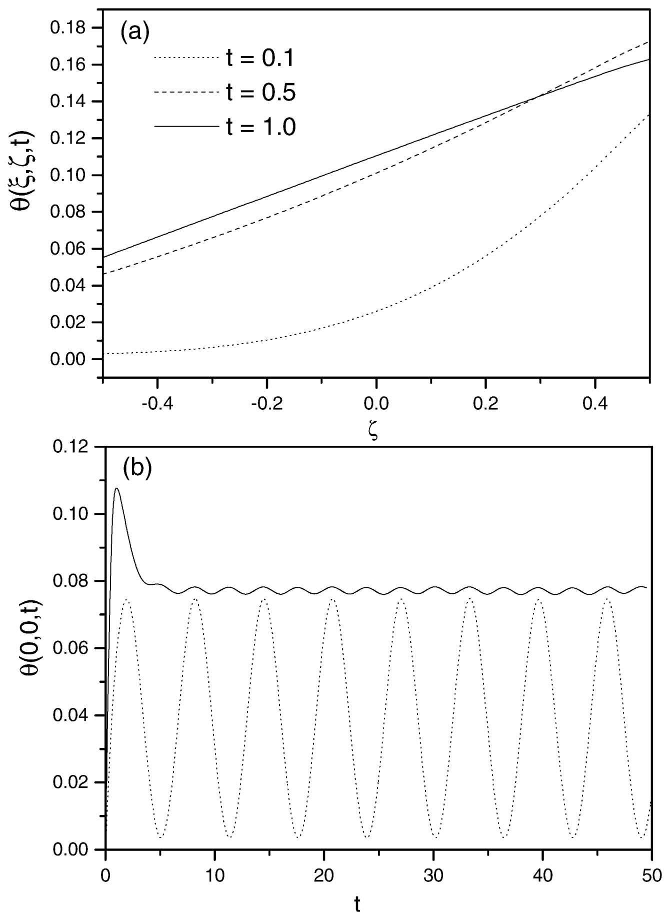

Fig. 4. Behavior of $\theta(\xi,\zeta,t)$ versus ζ is illustrated in figure (a) by considering an oscillating external field, i.e., $\alpha^2(t) = \alpha^2\cos^2(t)$ with $\alpha^2 = 0.1$ for a typical values of t with $\xi = 1$. The condition applied on the surface for this case is $\Theta_-(\xi,t) = 0$ and $\Theta_+(\xi,t) = \Theta(1+e^{-t})$. Figure (b) illustrates the behavior of $\theta(0,0,t)$ versus t for the previous oscillating external field taking the boundary conditions $\Theta_-(\xi,t) = 0$ and $\Theta_+(\xi,t) = \Theta(1+e^{-t})$ (solid line) and $\Theta_-(\xi,t) = 0$ and $\Theta_+(\xi,t) = \Theta(1+\sin(t))/2$ (dot line) into account. In all cases, we consider $\theta_0(\xi,\zeta) = 0$ and $L = 0.5$.

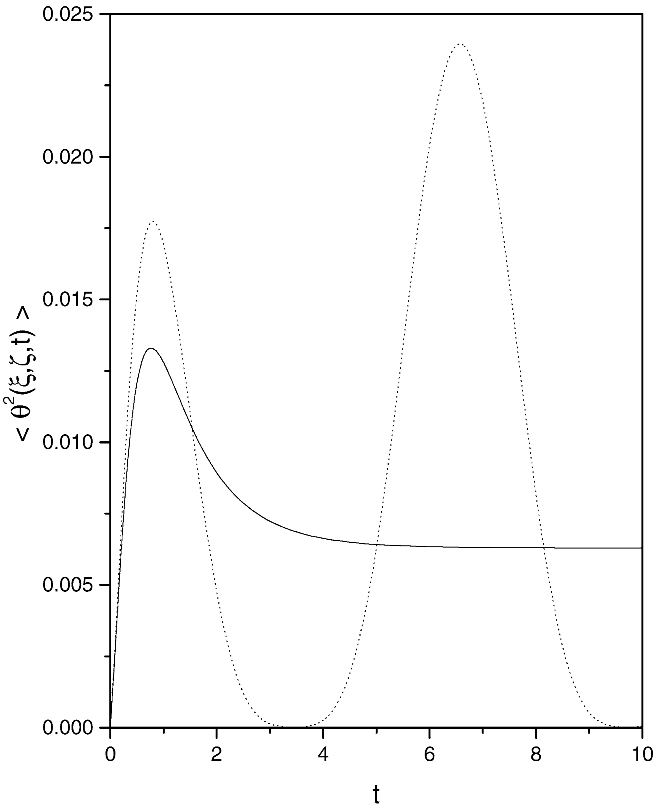

Fig. 5. Behavior of $\langle\theta^2(\xi,\zeta,t)\rangle$ versus t is illustrated by considering a constant external field, i.e., $\alpha^2(t) = \alpha^2$ with $\alpha^2 = 0.1$, $\theta_0(\xi,\zeta) = 0$ and $L = 0.5$. The solid line corresponds to the case $\Theta_-(\xi,t) = 0$ and $\Theta_+(\xi,t) = \Theta(1+e^{-t})$ and the dot line represents the case $\Theta_-(\xi,t) = 0$ and $\Theta_+(\xi,t) = \Theta(1+\cos(t))$. In both cases, we use $\Theta = \pi/20$.

thermore, $R = 1 - (n_o/n_e)^2$, and n_o and n_e are, respectively, the ordinary and extraordinary refractive indices. In Fig. 5, we illustrate the behavior of Eq. (17) for the weak anchoring case.

4. Summary and conclusion

A general 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 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 to investigate reorientation process governed by external fields near the Fréedericksz threshold, the results have been obtained in exact manner for the general case of weak anchoring at the surfaces, in the case in which these surfaces are characterized by a inhomogeneous distribution of easy directions, which, in addition, is time dependent, as in systems whose surfaces are covered by photopolymeric films.

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