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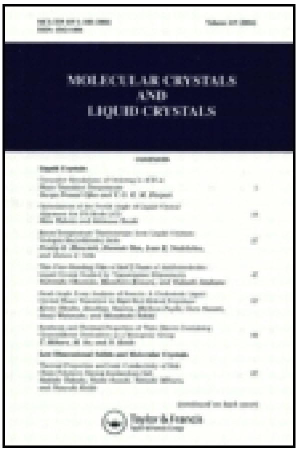

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Modeling Nematic Liquid Crystals: Analytical Solution for the Balance of Torques Equation With Moment of Inertia and Surface Viscosity

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Modeling Nematic Liquid Crystals: Analytical Solution for the Balance of Torques Equation With Moment of Inertia and Surface Viscosity

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We investigate the director relaxation of a nematic liquid crystal cell by considering the molecular moment of inertia, surface viscosity and anchoring energies at the boundaries. The problem solved here corresponds to a more complete description of the nematic director reorientation, since it incorporates ingredients that are usually neglected due to the mathematical difficulty raised by the moment of inertia and surface viscosity. In order to face this problem, we apply the half space approximation for the sample with the surfaces characterized by a time dependent easy direction, which can be mechanically or optically induced in the system. The results show that both, the molecular moment of inertia and the surface viscosity, have influence on the relaxation process of the director. In particular, the presence of the molecular moment of inertia introduces a finite phase velocity and, consequently, leads to a non-instantaneous response time for the distortion propagation in a liquid crystal cell.

Keywords Surface viscosity; Cattaneo's equation; reorientation

I. Introduction

The anisometric shape of thermotropic liquid crystal molecules dictates steric and dispersive forces that cause them, in the nematic phase, to orient along a common direction, called director, described by a vector $\vec{n}(r)$ which may vary from point to point. If an applied external stress does not perturb this orientation, the material response is to flow. Alternatively, when the stress does perturb the preferential direction at a certain point, the material responds with a restorative force in order to retrieve the uniform orientation. This dual response is described in the continuum theory limit where this coupling of elasticity and flow is given by the general treatment from the Leslie-Ericksen formalism [1]. This theory bases itself on the balance of torques acting to rotate or translate the nematic director. Basically, three torques enter in this problem: the elastic torque $\vec{\Gamma}_e$, due to the molecular field (responsible for the elastic-like behavior) and the external field (e.g electric), the viscous torque, $\vec{\Gamma}_v$, associated to the viscous forces between adjacent layers during the director reorientation process and $\vec{\Gamma}_f$, which accounts for the viscosity during the translational motion of the

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director. From Newton's second law, these torques are related as

$$I\frac{\partial\vec{\Omega}}{\partial t} = \vec{\Gamma}_e + \vec{\Gamma}_v + \vec{\Gamma}_f \tag{1}$$

where $\vec{\Omega}$ is the local angular velocity of the director and I is the moment of inertia. Equation 1 contains the ingredients for the continuum description of nematic liquid crystals. This is very important because one can solve this equation with proper boundary conditions to encounter the director orientation in any type of liquid crystal cell. For example, in commercial displays, which is the foremost important application of liquid crystals, the orientation of the bulk director is changed by the presence of an external electric field, whereas at the surfaces the anchoring at the substrate guarantees the uniformity at zero field. In general, from the display application point of view, the flow (or the backflow) is discarded because the electric field effect is solely to rotate the director, so in this article we assume $\vec{\Gamma}_f = 0$. Moreover, the liquid crystal dynamics is considered overdamped [2], so the inertia term is, usually, neglected. The expression $\vec{\Gamma}_v = \vec{\Gamma}_e$ is the famous torque balance found in many textbooks [2,3], where $\vec{\Gamma}_v = -\gamma_1\partial\vec{n}/\partial t$ and $\vec{\Gamma}_e = \delta F_e/\delta\vec{n}$, with

$$\frac{\delta F_e}{\delta\vec{n}} = \frac{\partial F_e}{\partial\vec{n}} - \frac{d}{dr}\frac{\partial F_e}{\partial\vec{n}'}, \tag{2}$$

is the Euler-Lagrange equation and F_e is the free energy corresponding to the Frank (elastic) energy plus the dielectric contribution [2, 3]. Nevertheless, the inertial term has been considered before in the description of picoseconds laser induced director reorientation [4] and induced density, temperature, and flow-reorientation [5] because in this fast dynamic regime, the second derivative term becomes important. It has also been used to allow a complete description of the nematic distortion because the diffusion-like equation does not satisfy the boundary conditions at $t = 0$ [6]. It may also be important in the dynamics of nanoseconds pulses recently used for separating the effect of field-induced biaxial order and differential quenching of uniaxial order [7]. Furthermore, the second derivative term represents a more physical problem because it introduces a finite time for the propagation of the distortion, which is clear from the fact that the equation governing the problem is mathematically the same as the Cattaneo equation [8–10]. Nevertheless, it is clear that the inertial term has not been widely used so far due to the complexity of the mathematical problem.

On the other hand, as a part of a complete formalism for liquid crystals, the scientific community has given considerable attention lately to the surface viscosity [11–17]. Basically, the surface viscosity concepts raises from the fact that for finite anchoring energies (here described in the Rapini-Papoular framework [18]), the director relaxation back to the uniform position happens in a finite time, relaxing at a different pace from the bulk due to the surface anchoring. From the display industry point of view, this is a very important concept, from the design, where liquid crystal simulations such as the relaxation method are heavily employed [2] to practical situations. It is also necessary from the mathematical point of view [19,20]. Nonetheless, similarly to the inertial moment case, the surface viscosity has been neglected in liquid crystal problems due to mathematical complications. Both, moment of inertia and surface viscosity are legitimate contributions in the continuum theory of liquid crystals that rise from basic derivations.

The scope of this article is to deal with the reorientation of the nematic director by taking into account the moment of inertia and surface viscosity, which represents a suitable scenario for the nematic description with direct importance for electronic devices such as displays. The analytical solution is encountered by means of the *Green* function method [21].

II. The Problem

We consider a nematic liquid crystal cell in 1D. For simplicity, we assume that one surface is located at $z = 0$ while the other surface is located at $z = d$, far away, hence the cell thickness can be thought as infinity, also known as half space approximation [22]. Within this approach, the only meaningful angle is the polar angle $\phi(z, t)$ between the director $\vec{n}$ and the x-axis ($x \perp z$), representing the distortion. By using the one constant approximation, the combination of equations 1 and 2, neglecting flow is

$$I \frac{\partial^2}{\partial t^2}\phi(z, t) + \gamma_b \frac{\partial}{\partial t}\phi(z, t) = k \frac{\partial^2}{\partial z^2}\phi(z, t), \tag{3}$$

where k is the elastic constant, γ_b is the (effective) bulk viscosity, and I is the molecular moment of inertia per unit volume. The boundary conditions to be satisfied by ϕ, which incorporate a finite anchoring energy and the surface viscosity γ_s [23], are given by

$$-k \frac{\partial}{\partial z}\phi(z, t) + \omega\phi(z, t) + \gamma_s \frac{\partial}{\partial t}\phi(z, t)\bigg|_{z=0} = \omega\phi_s(t), \tag{4}$$

$$\frac{\partial}{\partial z}\phi(z, t)\bigg|_{z=d/2} = 0. \tag{5}$$

We have assumed the parabolic approximation form of the Rapini-Papoular expression as $f_s = \left(1/2\right) \omega \left[\phi - \phi_s(t)\right]^2$ where the arbitrary time dependent function $\phi_s(t)$ represents the surface easy axis and the symmetry of the problem implies that $\phi(z, t) = \phi(d - z, t)$. In equation (4), the first term represents the elastic torque transmitted by the liquid crystal to the limiting surface. It is balanced by the restoring torque due to the anisotropic interaction (surface energy) of the nematic with the surface (second term) and by the viscous torque due to the surface dissipation (third term).

For $t \leq 0$, for simplicity, the director angle profile is initially given by $\phi(z, t) = \Phi(z)$ with $\partial_t\phi = 0$, where $\Phi(z)$ is an arbitrary function that represents the initial tilt angle profile. From equations (3), (4) and the initial conditions imposed to the tilt angle, it follows that

$$\left(\frac{\partial\phi}{\partial t}\right)_{surface,t=0} = \left(\frac{\partial\phi}{\partial t}\right)_{bulk,t=0}, \tag{6}$$

i.e, the time derivative at the surface evaluated by means of the bulk equation, equation (3), and the same quantity, evaluated by means of the boundary condition, equation (4), coincide at $t = 0$, thus avoiding the incompatibility problem pointed out in [24] (a detailed discussion can be found in Refs. [11,19,20,24–27]). Therefore, an arbitrary profile can be consistently considered as an initial condition to represent the initial state of the system, in contrast to the situations where the molecular moment of inertia is absent.

In order to investigate the dynamic reorientation profile of the system governed by equation (3), and subjected to the boundary conditions given by equations (4) and (5), the Green function approach and integral transforms were used. In this sense, we start by applying the *Laplace* transformation on equations (3), (4), and (5) which leads us to the following equation

$$k\frac{\partial^2}{\partial z^2}\phi(z,s) - (Is+\gamma_b)s\phi(z,s) = -(Is+\gamma_b)\phi(z,0), \tag{7}$$

with

$$-k\frac{\partial}{\partial z}\phi(z,s) + (\omega + s\gamma_s)\phi(z,s)\bigg|_{z=0} = \omega\phi_s(s) + \gamma_s\phi(z,0)|_{\mathrm{z=0}} \tag{8}$$

$$\frac{\partial}{\partial z}\phi(z,s)\bigg|_{z=d/2} = 0. \tag{9}$$

The solution of equation (7) subjected to equations (8) and (9) in terms of the *Green* function approach is given by

$$\phi(z',s) = -(Is+\gamma_b)\int_0^{d/2} dz\Phi(z)G(z,z';s) - k\phi(z,s)G(z,z';s)|_{z=0}. \tag{10}$$

The first term in the integrand describes the NLC's relaxation from the initial deformation. The second term of the solution represents the surface effect on the relaxation of the director's angle. In this sense, it is also interesting to observe that the stationary state of the NLC obtained in the limit of long times essentially depends on the surface effects. The Green function is obtained by solving the following equation

$$k\frac{\partial^2}{\partial z^2}G(z,z';s) - (Is+\gamma_b)sG(z,z';s) = \delta(z-z'), \tag{11}$$

subjected to the boundary conditions

$$\begin{aligned}-k\frac{\partial}{\partial z}G(z,z';s) + (\omega+s\gamma_s)G(z,z';s)\bigg|_{z=0} &= 0\\ \frac{\partial}{\partial z}G(z,z';s)\bigg|_{z=d/2} &= 0.\end{aligned} \tag{12}$$

After performing some calculations, it is possible to show that the Green function is given by

$$G(\mathrm{z},\mathrm{z}';\mathrm{s}) = -\frac{1}{\alpha F(\alpha)}(\alpha(\cosh(\alpha z)) + (w/k + \gamma_s s/k)\sinh(\alpha z))\cosh(\alpha(d/2-z')), \tag{13}$$

for $0 \le z \le z'$ and

$$G(\mathrm{z},\mathrm{z}';\mathrm{s}) = -\frac{1}{\alpha F(\alpha)}(\alpha(\cosh(\alpha z')) + (w/k + \gamma_s s/k)\sinh(\alpha z'))\cosh(\alpha(d/2-z)), \tag{14}$$

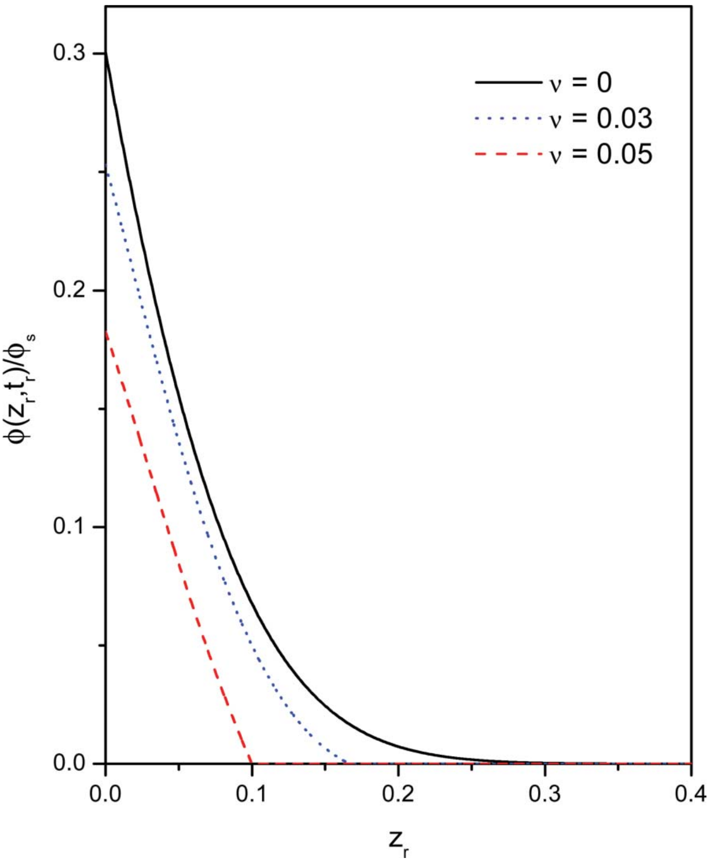

Figure 1. This figure illustrates $\phi(z_r, t_r)/\phi_s$ versus z_r for different values of ν with $t_r = 5 \times 10^{-3}$. The deformation progressively propagates into the sample and the stationary state is reached in the asymptotic limit of long times (see Fig. (3)). For simplicity, we also consider the initial condition $\Phi(z_r) = 0$, $u = 5$, and $v = 0$.

for $z' \leq z \leq d/2$, where $\alpha = \sqrt{s(Is + \gamma_b)/k}$ and $F(\alpha) = \alpha \sinh(\alpha d/2) + (w/k + s\gamma_s/k)\cosh(\alpha d/2)$.

Following, we consider, without loss of generality, the previous results in the half space approximation, which corresponds to take the limit of large thickness, i.e., $z << d$, to analyze how the molecular inertial moment influences the reorientation process. Incorporating this approximation in the previous equations, we obtain

$$G(z, z'; s) = -\frac{1}{2\sqrt{s(Is + \gamma_b)/k}} \left(e^{-\sqrt{s(Is+\gamma_b)/k}|z-z'|} + e^{-\sqrt{s(Is+\gamma_b)/k}|z+z'|} \right) - \frac{1}{\sqrt{s(Is + \gamma_b)/k} + w/k + \gamma_s s/k} e^{-\sqrt{s(Is+\gamma_b)/k}|z+z'|} \tag{15}$$

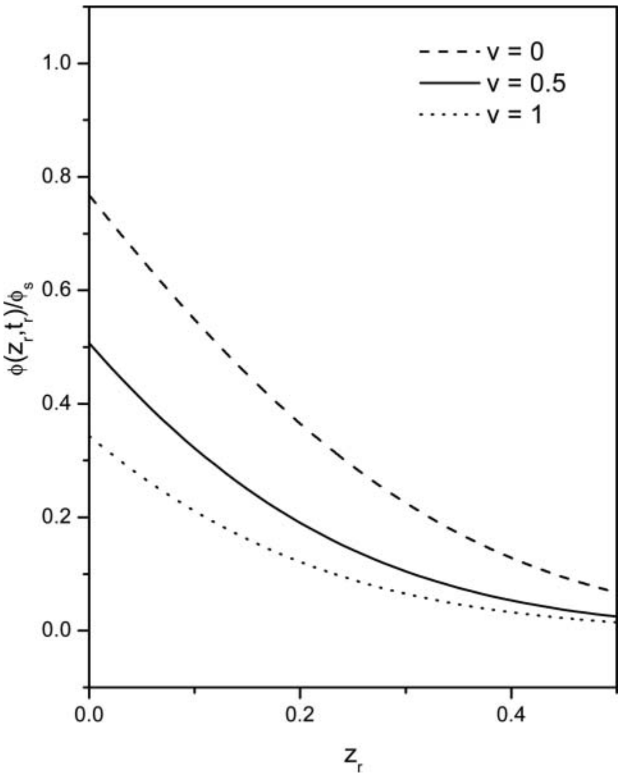

Figure 2. This figure illustrates $\phi(z_r, t_r)\big/\phi_s$ versus z_r for different values of v. The relaxation of the tilt angle becomes slower as the surface viscosity is increased. We consider, for simplicity, the initial condition $\Phi(z_r) = 0$, $u = 10$, $\nu = 10^{-3}$, and $t_r = 10^{-3}$.

By performing the inverse *Laplace* transform in equation (15) and, for simplicity, introducing the reduced variables $t_r = t/\tau$, $\tau = \gamma_b d^2\big/k$, $z_r = z/d$, $u = \omega d/k$, $\nu^2 = Ik/(\gamma_b d)^2$, and $v = \gamma_s/\,(\gamma_b d)$, we obtained

$$G(z_r, z_r'; t) = G_1(z_r, z_r'; t) + \Im_1(z_r, z_r'; t) + \Im_2(z_r, z_r'; t), \tag{16}$$

with

$$\begin{aligned} G_1(z_r, z_r'; t) = -\frac{1}{2\nu}e^{-t_r/2\nu^2}\Bigg\{&\theta(t_r - \nu|z_r - z_r'|)\mathrm{I}_0\left(\frac{1}{2\nu^2}t_r - \nu^2(z_r - z_r')^2\right) \\ &-\theta(t_r - \nu|z_r + z_r'|)\mathrm{I}_0\left(\frac{1}{2\nu^2}t_r - \nu^2(z_r + z_r')^2\right)\Bigg\}, \end{aligned} \tag{17}$$

$$\begin{aligned} &\Im_1(z_r, z'_r; t) \\ &= -\theta(t_r - \nu|z_r + z'_r|)\int_0^1 d\eta\eta e^{-t_r/2\nu^2}\frac{\eta\sqrt{1-\eta^2}\cos(|z_r + z_r'|\eta\big/\nu\sqrt{1-\eta^2})}{\pi\nu[(\omega - \eta^2 v\big/\nu^2)^2 + (1-\eta^2)\eta^2\big/\nu^2]}, \end{aligned} \tag{18}$$

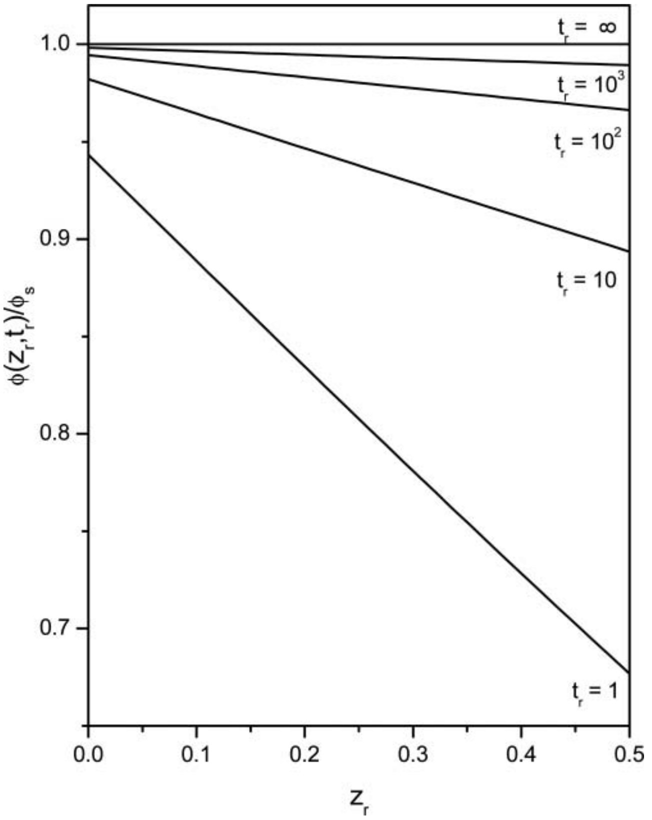

Figure 3. This figure illustrates $\phi(z_r, t_r)/\phi_s$ versus z_r for different t_r. It shows that the stationary state is reached in the asymptotic limit of long times. We consider, for simplicity, the initial condition $\Phi(z_r) = 0$, $u = 10$, $\nu = 10^{-3}$, and $v = 0.1$.

and

$$\Im_2(z_r, z_r'; t)$$

$$= -\theta(t_r - \nu|z_r + z_r'|)\int_0^1 d\eta\eta e^{-t_r/2\nu^2}\frac{(\omega - \eta^2 v/\nu^2)\sin(|z_r + z_r'|\eta/\nu\sqrt{1-\eta^2})}{\pi[(\omega - \eta^2 v/\nu^2)^2 + (1-\eta^2)\eta^2/\nu^2]}, \quad (19)$$

where $\mathrm{I}_0(x)$ is a modified Bessel function [21] and $\theta(x)$ is the step function [21].

Note that the inertial effects are expected to play an important role at initial times since that for long times the results are essentially governed by a diffusive-like process. In fact, the presence of the inertial term in the relaxation process introduces a finite phase velocity which is not present in the usual relaxation processes governed only by the dissipative term, i.e., γ_b, indicating that the deformations produced by the surface and bulk effects progressively propagate into the sample rather than instantaneously. In this sense, the presence of the step functions shows that the reorientation process starts with terms for which $t_r > \nu|z_r - z_r'|$ and, after, incorporate the terms containing $t_r > \nu|z_r + z_r'|$, indicating that the process is not instantaneous. This point is illustrated in Fig. (1) for two different values of the molecular inertial momentum, $I = 9 \times 10^{-7} kg/m$ (blue dotted line) and $I = 25 \times 10^{-7} kg/m$ (red

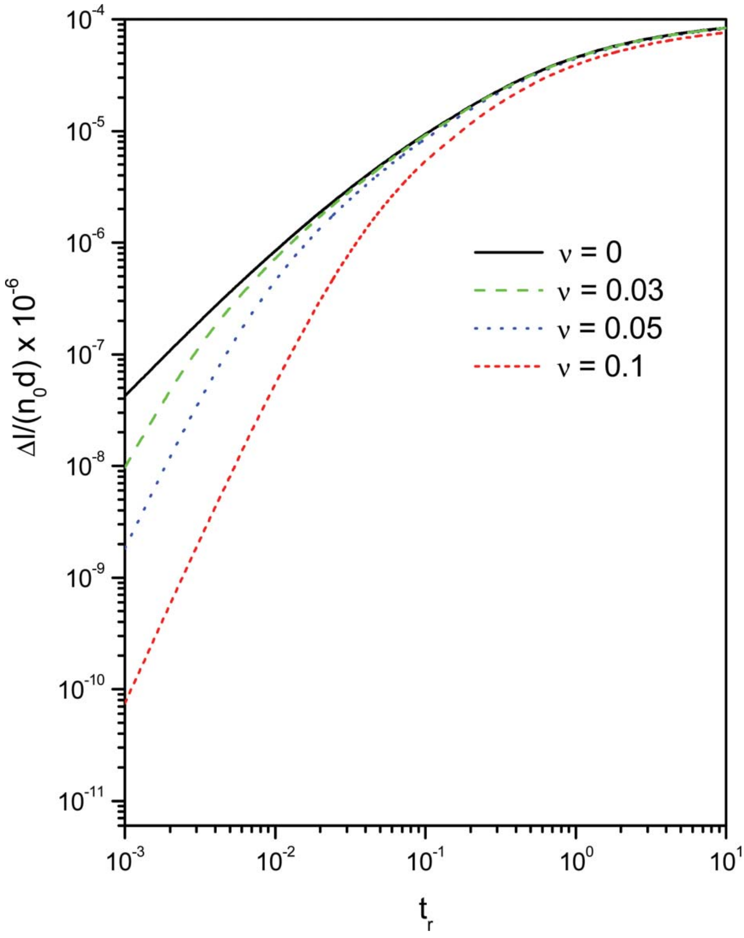

Figure 4. This figure illustrates Δl versus t_r for different values of ν in order to show effect of molecular moment of inertia on the optical path difference. The effect becomes greater as the molecular inertial momentum increases and for long times the relaxation is essentially governed by the dissipative term. We consider, for simplicity, the initial condition $\Phi(z_r) = 0, n_0 = 1.53, n_e = 1.73,$ $\phi_s = 10^{-2}$, $v = 0$, and $u = 5$.

dashed line) in absence of surface viscosity. Note that the case characterized by the absence of the inertial momentum (black solid line) and surface viscosity has an infinity phase velocity and, consequently, distortion propagation in the liquid crystal cell is instantaneous. The influence of the surface viscosity is illustrated in Fig. (2) for a particular value of time and inertial moment. In particular, it shows that the relaxation process becomes slower when the surface viscosity is increased. In Fig. (3), we illustrate the time evolution of the tilt angle with the surfaces characterized by a constant easy axis ϕ_s in the presence of the inertial momentum and surface viscosity, in order to show that the stationary state is reached for long times. From the above results, it is possible to investigate the optical path difference Δl, between the ordinary and the extraordinary rays of a linear polarized beam impinging normally the sample, which is given by [3]

$$\Delta l = \int_0^d \Delta n(\phi) dz$$

$$\Delta n(\phi) = n_{eff}(\phi) - n_0 = n_0 \left\{ \frac{1}{\sqrt{1 - r\sin^2(\phi)}} - 1 \right\}, \tag{20}$$

with $r = 1 - \left(n_0/n_e\right)^2$, where n_0 and n_e are the ordinary and extraordinary refractive indices, respectively. This is shown in Fig. (4). The results essentially show that the moment of inertia is of significant importance for short times whereas for long times the behavior is governed by the dissipative term.

III. Discussion and Conclusion

We have investigated the relaxation process in a nematic liquid crystal cell by considering the molecular moment of inertia and the surface viscosity. The problem solved here corresponds to a more complete description of the relaxation process of the nematic director, since it includes two legitimate terms that are usually neglected due to the mathematical difficulty of the problem. It also corresponds to a more physical process because the Cattaneo-like equation solved here accounts for the finite time of the distortion propagation in a liquid crystal cell. The results show that the relaxation process of the tilt angle in the sample is progressively propagated in the sample with characteristics time which starts after $t_r > \nu|z_r - z_r'|$ as indicated by the step functions present in the Green function. Hence, the deformation of the tilt angle has finite velocity propagation in the sample which is directly connected to the presence of the inertial moment of the molecules. We have also considered the effect of the surface viscosity which has an influence on the relaxation process. In particular, we have observed that the larger the surface viscosity, the slower is the relaxation process, as shown in Fig. (2). In Fig. (3), we illustrated the time evolution of the solution for an initial condition in order to show that the stationary state is reached for long times. The optical path difference is shown in Fig. (4) by taking into account the molecular inertial moment. The inertial effects are observed for short times whereas for long times the system is essentially governed by the dissipative term.

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