A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

December 2009

EPL, **88** (2009) 58003
doi: 10.1209/0295-5075/88/58003

www.epljournal.org

Influence of the anchoring energy on the relaxation of the nematic deformation

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received 16 October 2009; accepted in final form 16 November 2009
published online 15 December 2009

PACS 83.80.Xz – Liquid crystals: nematic, cholesteric, smectic, discotic, etc.
PACS 61.30.Hn – Surface phenomena: alignment, anchoring, anchoring transitions, surface-induced layering, surface-induced ordering, wetting, prewetting transitions, and wetting transitions.

Abstract – We analyze the influence of the anchoring energy strength on the relaxation of the nematic deformation, when the distorting field is removed, at $t=0$. The analysis is performed by assuming that the nematic sample is in the shape of a slab, the anchoring energy can be approximated by the form proposed by Rapini and Papoular, and the surface dissipation, responsible for the surface viscosity, is negligible with respect to the bulk one. The switching time of the distorting field is supposed finite, to avoid the non-physical discontinuity of the time derivative of the tilt angle at $t=0$. We show that the relaxation time of the nematic deformation is a multi-relaxation phenomenon. For large t, the relaxation phenomenon is simple, and the relaxation time is proportional to the diffusion time $\tau_D=\eta d^2/k$, where d is the thickness of the sample, η the viscosity and k the elastic constant of the nematic liquid crystal. For $t\ll\tau_D$, the time dependence of the tilt angle is well approximated by few exponential terms. The relation between the effective relaxation time and the anchoring energy strength is deduced. A critical discussion on the standard analysis based on the diffusion equation is also reported.

Nematic-liquid-crystal displays are based on the change of the optical properties of a nematic liquid crystal induced by an external electric field. The optical properties of a nematic-liquid-crystal sample depend on the average orientation molecular orientation described by a vectorial field $\mathbf{n}=\mathbf{n}(\mathbf{r})$, known as nematic director. In the presence of the electric field the nematic liquid crystal is aligned in such a manner that the total energy of the sample is minimized [1]. The total energy of the sample is due to the elastic energy of the liquid crystal, associated to the nematic deformation, to the electric energy related to the interaction between the nematic liquid crystal and the electric field, and to the surface energy due to the interaction of the liquid crystal with the limiting surfaces. The actual nematic orientation is such that the bulk density of torque is zero, and the elastic torque transmitted by the liquid crystal to the limiting surfaces is balanced by the surface torques related to the anisotropic surface tension [2]. If the external field inducing the deformation changes with time, the nematic director also is time dependent. Our aim is to investigate the time dependence of $\mathbf{n}$ when the field inducing the deformation is switched off, at $t=0$. We will show that the usual description of this phenomenon, based on a dynamical equation similar to the diffusion equation, does not allow a full description of the relaxation phenomenon, because the time derivative of the nematic deformation is discontinuous at $t=0$. This discontinuity can be responsible for fundamental problems related to the inertial properties of the liquid crystal [3–6]. These type of problems are absent if the switching time of the distorting field is assumed finite, as we will suppose in our analysis.

In order to simplify as much as possible the mathematical problem we assume that the nematic cell is in the shape of a slab of thickness d. The z-axis used for the description is perpendicular to the limiting surfaces, at $z=\pm d/2$, indicated by the subscript 1 and 2, respectively. The surface treatment on the limiting surfaces is the same. The easy axes of the two surfaces [7], are identical $\mathbf{n}_{e1}=\mathbf{n}_{e2}=\mathbf{n}_e$, and form an angle ϕ_s with the z-axis. The

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x-axis is in the plane individuated by the z-axis and the easy axes. The external field is $\mathbf{E} = E\,\mathbf{z}$, and the dielectric anisotropy of the nematic liquid crystal is assumed positive ($\varepsilon_a = \varepsilon_\parallel - \varepsilon_\perp > 0$, where $\parallel$ and $\perp$ refer to $\mathbf{n}$). The angle formed by $\mathbf{n}$ with the z-axis is indicated by ϕ, and called tilt angle. In this framework, in the absence of the external field, $\mathbf{n}$ is parallel to the surface easy axes, contained in the (x,z)-plane, and $\phi = \phi_s$. When the external field is present, the electric torque tends to orient $\mathbf{n}$ parallel the z-axis, and $\phi \leqslant \phi_s$. The surface anchoring energy, describing the interaction between the nematic liquid crystal and the limiting surface is assumed of the form proposed by Rapini and Papoular $f_{s1} = f_{s2} = -(w/2)(\mathbf{n}_s \cdot \mathbf{n}_e)^2$, where $\mathbf{n}_s$ is the nematic director at the surface (for symmetry reasons $\mathbf{n}_{s1} = \mathbf{n}_{s2} = \mathbf{n}_s$), and w the anchoring energy strength [7].

Let us consider first the nematic sample submitted to a constant electric field $\mathbf{E_0} = E_0\mathbf{z}$. The actual nematic orientation, $\Phi = \Phi(z)$, is an even function of z, for the symmetry of the problem, solution of the bulk differential equation [8]

$$k\frac{\mathrm{d}^2}{\mathrm{d}z^2}\Phi(z) - \frac{1}{2}\varepsilon_a E_0^2 \sin[2\Phi(z)] = 0, \qquad (1)$$

where k is the elastic constant of Frank, Φ is the angle formed by the nematic director with the z-axis, and ε_a the dielectric anisotropy of the liquid crystal. Equation (1) is valid in the one-constant approximation [1]. The actual $\Phi = \Phi(z)$ satisfies the boundary conditions

$$\pm k\frac{\mathrm{d}}{\mathrm{d}z}\Phi(z) + \frac{1}{2}w\sin[2(\Phi(z) - \phi_s)]\Big|_{z=\pm d/2} = 0, \qquad (2)$$

related to the weak-anchoring hypothesis, where w is the surface anchoring strength [8]. In our analysis we assume that ϕ_s is small, in such a manner that $\sin(2\phi_s) \sim 2\phi_s$. Since $\Phi(z) < \phi_s$, eqs. (1), (2) can be linearized, and the fundamental equations of the problem read

$$k\frac{\mathrm{d}^2}{\mathrm{d}z^2}\Phi(z) - \varepsilon_a E_0^2\,\Phi(z) = 0 \qquad (3)$$

and

$$\pm k\frac{\mathrm{d}}{\mathrm{d}z}\Phi(z) + w\Phi(z)\Big|_{z=\pm d/2} = w\phi_s. \qquad (4)$$

The solution of eq. (3) with the boundary conditions (4) is

$$\Phi(z) = 2\phi_s u \times \frac{(d/\lambda)\cosh(d/2\lambda) + u\sinh(d/2\lambda)}{[(d/\lambda)^2 + u^2]\sinh(d/\lambda) + 2(u/\lambda)\cosh(d/\lambda)}\cosh(z/\lambda), \qquad (5)$$

where $\lambda = (1/E_0)\sqrt{k/\varepsilon_a}$ is the electric coherence length [1] and $u = wd/k$, where w/k is the inverse of the extrapolation length. As discussed in [1], the coherence length λ indicates the thickness of the surface layer where the surface torque dominates on the electric torque. In the limit $u \to \infty$, that corresponds to the strong-anchoring case, from eq. (5) we get

$$\Phi(z) = \phi_s\frac{\cosh(z/\lambda)}{\cosh(d/2\lambda)}, \qquad (6)$$

as expected. The tilt angle $\Phi(z)$ given by eq. (5) will be the initial condition for the tilt angle $\phi(z,t)$ when the external field is removed at $t = 0$, *i.e.* $\phi(z,0) = \Phi(z)$.

In the standard analysis, the relaxation of the initial deformation is described by the partial differential equation

$$k\,\frac{\partial^2}{\partial z^2}\phi_D(z,t) = \eta\,\frac{\partial}{\partial t}\phi_D(z,t), \qquad (7)$$

stating that during the relaxation, the elastic torque is balanced by the viscous torque. In eq. (7) η is the rotational viscosity of the nematic liquid crystal [1]. Equation (7) holds true when the inertial properties of the nematic molecules are negligible [9], and the electric field is removed with switching time zero. Since the anchoring is weak, we have the boundary condition

$$\pm k\frac{\partial}{\partial z}\phi_D(z,t) + w\phi_D(z,t)\Big|_{z=\pm d/2} = 0. \qquad (8)$$

We look for a solution of eqs. (7), (8) of the type $\phi_D(z,t) = \phi_s + \delta\psi(z,t)$, where $\delta\psi(z,0) = \Phi(z) - \phi_s$, and $\lim_{t\to\infty}\delta\psi(z,t) = 0$. By taking into account eq. (8), the solution of eq. (7), such that $\delta\psi(z,0) = \Phi(z) - \phi_s$, and $\lim_{t\to\infty}\delta\psi(z,t) = 0$ is

$$\delta\psi(z,t) = \sum_{n=0}^{\infty}\mathcal{A}_n\,\varphi_n(z)\,e^{-\frac{k}{\eta}a_n^2 t}, \qquad (9)$$

where $\varphi_n(z) = \cos(a_n z)$, and the eigenvalues a_n are obtained by

$$(w/k)\cos(a_n d/2) - a_n\sin(a_n d/2) = 0. \qquad (10)$$

For $w \to \infty$, $a_n \to (2n+1)(\pi/d)$, whereas for $w \to 0$, $a_n = \sqrt{2w/(kd)}$. We observe that the eigenvalues equation, eq. (10), does not depend on the coherence length λ. Consequently, the relaxation times of the dynamical evolution of the tilt angle profile does not depends on the initial deformation related to E_0. The coefficients $\mathcal{A}_n$ are given by

$$\mathcal{A}_n = \frac{1}{\mathcal{N}_n}\int_{-d/2}^{d/2}\varphi_n(z)\,[\Phi(z) - \phi_s]\,\mathrm{d}z, \qquad (11)$$

where

$$\mathcal{N}_n = \int_{-d/2}^{d/2}\varphi_n^2(z)\,\mathrm{d}z = \frac{d}{2}\left(1 + \frac{\sin(a_n d)}{a_n d}\right). \qquad (12)$$

Note that the solution for this case was obtained by using the eigenfunction and eigenvalues of the Sturm-Liouville problem related to the spatial operator of eq. (7), *i.e.*, $\partial_z^2\varphi_n = -a_n^2\varphi_n$ with φ_n accomplishing the boundary

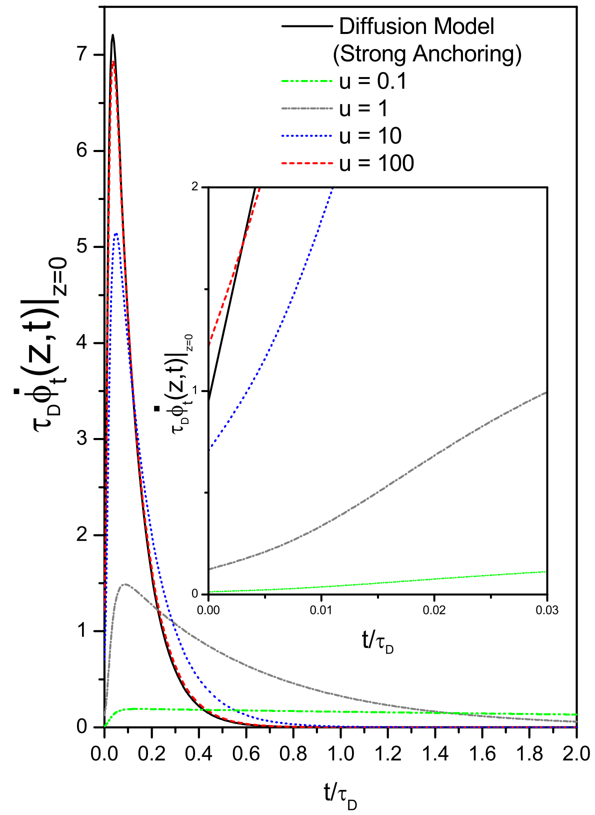

Fig. 1: (Color online) $\tau_D\dot{\phi}_t$ *vs.* t/τ_D (where $\dot{\phi}_t \equiv \partial\phi/\partial t$) evaluated for $z=0$ for the diffusion model for a few values of the dimensionless anchoring energy $u=dw/k$. The black line corresponds to the diffusion model with strong anchoring.

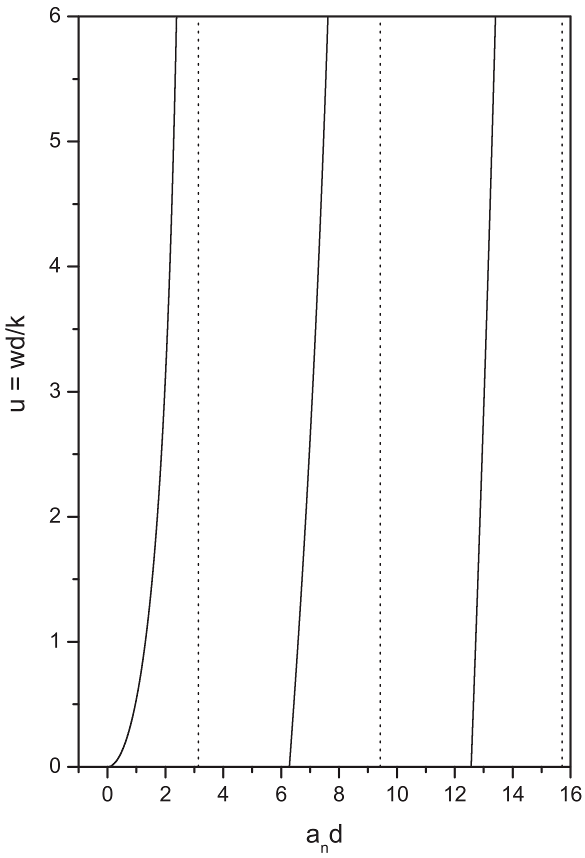

Fig. 2: $u=wd/k$ *vs.* $a_n d$ to show the influence of the surface anchoring strength on a_n. The vertical dotted lines, that are the asymptote of the continuous curves, define the eigenvalues in the strong-anchoring case, where $a_n=(2n+1)(\pi/d)$.

conditions given by eq. (8)[1]. We note that the value of w, *i.e.*, surface anchoring strength, defines the eigenvalues and consequently has influence on the relaxation process of the system.

Figure 1 illustrates the effect of the surface energy on $\tau_D\dot{\phi}_t$ (where $\dot{\phi}_t \equiv \partial\phi/\partial t$), at $z=0$, *vs.* t derived with the model based on the diffusion equation. This figure shows that according to the surface energy we may have a fast or slow relaxation for the tilt angle. In this direction, it is interesting to note that the eigenvalues and eigenfunctions by means of which we can build the solution of our problem depend on w (see fig. 2). Consequently, the relaxation process depends on the anchoring energy strength [10]. The case corresponding to the strong-anchoring hypothesis is also shown in fig. 1. The inset of fig. 1 shows that at $t=0$ the model based only on diffusion equation, *i.e.*, removing the electric field in a discontinuous manner at $t=0$, predicts

$$\left(\frac{\partial\phi}{\partial t}\right)_{t=0^-}=0, \quad \text{and} \quad \left(\frac{\partial\phi}{\partial t}\right)_{t=0^+}=\frac{\eta}{k}\frac{\mathrm{d}^2\Phi}{\mathrm{d}z^2}\neq 0. \qquad (13)$$

[1]A simple calculation allows to verify that the set of eigenfunctions $\varphi_n(z)=\cos(a_n z)$ are orthogonal in $-d/2\leqslant z\leqslant d/2$ when a_n are given by eq. (10).

This means that the first-order time derivative of the tilt angle is discontinuous at $t=0$, and hence

$$\left(\frac{\partial^2\phi}{\partial t^2}\right)_0 \to \infty. \qquad (14)$$

Figure 3 shows the behavior of the tilt angle profile *vs.* t at $z=0$. Note that the relaxation process, *i.e.*, the time-dependent behavior of $\phi(z,t)$, is dominated by the first terms of the series expansion of $\phi(z,t)$. In the analysis presented above we have considered the boundary condition for the dynamical problem under consideration in the form of eq. (8). This implies that we have not considered a specific dissipation at the surface related to the surface viscosity, as discussed by Derzhanskii and Petrov [11]. According to this point of view, eq. (8) should be written as

$$\pm k\frac{\partial}{\partial z}\phi_D(z,t)+w\phi_D(z,t)+\eta_s\frac{\partial}{\partial t}\phi_D(z,t)\Big|_{z=\pm d/2}=0, \qquad (15)$$

where η_s is the surface viscosity. A simple analysis shows that the problem of the initial discontinuity of the first-order time derivative of the tilt angle is not solved when the surface viscosity is taken into account. In fact, even in

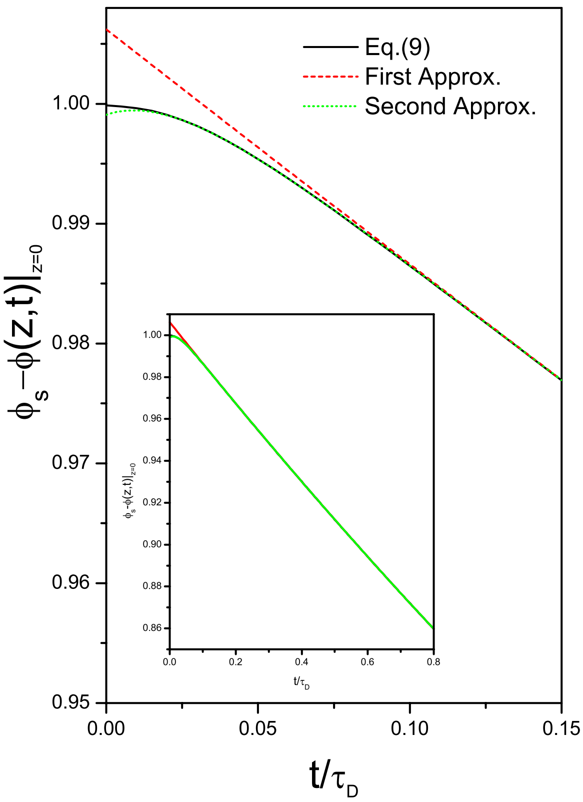

Fig. 3: (Color online) $\phi_s-\phi(z,t)$ *vs.* t/τ_D evaluated for $z=0$ for the diffusion model. For large t the relaxation phenomenon is characterized by a single relaxation time. For small t, with respect to τ_D, a few terms of the series giving $\phi(z,t)$ are enough to approximated the complete solution.

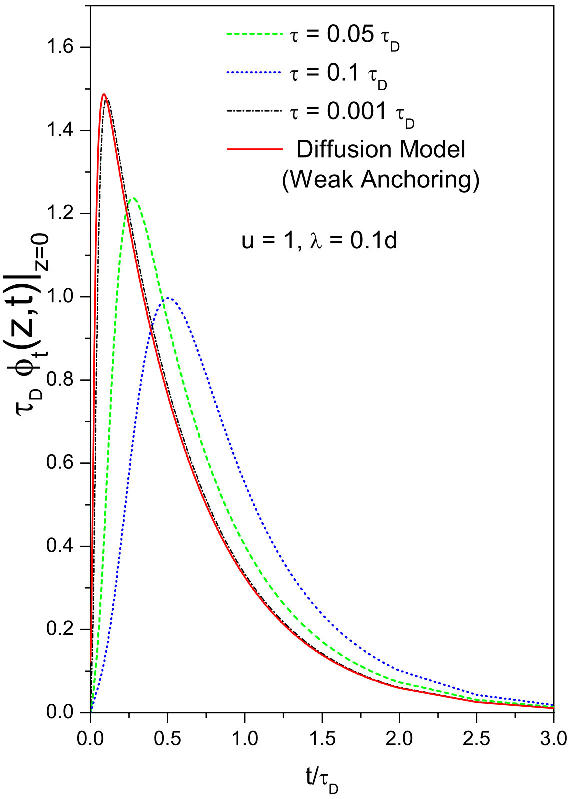

Fig. 4: (Color online) $\tau_D\dot{\phi}_t$ *vs.* t/τ_D evaluated for $z=0$ for different relaxation times (τ) by assuming $u=1$ and $\lambda=0.1d$.

the case in which eq. (15) hold, eqs. (13) are still valid, and hence the second time derivative of $\phi(z,t)$ is still discontinuous. In the framework of this model there is another difficulty related to eq. (7) and eq. (15) connected to the compatibility of the initial deformation $\Phi(z)$, as discussed in [3–6]. To avoid this type of problem, we limit our analysis to the case where $\eta_s=0$.

In the previous analysis, the distorting field was assumed to be removed in a discontinuous manner. This means that the switching time was supposed zero. Of course, in real systems, the switching time is finite. We analyze now the influence of a finite switching time on the relaxation of the initial deformation of the nematic liquid crystal. We will base our investigation on the equation

$$k\frac{\partial^2}{\partial z^2}\phi_E(z,t)-\varepsilon_a E^2(t)\phi_E(z,t)=\eta\frac{\partial}{\partial t}\phi_E(z,t), \tag{16}$$

where $E^2(t)=E_0^2\,f(t)$, with $f(t)=1$ for $t\leqslant 0$, and $f(t)\to 0$ for $t\to\infty$. In the following we will consider the simple case $f(t)=\exp(-t/\tau)$, where τ is the switching time. Equation (16) is the dynamical equilibrium of the torques, when the inertial properties of the liquid crystal can be neglected [9], and in the following will be rewritten as

$$\frac{\partial^2}{\partial z^2}\phi_E(z,t)-\frac{1}{\lambda^2}\,f(t)\phi_E(z,t)=\frac{\eta}{k}\frac{\partial}{\partial t}\phi_E(z,t). \tag{17}$$

Equation (17) has to be solved by taking into account the boundary conditions

$$\pm k\frac{\partial}{\partial z}\phi_E(z,t)+w\phi_E(z,t)\bigg|_{z=\pm d/2}=w\phi_s \tag{18}$$

and $\phi_E(z,0)=\Phi(z)$, where $\Phi(z)$ is given by (5). In order to solve the above equation, we use the eigenfunctions related to the spatial operator of the diffusion equation, which is a Sturm-Liouville problem. In this way the solution for the problem under consideration is given by

$$\phi_E(z,t)=\phi_s+\sum_{n=0}^{\infty}\mathcal{K}_n(t)\,\varphi_n(z), \tag{19}$$

where $\mathcal{K}_n(0)=\mathcal{A}_n$ and $\varphi_n(z)$ are the eigenfunctions used in the previous analysis. By substituting (19) into eq. (17), after simple calculations, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}_n(t)+\mathcal{H}_n(t)\,\mathcal{K}_n(t)=-\mathcal{G}_n(t), \tag{20}$$

where

$$\begin{aligned}\mathcal{H}_n(t)&=\frac{k}{\eta}\left(a_n^2+\frac{1}{\lambda^2}\,f(t)\right),\\ \mathcal{G}_n(t)&=\frac{2k\phi_s f(t)}{\eta\lambda^2 a_n\mathcal{N}_n}\sin\left(\frac{d}{2}a_n\right),\end{aligned} \tag{21}$$

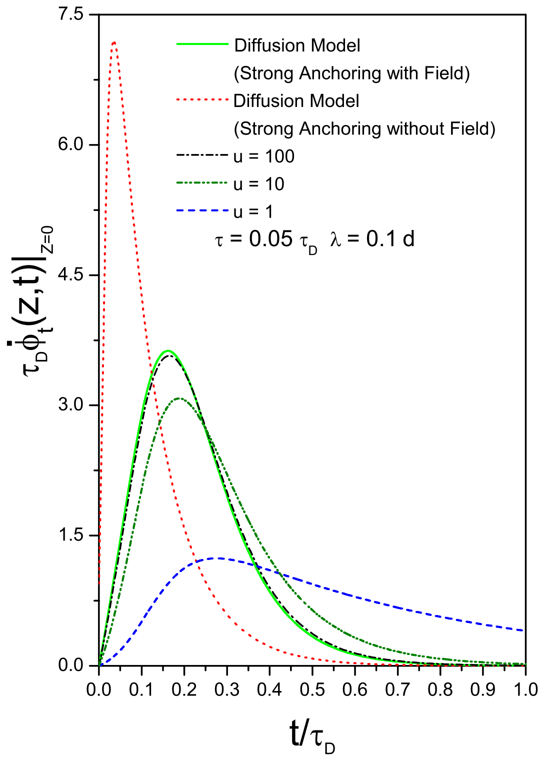

Fig. 5: (Color online) $\tau_D\dot{\phi}_t$ *vs.* t/τ_D for the case of a distorting field and for the diffusion model by considering different values of $u = wd/k$ for $\tau = 0.05\tau_D$ and $\lambda = 0.1d$. The red dotted line corresponds to the diffusion model for the strong-anchoring case in the absence of the field ($\tau = 0$). The green solid line is the case characterized by the strong-anchoring case in the presence of an electric field. The other lines represent the case of weak anchoring in the presence of an electric field.

with $\mathcal{N}_n$ defined by eq. (12). The solution we are looking for $\mathcal{K}_n(t)$ is

$$\mathcal{K}_n(t) = e^{-u_n(t)}\left\{\mathcal{A}_n - \int_0^t e^{u_n(t')}\,\mathcal{G}_n(t')\,\mathrm{d}t'\right\}, \qquad (22)$$

where

$$u_n(t) = \int_0^t \mathcal{H}_n(t')\,\mathrm{d}t'. \qquad (23)$$

In the simple case where $f(t) = \exp(-t/\tau)$ a simple calculation gives

$$u_n(t) = \frac{k}{\eta}\left\{\frac{\tau}{\lambda^2}\left(1 - e^{-t/\tau}\right) + a_n^2\,t\right\}. \qquad (24)$$

From eq. (24) it follows that for large t, $u_n(t) \to (k/\eta)a_n^2 t$, and hence $\phi_E(z,t) \to \phi_D(z,t)$.

In fig. 4, we show $\tau_D\dot{\phi}_t$ *vs.* t evaluated for $z = 0$ derived by means of the model where the switching time of the distorting field is taken into account by considering the situation where $E^2(t) = E_0^2\exp(-t/\tau)$. The numerical calculations have been performed by assuming $u = 1$ ($u = wd/k$), and $\lambda = 0.1d$. The condition $\partial\phi/\partial t = 0$ for $t = 0$ is automatically satisfied, in contrast to the diffusion model (see inset of fig. (1)). For $\tau \to 0$ the diffusion model with weak anchoring (black dash-dotted line) is recovered. In fig. 5 we show $\tau_D\dot{\phi}_t$ *vs.* t evaluated for $z = 0$, for three values of u, for the same switching time τ.

The analysis reported above shows that to avoid the discontinuity of the first-order time derivative of the tilt angle for $t = 0$ it is necessary to take into account that the switching time of the distorting field is different from zero. In this framework, the dynamical equation describing the relaxation of the nematic deformation, differs from the diffusion equations in a time interval comparable with the switching time for the presence of the torque due to the electric field. According to this description, the first-order time derivative of the tilt angle is continuous at $t = 0$. Our analysis shows also that the relaxation time strongly depends on the anchoring energy strength.

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