Dynamics of the director reorientation in confined nematic liquid crystals imposed by a strong orthogonal electric field

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Abstract. The dynamics of the periodic distortions in confined nematic liquid crystals (LCs) has been investigated theoretically basing on the hydrodynamic theory including the director motion with appropriate boundary and initial conditions. Analysis of the numerical results for the turn-on process provides an evidence for the appearance of the spatially periodic patterns in confined LC film, only in response to the suddenly applied strong electric field. It has been shown that there is a threshold value of the amplitude of the thermal fluctuations of the director over the LC sample which provides the nonuniform rotation mode rather than the uniform one, whereas the lower values of the amplitude dominate the uniform mode. During the turn-off process the reorientation of the director to the direction preferred by the surfaces is characterized by the complex destruction of the initially periodic structure to a monodomain state.

1. Introduction
In this paper we will particularly refer to the electrically driven director reorientation in a thin nematic liquid crystal (LC) film confined between two transparent electrodes and subjected to a strong orthogonal electric field. When the applied field $E$ is much larger than a critical field, then the LC system is suddenly placed far from the equilibrium. It responds by creating a distortion which maximizes the rate at which the LC lowers its total free energy. In this case, the final form of deformation depends on viscous, elastic and electric torques, as well as the boundary and initial conditions. In this work we are focusing on such geometry where the electric field is orthogonal (or approximately orthogonal) to the horizontal boundaries. In this configuration the state of the system immediately becomes unstable after applying the orthogonal electric field. When the misalignment of the director with respect to the direction preferred by the surfaces is due to the thermal fluctuations with small amplitudes, the reorientation following the sudden application of a sufficiently strong and orthogonal electric field manifests itself by the growing of one particular Fourier mode. After switching-off the field the long-range elastic interactions ensure that the molecules reorient themselves in the direction preferred by surfaces.

In this work, switching will be driven by a series of a voltage pulses: $V>0$, for $0 < t < t_0$; $V=0$, for $t_0 \leq t \leq t_1$; and $V<0$, for $t_1 < t < t_2$. So, the aim of this paper is to shows how in the
LC system of this geometry switching can be driven by the electric field and to demonstrate the kinetic pathway along which the switching proceeds.

2. Formulation of the relevant equations for dynamical reorientation of the director field

We consider a nematic system such as cyanobiphenyls which is delimited by two horizontal and two lateral surfaces at mutual distances 2d and 2L on a scale in the order of tens micrometers. According to this geometry, the LC system may be seen as two-dimensional, since the director field \( \hat{n} \) is directed parallel to the horizontal surfaces, \( \hat{k} \) is a unit normal vector which coincides with the direction of the electric field \( \mathbf{E} \), and \( \mathbf{j} = \hat{k} \times \hat{\mathbf{i}} \). We can suppose that the components of the director, \( \hat{n} = n_x \hat{i} + n_z \hat{k} = \cos \theta(x, z, t) \hat{i} + \sin \theta(x, z, t) \hat{k} \) depend only on x- and z-components and on time t. Here \( \theta \) denotes the angle between the director and the unit vector \( \hat{i} \). In the case of the quasi-two-dimensional LC system the dimensionless torque balance equation describing the reorientation of \( \hat{n} \) to its equilibrium orientation \( \hat{n}_{eq} \) can be written as (for details, see the Refs.[1, 2, 3])

\[
\theta_{,\tau} = \delta_1 \left[ \Delta_1 (\theta) \theta_{,xx} + \Delta_2 (\theta) \theta_{,xx} + \Delta_3 (\theta) \left( -2\theta_{,xx} + \theta^2_{,x} - \theta^2_{,z} \right) + \Delta_4 (\theta) \theta_{,x}\theta_{,z} \right] +
\frac{1}{2} E^2 (z) \sin 2(\alpha - \theta) + \frac{1}{2} (\psi_{,xx} + \psi_{,xz}) - \psi_{,x}\theta_{,x} + \psi_{,x}\theta_{,z} +
\gamma \left[ \sin 2\theta\psi_{,xx} + \frac{1}{2} (\psi_{,xx} - \psi_{,xz}) \right],
\]

(1)

where \( \Delta_1 (\theta) = \sin^2 \theta + K_{31} \cos^2 \theta \), \( \Delta_2 (\theta) = \cos^2 \theta + K_{31} \sin^2 \theta \), \( \Delta_3 (\theta) = \frac{1 - K_{31}}{\epsilon_0 \alpha_{e_0 V^2}} \sin 2\theta \), and \( \Delta_4 (\theta) = (K_{31} - 1) \cos 2\theta \) are four functions of the angle \( \theta \), whereas \( \delta_1 = \frac{4K_{31}}{\epsilon_0 \alpha_0 V^2} \), \( \gamma = \frac{\pi}{\gamma_1} \), and \( K_{31} = \frac{K_3}{K_1} \) are three parameters of the system. Here \( \gamma_1 \) and \( \gamma_2 \) are two rotational viscosity coefficients (RVCs), and \( K_1 \) and \( K_3 \) are the splay and bend elastic constants of the nematic phase, \( d \) is the film thickness, \( \epsilon_0 \) is the absolute dielectric permittivity of free space, and \( \epsilon_a \) is the dielectric anisotropy of the nematic LC phase. The dimensionless Navier-Stokes equation for the velocity field \( \mathbf{v} = u (x, z, \tau) \hat{i} + w (x, z, \tau) \hat{k} \) takes the form (for details, see the Refs.[1, 2, 3])

\[
\delta_2 \left[ (\Delta \psi)_{,x} + \psi_{,x} (\Delta \psi)_{,x} - \psi_{,x} (\Delta \psi)_{,z} \right] = \hat{\mathbf{\nabla}} \psi + \mathcal{F},
\]

(2)

where the dimensionless components of the velocity field vector \( \mathbf{v} = u \hat{i} + w \hat{k} \) are expressed by the dimensionless stream function \( \psi (x, z, \tau) \) as \( u = \frac{\partial \psi}{\partial z} \) and \( w = -\frac{\partial \psi}{\partial x} \), respectively, \( \Delta \psi = \psi_{,xx} + \psi_{,zz} \), both the operator \( \hat{\mathbf{\nabla}} \psi \) and the function \( \mathcal{F} \) are listed in the Ref.[4]), whereas \( x = x/d \) and \( z = z/d \) are the dimensionless space variables, \( d \) is the film thickness, \( \tau = \frac{\epsilon_0 \alpha_{e_0 V^2}}{\gamma_1} \left( \frac{V}{d} \right)^2 t \) is the dimensionless time, \( \delta_2 = \frac{\epsilon_0 \alpha_{e_0 V^2}}{4\gamma_1} \) is an additional parameter of the system, whereas the electric field \( \mathbf{E} = E_x \hat{i} + E_z \hat{k} = E (z) \cos \alpha \hat{i} + E (z) \sin \alpha \hat{k} \) makes the angle \( \alpha \) with the horizontal surfaces, and its values are varied in the vicinity of \( \frac{\pi}{2} \). Notice that the overbars in the space variables \( x \) and \( z \) have been (and will be) eliminated in the last as well as in the following equations.

The application of the voltage across the nematic film results in a variation of \( E(z) \) through the film which is obtained from [1, 2, 3]

\[
\frac{\partial}{\partial z} \left[ \left( \frac{\epsilon_1}{\epsilon_0} \sin^2 \theta \right) E(z) \sin \alpha \right] = 0,
\]

\[
1 = \int_{-1}^{1} E(z) dz,
\]

(3)
where \( \mathcal{E}(z) = \frac{2dE(z)}{V} \), and \( V \) is the voltage applied across the cell, \( \epsilon_0 \) is the absolute dielectric permittivity of free space, and \( \epsilon_a \) is the dielectric anisotropy of the nematic LC phase. Consider now the nematic film between two electrodes when the director is weakly anchored at the horizontal surfaces and the anchoring energy takes the form \( W^{an} = \frac{1}{2} A \sin^2 (\theta_s - \theta_0) \), where \( \theta_s \) and \( \theta_0 \) are the angles corresponding to the director orientation on the solid surface, \( \mathbf{n}_s \), and easy axis, \( \mathbf{n}_0 \), respectively. In order to elucidate the role of the thermal fluctuations in maintaining of the spatially periodic patterns in the LC sample under the influence of the strong orthogonal electric field, we have performed a numerical study of Eqs.(1)-(3) with the mixed boundary condition for the angle \( \theta \), which reads in the dimensionless form as (hereafter referred to as case A)

\[
\theta(x) = \pm \delta_3 \theta(x = 10, -1 < z < 1) = 0,
\]

where \( \delta_3 = \frac{Ad_{el}}{K_1} \), and with the strong anchoring condition for the angle \( \theta \), which reads in the dimensionless form as (hereafter referred to as case B)

\[
\theta(x = 10, -1 < z < 1) = 0.
\]

Moreover, we will assume the no-slip boundary conditions for the nematogenic molecules on these boundary surfaces, i.e.,

\[
\begin{align*}
(\psi_x)_{-10 < x < 10, z = \pm 1} &= \psi_{x, \pm 1} = 0, \\
(\psi_x)_{-10 < x < 10, z = \pm 1} &= \psi_{x, \pm 1} = 0.
\end{align*}
\]

In order to observe the formation of the spatially periodic patterns developing spontaneously from homogeneous state and excited by the strong orthogonal electric field, we consider the initial condition in the form

\[
\theta(x, z, 0) = \theta_0 \cos(q_\alpha x) \cos(q_\beta z),
\]

which defines the thermal fluctuations of the director over the LC sample with the amplitude \( \theta_0 \) and wavelengths \( q_\alpha \) and \( q_\beta \) of an individual Fourier component of the modulation. In the case A, the wavelengths \( q_\alpha \) and \( q_\beta \) of an individual Fourier components are described as

\[
q_\alpha = \frac{\pi}{2k}(2k + 1),
\]

where \( k = 0, 1, 2, ... \) and \( q_\beta = \mp (\delta_3 \cot q_\beta)_{z = \pm 1} \), whereas in the case B, as

\[
q_\alpha = \frac{\pi}{2}(2k + 1),
\]

where \( \alpha = x, z \) and \( k = 0, 1, 2, ... \). In turn, the initial velocity field is \( \mathbf{v}(x, z, 0) = 0 \), so the initial condition for the dimensionless stream function has the form

\[
\psi(x, z, 0) = 0.
\]

In the following the reorientation of the director in the nematic film, under the influence of the strong electric field directed perpendicular to the horizontal bounding surfaces, will be obtained by solving the nonlinear differential equations (1) and (3), with appropriate bounding conditions for the angle \( \theta \) (Eq.(4) (case A) or (Eq.(5) (case B)), and for the dimensionless stream function \( \psi \) (Eq.(6), together with the initial conditions both for the angle \( \theta \) (Eq.(7)) and \( \psi \) (Eq.(8)), respectively. The optimal dimensionless wavelengths \( q_\alpha \) and \( q_\beta \) are determined by the minimum condition of the total energy \( W = W_{elast} + W_{el} \) (for details, see the Refs.[1, 2, 3]). Thus we have obtained a closed system of nonlinear differential equations (1)-(3) with appropriate boundary (4)-(6) and initial conditions (7) and (8) which can provides the nonuniform rotation mode rather than the uniform one.
2.1. Turn–on process in the positive sense (case A)

When a strong electric field $\mathbf{E}$ is applied in the positive sense at the angle $\alpha$ close to the right angle to the unit vector $\hat{\mathbf{i}}$, the director moves from being parallel to the direction preferred by the surfaces to being parallel to the electric field (the turn-on process), because dielectric anisotropy is positive for all cyanobiphenyls. For the case of 4-cyano-4′-pentylbiphenyl (5CB), at the temperature $300^\circ K$, corresponding to nematic phase and the density $10^3$ kg/m$^3$, the set of $\delta$-parameters, which is involved in Eqs.(1)-(4), takes the values $[2, 3] \delta_1 = 8.6 \times 10^{-6}$, $\delta_2 = 0.19$, and $\delta_3 = 19.5$. These nonlinear differential equations has been solved by the numerical relaxation method [4]. The relaxation criterion $\epsilon = |(\theta_{(n+1)}(\tau) - \theta_{(n)}(\tau))/\theta_{(n)}(\tau)|$ for calculating procedure was chosen equal to be $5 \times 10^{-4}$, and the numerical procedure was then carried out until a prescribed accuracy was achieved. The evolution both of the angle $\theta(x, z = 0, \tau)$ (Fig.1(a)) and the velocity components $w(x, z = 0, \tau)$ and $u(x, z = 0, \tau)$ (Fig.1(b)) of the vector $\mathbf{v} = u\hat{\mathbf{i}} + w\hat{\mathbf{k}}$ along the $x$-axis ($-10 \leq x \leq 10$), for a number of times $\tau = 2$ (12 ms), $4$ (24 ms), $6$ (36 ms), $8$ (48 ms), and $10$ (60 ms), are shown in Fig.1(a) and (b), respectively. The values of the dimensionless time $\tau = (\rho a c_0^2 V^2)/2a$ is accounted for after switching on the electric field. The time propagation of the angle $\theta(x, z = 0, \tau)$ along the $x$-axis ($-10 \leq x \leq 10$) with the value of the amplitude $\theta_0$ which is equal to 0.01 ($\sim 1.1^\circ$) is characterized by the well developed periodic structure with the lattice points at $x = \pm 2.175$ and $\pm 5.83$ (case A). According to our calculations, the evolution process of the dimensionless velocities $w(x, z = 0, \tau)$ (Fig.1(b), solid curves) and $u(x, z = 0, \tau)$ (Fig.1(b), dash dotted curves) is characterized by the increase of these components upon increasing of $\tau$ up to 8 (48 ms), before getting to the distributions of $w(x, z = 0, \tau = 8)$ and $u(x, z = 0, \tau = 8)$ along the $x$-axis ($-10 \leq x \leq 10$). That distribution of $w$ is characterized by the maximum $w(x, z = 0, \tau = 8) \sim 0.15$ ($\sim 5$ mm/s) in the vicinity of the lattice points at $x = \pm 2.175$ and $\pm 5.83$. In that case the distribution of the velocity field $\mathbf{v}$ in the LC sample under the influence of the strong electric field is characterized by maintaining the well developed vortices, in the framework of the cells delimited by the scaled distances $-10 < x < -5.83$, $-5.83 < x < -2.175$, $-2.175 < x < 2.175$, $2.175 < x < 5.83$, $5.83 < x < 10$.
Figure 2. The evolution of the angle $\theta(x, z = 0, \tau)$ during the turn-on process ($E > 0$ and $\alpha = 1.57$ ($\sim 89.96^\circ$)) along the length of the dimensionless LC film ($-10 \leq x \leq 10$), for a number of dimensionless times $\tau = 2$ ($\sim 12$ ms), 6 ($\sim 36$ ms), 8 ($\sim 48$ ms), 12 ($\sim 72$ ms), and 20 ($\sim 0.12$ s), respectively. Part (a) shows the case of strong anchoring (case B), while (b) shows the case of weak anchoring (case A). In all these cases the amplitude of the thermal fluctuation $\theta_0$ is equal to 0.01 ($\sim 1.1^\circ$). and $5.83 < x < 10$, as shown in Fig.1(a). For both cases A and B, and for the values of $\theta_0 = 0.01$ ($\sim 1.1^\circ$ and $\alpha = 1.57$), the time propagation of the angle $\theta(x, z = 0, \tau)$ profile along the x-axis ($-10 \leq x \leq 10$) is characterized by well-developed periodic structure with the lattice points at $x = \pm 2.175$ and $\pm 5.83$ (case A) (Fig.2(a)) and $x = \pm 2.19$, and $\pm 5.80$ (case B) (Fig.2(b)), respectively. Physically, this means that the character of the molecules anchoring to the bounding surfaces does not influence on the final maintaining of the spatially periodic patterns (see Fig.2). At the value of the angle $\alpha = 1.57$ the optimal dimensionless wavelengths $q_x$ and $q_z$ provide the minimal values of the total energy $W = W_{\text{elast}} + W_e$. In our case, the equilibrium $\theta_{\text{eq}}^{\text{ON}}(x, z)$ value of the angle $\theta(x, z, \tau = 12)$ corresponding to the turn-on process is achieved after the dimensionless time term $\tau = 12$. It is also shown that only for the values of $q_x = 0.785$, $q_z = 64.336$, $\alpha = 1.57$, and $\theta_0 = 0.01$ ($\sim 1.1^\circ$) and higher the periodic structure may appear spontaneously from homogeneous nematic phase under the above-mentioned conditions. These values of $q_x$ and $q_z$ provide the minimal values of the total energy $W$.

2.2. Turn–off process (case B)

After the electric field is removed, the director relaxes back to the direction preferred by the surfaces (the turn-off process). Now the reorientation of the director in the nematic film under the influence of the long-range elastic interactions can be obtained by solving the nonlinear differential equations (1) and (3), for the case of $E = 0$, and both with the mixed Eq.(4) (case A) or strong Eq.(5) (case B) boundary conditions for the angle $\theta$. The initial condition is taken in the form $\theta(x, z, 0) = \theta_{\text{eq}}^{\text{ON}}(x, z)$, where $\theta_{\text{eq}}^{\text{ON}}$ is defined as an equilibrium distribution of the director over the LC film, obtained during the turn-on process and at the value of the angle $\alpha$ being equal to 1.57. Figure 3 shows the evolution of the angle $\theta(x, z = 0, \tau)$ during the turn-off process along the length of the dimensionless LC film ($-10 \leq x \leq 10$), for two cases, A (Fig.3(a)) and B (Fig.3(b)), respectively, and for a number of times $\tau = 2$ (22) ($\sim 12$ ms), 6 (26) ($\sim 36$ ms), 8 (28) ($\sim 48$ ms), 12 (32) ($\sim 72$ ms) and 20 (40) ($\sim 0.12$ s). Here in our notation the first value denotes the dimensionless $(\tau = \frac{\epsilon_0 \epsilon_\alpha}{k_1} \left(\frac{V}{2\pi}\right)^2 t)$ time after switching- off the electric field, whereas the second value is the total time after starting the process. It is shown that after
Figure 3. The evolution of the angle \( \theta(x, z = 0, \tau) \) during the turn-off process (\( E = 0 \)) along the length of the dimensionless LC film \((-10 \leq x \leq 10)\), and for a number of dimensionless times \( \tau = 2 (22), 6 (26), 8 (28), 12 (32) \) and \( 20 (40) \), respectively. Part (a) shows the case of strong anchoring (case B), while (b) shows the case of weak anchoring (case A), respectively.

2.3. Turn-on process in the negative sense (case C)

When the strong electric field \( E \) is applied again but in the negative sense at the angle \( \alpha \sim -\frac{\pi}{2} \), the director moves from being parallel to the \( \mathbf{n}^{\text{OFF}} \) to being parallel to the electric field. Here \( \mathbf{n}^{\text{OFF}} \) is the final orientation of the director after the time term \( \tau_{\text{OFF}} \), when the electric field was removed. Now the reorientation of the director in the nematic film under the influence of the external forces can be obtained by solving the nonlinear differential equations (1) and (3), with the appropriate boundary Eqs.(4)-(5) and initial conditions. In that case the initial condition is taken in the form \( \theta(x, z, 0) = \theta^{\text{OFF}}(x, z) \), where \( \theta^{\text{OFF}}(x, z) \) is defined as the final distribution of the director over the LC film, obtained during the turn-off process when the electric field was removed. Two scenarios of the evolution of the director distribution across the LC film, under the influence of the strong electric field directed in the negative sense at the angle \( \alpha = -1.57 \) to the horizontal bounding surfaces are shown in Fig.4. That evolution is shown for time sequences \( \tau = 0 (248), 2 (250), 4 (252), 6 (254) \) and \( 8 (256) \) (see Fig.4), respectively. Here the first value denotes the dimensionless time after switching-on the process in the negative sense, whereas the second value is the total time after starting the process. In that case, the electric field was switching-on again after the dimensionless time terms \( \tau = 248 (\sim 1.488 \text{ s}) \). So, in that case the electric field was removed during \( \tau_{\text{OFF}} = 228 \) (20 \( \leq \tau \leq 248) \) dimensionless units. The main result of these calculations is that the final maintaining of the spatially periodic patterns, at \( \alpha = -1.57 \), is possible only when the electric field was removed during 228 dimensionless time units or \( 20 \leq \tau_{\text{OFF}} \leq 248 \) (0.12 s \( \leq \tau_{\text{OFF}} \leq 1.488 \text{ s}) \) (see Fig.4). This result confirm our previous suggestion that there is a threshold value of the amplitude \( \theta_0 \) which provides the nonuniform rotation mode rather than the uniform one, whereas the lower value of \( \theta_0 \) dominates the uniform mode [4]. Notice that the final maintaining of the spatially periodic (Fig.4) structure is achieved...
Figure 4. Formation of the nonuniform periodic evolution of the angle $\theta(x, z = 0, \tau)$ along the length of the dimensionless LC film ($-10 \leq x \leq 10$), for the turn-on process in the negative sense ($E < 0$), and for a number of dimensionless times $\tau = 0$ (248), 2 (250), 4 (252), 6 (254), and 8 (256). Part (a) shows the case of strong anchoring (case B), while (b) shows the case of weak anchoring (case A), respectively. Here $\alpha = -1.57$ ($\sim -89.96^\circ$), and the value of the amplitude $\theta_0$ is equal to 0.01 ($\sim 1.1^\circ$).

after the same dimensionless time 8 ($\sim 48$ ms).

3. Conclusion
In summary, we have numerically investigated the peculiarities in the director relaxation during both the turn-on and turn-off aligning processes in the nematic phase. Analysis of the numerical results for the turn-on process provides the evidence for the appearance of the spatially periodic patterns in confined 5CB LC film only in response to the suddenly applied strong electric field directed orthogonal (or approximately orthogonal) to the horizontal bounding surfaces. During the turn-off process ($\tau_{OFF}$), when the electric field is removed, the director relaxes back to the direction preferred by the surfaces and that process is characterized by the complex destruction of the initially periodic structure to a monodomain state.

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