# Field-induced director dynamics in confined nematic liquid crystals imposed by a strong orthogonal electric field

A. A. Vakulenko<sup>\*</sup> and A. V. Zakharov<sup>†</sup>

Saint Petersburg Institute for Machine Sciences, The Russian Academy of Sciences, Saint Petersburg 199178, Russia (Received 10 June 2013; published 21 August 2013)

The field-induced director dynamics for a low molar mass nematic liquid crystal (LC) has been investigated theoretically based 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 evidence for the appearance of the spatially periodic patterns in 4-*n*-pentyl-4'-cyanobiphenyl LC film, only in response to the suddenly applied strong electric field orthogonal to the magnetic field. It has been shown that at the values of the voltage of 200 V across the 194.7  $\mu$ m LC film and the magnetic field of 7.05 T directed at the angle  $\alpha = 1.57$  (~89.99°) between two fields, 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 mode. During the turn-off process, the reorientation of the director to its equilibrium orientation is characterized by the complex destruction of the initially periodic structure to a monodomain state.

DOI: 10.1103/PhysRevE.88.022505

PACS number(s): 61.30.Cz, 65.40.De

### I. INTRODUCTION

It is important, both from an academic and a technological point of view, to investigate the dynamic director reorientation in a thin nematic liquid crystal (LC) film confined between two transparent electrodes and subject to competing constraints. In the presence of external electric and magnetic fields, and surface anchoring in a nematic film, the motion of the director,  $\hat{\mathbf{n}}(r,t)$ , to its equilibrium orientation,  $\hat{\mathbf{n}}_{eq}(r)$ , across the LC film is governed by elastic, electric, magnetic, and viscous torques. Nuclear magnetic resonance (NMR) spectroscopy is by now a well-established method for investigating orientational order and dynamic properties in thermotropic liquid crystalline phases [1]. Recently, time-resolved deuterium NMR spectroscopic measurements of field-induced director reorientations have been performed [2-6]. Taking into account that the quadrupolar splitting is related to the angle  $\theta$  made by the director  $\hat{\mathbf{n}}$  with the magnetic field **B** (see Fig. 1), deuterium NMR spectroscopy is found to be a powerful method with which to investigate the dynamic director reorientation in nematic films. When the deuterated  $4-\alpha$ ,  $\alpha$ - $d_2$ -pentyl-4'-cyanobiphenyl  $(5CB-d_2)$  is subject to the strong electric field **E** applied at the angle  $\alpha$  to the magnetic field **B**, the director moves from being parallel to the magnetic field to being parallel to the electric field (the turn-on process), with the relaxation time  $\tau_{ON}$ , because both dielectric and magnetic anisotropies are positive for 5CB. After the electric field is switched off, the director relaxes back to being parallel to the magnetic field (the turn-off process), with the relaxation time  $\tau_{OFF}$ . Such a reorientation process has a typical deuterium NMR signature: the initial quadrupolar doublet characterizing the initially aligned LC sample gives rise to an additional broad doublet with time-dependent slitting while simultaneously the initial steady doublet with constant splitting progressively vanishes.

Some recent experimental data show NMR spectra with a different time evolution [2,7]. In this case, the application of the strong orthogonal electric field gives rise to the appearance of a new doublet with vanishing amplitude that progressively grows with constant splitting so that the total spectra intensity is essentially transferred from the initial doublet to the new one, with half of the quadrupolar splitting. These results strongly suggest that the initial state is not simply homogeneous and perturbed by thermal fluctuations. It is, therefore, necessary to analyze the nematic response from an initial state disturbed over the LC sample to its final distribution, imposed by the strong electric field. This can be done based on the predictions of hydrodynamic theory including both the director motion and fluid flow, providing evidence for the appearance of the spatially periodic patterns at the angles  $\alpha > 60^\circ$ , in response to the suddenly applied E. These periodic distortions produce a lower effective rotational viscosity and give a faster response of the director rotation than for a uniform mode, as observed in NMR experiment [7].

In this work, we focus on the geometry where the electric and magnetic fields are orthogonal (or approximately orthogonal) to each other. In this configuration, the state of the system immediately becomes unstable after applying an orthogonal electric field. When the misalignment of the director with respect to the direction imposed by the aligning magnetic field 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. In this case, the spectral line shape characterizing the initially aligned sample broadens with time-dependent splitting while the initial steady doublet with constant splitting progressively vanishes [2-4], and the application of the strong orthogonal electric field gives rise to the appearance of a new doublet with vanishing amplitude that progressively grows with constant splitting so that the total spectral intensity is transferred from the initial doublet to the new one, with half the quadrupolar splitting. These results strongly suggest that the initial state is not homogeneous and perturbed by thermal fluctuations.

<sup>\*</sup>avak2vale@mail.ru; www.ipme.ru

<sup>&</sup>lt;sup>†</sup>Author to whom all correspondence should be addressed: avz0911@yahoo.com



FIG. 1. (Color online) The geometry used for the calculations. The z axis is normal to the electrodes. The magnetic field **B**, electric field **E**, and director  $\hat{\mathbf{n}}$  are in the xz plane. The director makes an angle  $\theta$  both with the x axis and the magnetic field **B**, and the electric field makes a right angle with the magnetic field.

It is, therefore, necessary to analyze the nematic response to an initial state exhibiting some thermal fluctuations of the director under the influence of the strong electric field. Since anomalous changes of the spectral line shapes do not give any information about the average director orientation, the additional numerical investigations of the system that include both director reorientation and fluid flow should be done. So, the aim of this paper is to investigate the response of a strongly aligned LC phase confined between two surfaces and subject to a suddenly applied orthogonal electric field to the magnetic one. However, this raises a question: how much does the initial perturbing of the director with respect to the direction imposed by the aligning magnetic field, and caused by the thermal fluctuations with small amplitudes, influence the character of the further evolution of the director field to its equilibrium orientation? Physically, this means that for certain values of the electric and magnetic fields, there is a threshold value of the amplitude which provides the nonuniform rotation mode rather than the uniform one. The outline of this paper is as follows. In the next section, we describe the theoretical treatment including the director motion in the nematic film and the numerical results for a number of hydrodynamical regimes. The discussion of these results is summarized in Sec. III.

## II. FORMULATION OF THE RELEVANT EQUATIONS FOR DYNAMICAL REORIENTATION OF THE DIRECTOR FIELD

The coordinate system defined by our experiment assumes that the electric field **E** is applied normal (or close to the normal) both to the electrodes and the magnetic field **B** (see Fig. 1). We consider a nematic system such as cyanobiphenyl, which is delimited by two horizontal and two lateral surfaces at mutual distances 2d and 2L on a scale on the order of tens of micrometers. According to this geometry, the system may be seen as two-dimensional, since the director is maintained within the xz plane (or in the yz plane) defined by the two fields, where  $\hat{\mathbf{i}}$  is the unit vector directed parallel to the horizontal surfaces, which coincides with the direction of the magnetic field **B**,  $\hat{\mathbf{k}}$  is a unit normal vector, which coincides with the direction of the electric field **E**, and  $\hat{\mathbf{j}} = \hat{\mathbf{k}} \times \hat{\mathbf{i}}$ . We can suppose that the components of the director,  $\hat{\mathbf{n}} = n_x \hat{\mathbf{i}} + n_z \hat{\mathbf{k}} = \cos \theta(x, z, t) \hat{\mathbf{i}} + \sin \theta(x, z, t) \hat{\mathbf{k}}$  (see Fig. 1), depend only x, z components and time t. Here  $\theta$  denotes the angle between the director and the magnetic field. Our recent investigation of the field-induced relaxation of the director field under the influence of a strong electric field suggests that in order to describe the dynamical reorientation of the director correctly, we do not need to include a proper treatment of backflow [8]. This means that the role of the viscous forces becomes negligible in comparison to the electric, magnetic, elastic, and flexoelectric contributions. In that case, the torque balance equation  $\mathbf{T}_{el} + \mathbf{T}_{mg} + \mathbf{T}_{vis} + \mathbf{T}_{elast} + \mathbf{T}_{fl} = \mathbf{0}$  takes the form [8] (for details, see the Appendix)

$$\begin{aligned} \gamma_{1}\theta_{,t} &= (K_{1}\sin^{2}\theta + K_{3}\cos^{2}\theta)\theta_{,xx} \\ &+ (K_{1}\cos^{2}\theta + K_{3}\sin^{2}\theta)\theta_{,zz} + (K_{3} - K_{1})\sin 2\theta\theta_{,xz} \\ &+ \frac{1}{2}(K_{1} - K_{3})\sin 2\theta (\theta_{,x}^{2} - \theta_{,z}^{2})(K_{3} - K_{1})\cos 2\theta\theta_{,x}\theta_{,z} \\ &+ \frac{1}{2}\epsilon_{0}\epsilon_{a}E^{2}\sin 2(\alpha - \theta) - \frac{1}{2}\frac{\chi_{a}}{\mu_{0}}\sin 2\theta B^{2} \\ &- \frac{1}{2}(e_{1} + e_{3})E_{,z}\sin\alpha\sin 2\theta, \end{aligned}$$
(1)

where  $\epsilon_0$  is the dielectric permittivity,  $\epsilon_a$  is the dielectric anisotropy of the nematic sample,  $\mu_0$  is the magnetic constant,  $\chi_a$  is the magnetic anisotropy of the nematic sample,  $\gamma_1$  is the rotational viscosity coefficient,  $K_1$  and  $K_3$  are the splay and bend elastic constants, and  $e_1$  and  $e_3$  are the flexoelectric constants. Here the electric field  $\mathbf{E} = E_x \hat{\mathbf{i}} + E_z \hat{\mathbf{k}} =$  $E(z) \cos \alpha \hat{\mathbf{i}} + E(z) \sin \alpha \hat{\mathbf{k}}$  makes the angle  $\alpha$  with the magnetic field  $\mathbf{B}$ , the values of which are varied in the vicinity of  $\frac{\pi}{2}$ . In the case of the two-dimensional LC system, the dimensionless torque balance equation describing the reorientation of  $\hat{\mathbf{n}}$  to its equilibrium orientation  $\hat{\mathbf{n}}_{eq}$  can be written as

$$\begin{aligned} \theta_{,\tau} &= \delta_1 [(\sin^2 \theta + K_{31} \cos^2 \theta) \theta_{,xx} + (\cos^2 \theta + K_{31} \sin^2 \theta) \theta_{,zz}] \\ &+ \delta_1 [(K_{31} - 1) \sin 2\theta \theta_{,xz} + \frac{1}{2} (1 - K_{31}) \\ &\times \sin 2\theta (\theta_{,x}^2 - \theta_{,z}^2)] + \delta_1 (K_{31} - 1) \cos 2\theta \theta_{,x} \theta_{,z} \\ &+ \frac{1}{2} [-\delta_2 \sin 2\theta + f^2(\theta) \sin 2(\alpha - \theta)] \\ &- \delta_3 f_z \sin \alpha \sin 2\theta. \end{aligned}$$
(2)

Here  $\overline{x} = x/d$  and  $\overline{z} = z/d$  are the dimensionless space variables which have been (and will be) eliminated in the preceding as well as in the following equations,  $\tau = \frac{\epsilon_0 \epsilon_a}{\gamma_1} (\frac{U}{2d})^2 t$  is the dimensionless time,  $f(\theta) = \frac{C - \delta_3 \sin 2\theta \theta_z}{\epsilon_\perp / \epsilon_a + \sin^2 \theta}$ ,  $C = [\int_{-1}^{1} (\epsilon_\perp / \epsilon_a + \sin^2 \theta)^{-1} dz]^{-1}$ , and  $\delta_1 = \frac{4K_1}{\epsilon_0 \epsilon_a U^2}$ ,  $\delta_2 = \frac{4\chi_a B^2 d^2}{\mu_0 \epsilon_0 \epsilon_a U^2}$ ,  $\delta_3 = \frac{e_1 + e_3}{\epsilon_0 \epsilon_a U}$ , and  $K_{31} = \frac{K_3}{K_1}$  are four parameters of the system.

The application of the voltage across the nematic film results in a variation of E(z) through the film which is obtained from [8]

$$\frac{\partial}{\partial z} \left[ \left( \frac{\epsilon_{\perp}}{\epsilon_a} + \sin^2 \theta \right) \overline{E}(z) + \delta_3 \theta_{,z} \sin 2\theta \right] = 0,$$

$$1 = \int_{-1}^1 \overline{E}(z) dz,$$
(3)

where  $\overline{E}(z) = \frac{2dE(z)}{U}$ , and U is the voltage applied across the cell. Notice that the overbars in the electric field  $\overline{E}$  will be

eliminated too in the following equations. Consider now the nematic film between the two electrodes when the director is weakly anchored at the surfaces and the anchoring energy takes the form [9]  $W^{an} = \frac{1}{2}A\sin^2(\theta_s - \theta_0)$ , where  $\theta_s$  and  $\theta_0$  are the angles corresponding to the director orientation on the solid surface,  $\hat{\mathbf{n}}_s$ , and easy axis,  $\hat{\mathbf{n}}^0$ , respectively. The torque balance transmitted to the surfaces assumes that the director has to satisfy the boundary conditions [7]

$$(\overline{n}_{,z})_{-10 < x < 10, z=\pm 1} = \frac{Ad}{K_1} \overline{n}_{-10 < x < 10, z=\pm 1}, \tag{4}$$

where  $\overline{n} = n_z - n^0$ ,  $n_{-10 < x < 10, z = \pm 1}$  is the director orientation on the bounding surfaces, and  $n^0$  is the projection of the easy axis orientation on the horizontal bounding surfaces, whereas on the rest two lateral surfaces assume the strong anchoring conditions

$$(\hat{\mathbf{n}})_{x=\pm 10,-1< z<1,} \parallel \hat{\mathbf{i}}.$$
 (5)

Now the reorientation of the director in the nematic film between the two electrodes, when the relaxation process is governed by viscous, elastic, flexoelectric, and magnetic torques, can be obtained by solving the system of nonlinear partial differential equations (2) and (3), with appropriate boundary (4) and (5) and initial  $\theta(x,z,\tau = 0)$  conditions.

### A. Turn-on process

When a strong electric field **E** is applied at the angle  $\alpha$  close to the right angle to the magnetic field **B**, the director moves from being parallel to the magnetic field to being parallel to the electric field (the turn-on process), because both dielectric and magnetic anisotropies are positive for 5CB. 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 (2) and (3) with appropriate boundary [(4) and (5)] and initial conditions. To elucidate the role of the thermal fluctuations in maintaining 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. (2) and (3) with the mixed boundary condition for the angle  $\theta$ , which read in the dimensionless form as (hereafter referred to as case A)

$$\theta_{,z}(-10 < x < 10, z = \pm 1) = \pm \delta_4 \theta(-10 < x < 10, z = \pm 1),$$
  
$$\theta(x = \pm 10, -1 < z < 1) = 0,$$
 (6)

where  $\delta_4 = \frac{Ad}{K_1}$ , and with the strong anchoring condition for the angle  $\theta$ , which reads in the dimensionless form as (hereafter referred to as case B)

$$\theta(-10 < x < 10, z = \pm 1) = 0,$$
  

$$\theta(x = \pm 10, -1 < z < 1) = 0.$$
(7)

To observe the formation of the spatially periodic patterns in cyanobiphenyl LC film, excited by the strong orthogonal electric field, we consider the initial condition in the form

$$\theta(x,z,0) = \theta_0 \cos(q_x x) \cos(q_z z), \tag{8}$$

which defines the thermal fluctuations of the director over the LC sample with amplitude  $\theta_0$  and wavelengths  $q_x$  and  $q_z$  of an individual Fourier component of the modulation. In case A, the latter are described as  $q_x = \frac{\pi}{2}(2k+1)$ , where k = 0, 1, 2, ... and  $q_z = \mp (\delta_4 \cot q_z)_{z=\pm 1}$ , whereas in case B, they are described as  $q_\alpha = \frac{\pi}{2}(2k+1)$ , where  $\alpha = x, z$  and k = 0, 1, 2, ...

For the case of  $5CB - d_2$ , at a temperature  $15 \,^{\circ}C$  and density  $10^3$  kg/m<sup>3</sup>, the measured data for the elastic constants are  $K_1 = 8.7$  and  $K_3 = 10.2$  pN [9], the calculated value of the dielectric anisotropy is equal to  $\epsilon_a = 11.5$  [10], and the experimental value of the rotational viscosity coefficient  $\gamma_1$ is equal to 0.136 Pas [11]. The value of the voltage across the nematic film, which is  $2d = 194.7 \ \mu$ m, was chosen to be U = 200 V, the value of A is equal to  $10^{-6}$  J/m<sup>2</sup>, and the ratio of L/d is equal to 10, whereas the calculated data for both flexoelectric coefficients,  $e_1$  and  $e_3$ , are equal to -11.6and -4.3 pC/m [12], respectively. The value of the magnetic anisotropy is equal to  $\chi_a = 1.17 \times 10^{-6}$  [13], whereas the value of the magnetic field is equal to B = 7.05 T. The set of  $\delta$  parameters, which is involved in Eqs. (2), (3), and (6), takes the values  $\delta_1 = 8.6 \times 10^{-6}$ ,  $\delta_2 = 0.424$ ,  $\delta_3 = -0.0009$ , and  $\delta_4 = 19.5$ .

The nonlinear partial differential equations (2) and (3), together with the boundary conditions (6) (case A) or (7) (case B) and the initial condition (8), have been solved by the numerical relaxation method. The relaxation criterion  $\epsilon =$  $|[\theta(\tau_R) - \theta_{eq}]/\theta_{eq}|$  for calculating the procedure was chosen to be equal to  $5 \times 10^{-4}$ , and the numerical procedure was then carried out until a prescribed accuracy was achieved. For the angle  $\alpha = 1.57 \ (\sim 89.96^\circ)$ , the values of  $\theta_0$  are equal to 0.01 ( $\sim$ 1.1°) and 0.001 ( $\sim$ 0.1°), whereas for the angle  $\alpha = 1.565$  (~88.81°), the values of  $\theta_0$  are equal to 0.02  $(\sim 2.2^{\circ})$  and 0.01  $(\sim 1.1^{\circ})$ , respectively. The main result of this calculation is that the periodic response appears for  $\alpha = 1.57$  only for the values of the amplitude  $\theta_0$  more than  $0.01 ~(\sim 1.1^{\circ})$  (see Fig. 2), whereas for the lower values of the amplitude [for instance, 0.001 ( $\sim 0.1^{\circ}$ ) (see Fig. 2)], the certain balance between the electric and magnetic fields provides only the uniform rotation mode. For the cases A and B, and for the values of  $\theta_0 = 0.01$  (~1.1°) and  $\alpha = 1.57$ , the time propagation of the  $\theta(x, z = 0, \tau)$  profile along the x axis  $(-10 \le x \le 10)$  is characterized by the well-developed periodic structure with the lattice points at  $x = \pm 2.3$  and  $\pm 5.7$ , and characterized by the different values of the relaxation time  $\tau_R$  (A) = 25 (~31.75 ms) for case A, and  $\tau_R$  (B) = 24.5 (~31.1 ms) for case B, respectively. In turn, for cases A and B, and for the smaller value of the amplitude  $\theta_0 = 0.001 \ (\sim 0.1^\circ)$ , the evolution of the angle  $\theta(x, z = 0, \tau)$ is characterized only by the wavelike profile along the x axis  $(-10 \le x \le 10)$  growing in the positive direction. In both of these cases, at the later stage of the evolution process, for  $\tau$  (A) > 15 in case A, and  $\tau$  (B) > 12.5 in case B, one deals with the completely convex profiles growing in the positive direction. These evolution processes are characterized by the different values of the relaxation times,  $\tau_R$  (A) ~ 26 (~33 ms) and  $\tau_R$  (B) ~ 25 (~31.75 ms), respectively. Physically, this means that in the latter case, when the value of the amplitude  $\theta_0$  is equal to or less than 0.001 (~0.1°), the value of the electric field is not enough to maintain the spatially periodic patterns; it is enough only for the formation of the wavelike deformations in the LC film. With the further decrease of the angle  $\alpha$  up to  $1.565 \ (\sim 88.81^\circ)$ , only the amplitudes greater than or equal



FIG. 2. (Color online) Two scenarios of evolution of the director distribution across the LC film under the influence of the strong electric field directed at the angle  $\alpha = 1.57$  (~89.96°) to the magnetic field for the turn-on process. Part (a) shows the case of the strong anchoring (case B), while (b) shows the case of the weak anchoring (case A), and with accounting for the flexoelectric effect. In all these cases, the amplitude of the thermal fluctuation  $\theta_0$  are equal to 0.01 (~1.1°) and  $\theta_0 = 0.001$  (~0.1°), respectively.

to 0.02 provide the nonuniform rotation mode rather than the uniform one (see Fig. 3). Physically, this means that with a decrease of  $\alpha$  up to 1.565 (~88.81°), the balance between the electric and magnetic forces enables only the nonperfect periodic patterns to be maintained with the lattice points at  $x = \pm 2.7$  and  $\pm 5.3$  for the value of the amplitude  $\theta_0 = 0.02$  $(\sim 2.2^{\circ})$  and higher and with the relaxation time  $\tau_R$  (A) = 20.5 (~26 ms) and  $\tau_R$  (B) = 20 (~25.4 ms), respectively. In the case of the smaller value of the amplitude  $\theta_0 = 0.01$  $(\sim 1.1^{\circ})$ , the time dependence of the  $\theta(x, z = 0, \tau)$  profile resembles the wavelike profile along the x axis growing in the positive direction, with the relaxation time  $\tau_R$  (A) = 22 (~28 ms) and  $\tau_R$  (B) = 21 (~26.7 ms), respectively. Only at the values of the angle  $\alpha = 1.565$  and higher do the optimal dimensionless wavelengths  $q_x$  and  $q_z$  provide the minimal values of the total energy W. It is can be written as [12]  $W = W_{elast} + W_{em}(\beta)$ , where  $\beta = A$  and B, respectively. Here

$$\frac{2}{\delta_1} W_{\text{elast}} = \int dx \, dz \Big[ -\sin\theta_{\text{eq}}^{\text{ON}}(x,z) \theta_{\text{eq},x}^{\text{ON}}(x,z) \\ + \cos\theta_{\text{eq}}^{\text{ON}}(x,z) \theta_{\text{eq},z}^{\text{ON}}(x,z) \Big]^2$$

$$+ K_{31} \int dx \, dz \Big[ \cos \theta_{\text{eq}}^{\text{ON}}(x, z) \theta_{\text{eq}, x}^{\text{ON}}(x, z) \\ + \sin \theta_{\text{eq}}^{\text{ON}}(x, z) \theta_{\text{eq}, z}^{\text{ON}}(x, z) \Big]^2 \tag{9}$$

is the elastic contribution, and

$$2W_{\rm em}(A) = \int dx \, dz f^2 \left[ \theta_{\rm eq}^{\rm ON}(x,z) \right] \cos^2 \left[ \theta_{\rm eq}^{\rm ON}(x,z) - \alpha \right] \\ + \int dx \, dz \left\{ \delta_2 \cos^2 \theta_{\rm eq}^{\rm ON}(x,z) - \delta_3 f \left[ \theta_{\rm eq}^{\rm ON}(x,z) \right] \sin \alpha \sin 2\theta_{\rm eq}^{\rm ON}(x,z) \right\}, \\ 2W_{\rm em}(B) = \int dx \, dz \left\{ \cos^2 \left[ \theta_{\rm eq}^{\rm ON}(x,z) - \alpha \right] + \delta_2 \cos^2 \theta_{\rm eq}^{\rm ON}(x,z) \right\}$$
(10)

are the electric and magnetic contributions to the total energy, for the cases A and B, respectively. Here  $\theta_{eq}^{ON}(x,z)$  is the equilibrium value of the angle  $\theta(x,z,\tau)$  corresponding to the turn-on process.

It is shown that only for the values of  $q_x = 0.785$ ,  $q_z = 64.3358$ ,  $\alpha = 1.57$ , and  $\theta_0 = 0.01 ~(-1.1^\circ)$  and higher does the solution show that the periodic structure may appear in the nematic phase under the above-mentioned conditions, whereas



FIG. 3. (Color online) The same as in Fig. 2, but the angle  $\alpha = 1.565$  (~88.81°), and for the values of the thermal fluctuation  $\theta_0 = 0.02$  (~2.2°) and 0.01 (~1.1°), respectively.



FIG. 4. (Color online) Formation of the periodic evolution of the angle  $\theta(x = 0, z, \tau)$  along the width of the dimensionless LC film  $(-1 \le z \le 1)$ , for the turn-on process, and for a number of times  $\tau = 4$ , 8, 12, and 16. Part (a) shows the case of strong anchoring (case B), while (b) shows the case of weak anchoring (case A), and with accounting for the flexoelectric effect. Here  $\alpha = 1.57$  (~89.96°), and the value of the amplitude  $\theta_0$  is equal to 0.01 (~1.1°).

for the angle  $\alpha = 1.565$ , these values are  $q_x = 0.785$  and  $q_z =$ 32.9521 for  $\theta_0 = 0.02 ~(\sim 2.2^\circ)$  and higher. These values of  $q_x$ and  $q_z$  provide the minimal values of the total energy W (see Figs. 2 and 3). When the value of  $\theta_0$  is less than 0.02 (~2.2°) for the angle  $\alpha = 1.565$ , or 0.01 (~1.1°) for the angle  $\alpha = 1.57$ , one sees that the periodic structure does not develop under the above-mentioned conditions, and for a certain balance between the electric and magnetic fields in the evolution of the director field across the LC sample, the uniform mode is dominated. So, the main feature of the numerical solutions is that the further decreasing of the angle  $\alpha$  [less than 1.565 (~88.81°)] leads to the destruction of the periodic structure, and the director is reoriented as a monodomain nematic. The evolution of the angle  $\theta(x = 0, z, \tau)$  for the turn-on process along the width of the dimensionless LC film  $(-1 \leq z \leq 1)$ , both for the cases A and B, and for the value of the amplitude  $\theta = 0 = 0.01 (\sim 1.1^{\circ})$  $(\alpha = 1.57)$ , is shown in Fig. 4(a) and 4(b). Here the evolution of the angle  $\theta(x = 0, z, \tau)$  for the turn-on process along the width of the dimensionless LC film is shown for a number of

times  $\tau = 4$  (~5.2 ms), 8 (~10.4 ms), 12 (~15.6 ms), and 16 (~20.8 ms), respectively.

It is obvious from Figs. 2–4 that for certain values of the electric and magnetic fields ( $2d = 194.7 \ \mu m$ ,  $U = 200 \ V$ ,  $B = 7.05 \ T$ ), for the values of the angle  $\alpha$  greater than or equal to 1.565 (~88.81°), there is a threshold value of the amplitude which provides the nonuniform rotation mode rather than the uniform one, whereas for the lower values, both the amplitude  $\theta_0$  and the angle  $\alpha$  dominate the uniform mode.

#### **B.** Turn-off process

After the electric field is removed, the director relaxes back to being parallel to the magnetic field (the turn-off process). Now the reorientation of the director in the nematic film under the influence of the magnetic force can be obtained by solving the nonlinear differential equation (1), for the case of E = 0, and both with the mixed (6) (case A) and strong (7) (case B) boundary conditions for the angle  $\theta$ . The initial condition is



FIG. 5. (Color online) The evolution of the angle  $\theta(x, z = 0, \tau)$  during the turn-off process along the length of the dimensionless LC film  $(-10 \le x \le 10)$ , and for a number of times  $\tau = 0, 4$  (~5.2 ms), 8 (~10.4 ms), 10 (~13.0 ms), 12 (~15.6 ms), 16 (~20.8 ms), and 20 (~26 ms), respectively. Part (a) shows the case of strong anchoring (case B), while (b) shows the case of weak anchoring (case A), respectively.



FIG. 6. (Color online) The evolution of the angle  $\theta(x,z,\tau)$  during the turn-off process at two points, x = 2.3 and 0, along the width of the dimensionless LC film ( $-1 \le z \le 1$ ), for cases A (b) and B (a), and for a number of times  $\tau = 4$  ( $\sim 5.2$  ms) (curve 1), 8 ( $\sim 10.4$  ms) (curve 2), 12 ( $\sim 15.6$  ms) (curve 3), 16 ( $\sim 20.8$  ms) (curve 4), 20 ( $\sim 26$  ms) (curve 5), and 24 ( $\sim 31.2$  ms) (curve 6), respectively.

taken in the form

$$\theta(x,z,0) = \theta_{eq}^{ON}(x,z), \qquad (11)$$

where  $\theta_{eq}^{ON}$  is defined as an equilibrium distribution of the director over the LC film obtained during the turn-on process and for the value of the angle  $\alpha$  equal to 1.57. Figure 5 shows the evolution of the angle  $\theta(x,z=0,\tau)$  during the turn-off process along the length of the dimensionless LC film  $(-10 \le x \le 10)$  for two cases, A and B, respectively, and for a number of times  $\tau = 4$  (~5.2 ms), 8 (~10.4 ms), 12 (~15.6 ms), 16 (~20.8 ms), and 20 (~26 ms), whereas Fig. 6 shows the evolution of the angle  $\theta(\tau, x, z)$  during the turn-off process at two points, x = 2.3 and 0, along the width of the dimensionless LC film  $(-1 \le z \le 1)$ , and for two cases, A and B, respectively, and for a number of times  $\tau = 4$  (~5.2 ms), 8 (~10.4 ms), 12 (~15.6 ms), 16 (~20.8 ms), and 20 (~26 ms). It is shown that after times  $\tau_R$  (B) ~ 24 (~31.2 ms) and  $\tau_R$  (A) ~ 26 (~33.8 ms), when the electric field is removed,

the director relaxes back to being parallel to the magnetic field and the angle  $\theta \to 0$ , when  $\tau \to \tau_R$ . So, according to our calculations, the reorientation of the director  $\hat{\mathbf{n}}$  to its equilibrium orientation with  $\theta_{eq}^{OFF}(x,z) = 0$  is characterized by the complex destruction of the initially periodic structure (see Fig. 5) especially in the vicinity of the lattice points  $x = \pm 2.3$ ,  $\pm 5.7$ , and z = 0, with a huge variation of  $\theta_{,x}(x,z)$ .

## **III. CONCLUSION**

Having obtained the evolution of the angle  $\theta(x, z, \tau)$  to its equilibrium distribution across the LC film  $[\theta_{eq}^{OFF}(x, z) = 0]$ , we can calculate the evolution of the spectra during the turnoff process. When the director field is inhomogeneous, the spectrum is a superposition of the elementary doublets  $I(\theta, \nu)$ weighted by the probability density  $P(\theta)$  for finding a director with orientation  $\theta$ . Accordingly, the full spectrum is given



FIG. 7. (Color online) The calculated time-resolved  $^{2}$ H spectra for the turn-off process at 14.8 °C, showing nonuniform director relaxation from being almost parallel to the electric field to being parallel to the magnetic field. Part (a) shows the case of strong anchoring, and (b) shows the case of weak anchoring.

by [2]

$$I(\nu) = \int I(\theta, \nu) P(\theta) d\theta, \qquad (12)$$

where the form of the elementary doublet associated with the orientation  $\theta$  with Gaussian line shapes is defined by

$$I(\theta, \nu) = \sum_{\epsilon \in [+, -]} \frac{1}{\sqrt{2\pi\sigma^2(\theta)}} \\ \times \exp\left[-\frac{1}{2} \left(\frac{\nu - \epsilon(\Delta\nu_0/2)P_2(\cos\theta)}{\sigma(\theta)}\right)^2\right], \quad (13)$$

where  $\sigma(\theta) = \sigma_0 + \sigma_2 P_2(\cos \theta) + \sigma_4 P_4(\cos \theta)$  is define as the linewidth. Here  $\sigma_0 = 1.14$ ,  $\sigma_2 = 0.523$ , and  $\sigma_4 = -0.373$  kHz [14]. Calculated time-resolved <sup>2</sup>H spectra for a turn-off process at 14.8 °C show nonuniform director relaxation from being almost parallel to the electric field (U = 200 V) to being parallel to the magnetic field (B = 7.05 T), for a number of times  $\tau = 4$  $(\sim 5.2 \text{ ms})$ , 8 ( $\sim 10.4 \text{ ms}$ ), 12 ( $\sim 15.6 \text{ ms}$ ), 16 ( $\sim 20.8 \text{ ms}$ ), and 20 ( $\sim$ 26 ms), as shown in Fig. 7. Figure 7(a) shows the case of strong anchoring, while Fig. 7(b) shows the case of weak anchoring. The spectral range used in the simulation is taken to be  $-40 \le \nu \le 40$  kHz. Such reorientation during the turn-off process has a typical NMR signature: the initial quadrupolar doublet characterizing the initially aligned LC sample gives rise to an additional broad doublet with time-dependent splitting while simultaneously the initial doublet with constant splitting progressively vanishes [see in Fig. 7 during the first time terms up to  $10(\sim 13 \text{ ms})$ ]. In this case, removing the strong electric field gives rise to the appearance of a new doublet that progressively grows with constant splitting so that the total spectral intensity is essentially transferred from the initial doublet to the new one, with double the quadrupolar splitting. These results strongly suggest that the nonuniform director distribution relaxes to the uniform one, parallel to the magnetic field.

In summary, we have numerically investigated the peculiarities in the director relaxation during both the turn-on and turn-off aligning processes. Analysis of the numerical results for the turn-on process provides evidence for the appearance of the spatially periodic patterns in the deuterated  $5CB-d_2$  LC film only in response to the suddenly applied strong electric field orthogonal to the magnetic field. The main result of this calculation is that the periodic response appears only for a certain balance between the electric and magnetic fields, and there is a threshold value of the amplitude of the director fluctuations over the LC sample which provides the nonuniform rotation mode rather than the uniform one, whereas for the lower values of the amplitude the uniform mode appears. During the turn-off process, the reorientation of the director to its equilibrium orientation is characterized by the complex destruction of the initially periodic structure to a monodomain state.

It is expected that the present investigation will shed some light on the problems of the reorientation processes in nematic films confined between two plates under the presence of a large electric field directed perpendicular to the magnetic field.

#### ACKNOWLEDGMENTS

We thank A. Sugimura for several helpful discussions. This work was supported by a Grant in Aid for Scientific Research (B-24360127) from JSPS.

#### **APPENDIX: TORQUE BALANCE EQUATION**

The torque balance equation  $T_{el} + T_{mg} + T_{vis} + T_{elast} +$  $\mathbf{T}_{\rm fl} = 0$  can be derived from the electric  $\mathbf{T}_{\rm el} = \frac{\delta \psi_{\rm el}}{\delta \hat{\mathbf{n}}} \times \hat{\mathbf{n}}$ , magnetic  $\mathbf{T}_{mg} = \frac{\delta \psi_{mg}}{\delta \hat{\mathbf{n}}} \times \hat{\mathbf{n}}$ , viscous  $\mathbf{T}_{vis} = \frac{\delta \mathcal{R}^{vis}}{\delta \hat{\mathbf{n}}_i} \times \hat{\mathbf{n}}$ , elastic  $\mathbf{T}_{\text{elast}} = \frac{\delta \psi_{\text{elast}}}{\delta \hat{\mathbf{n}}} \times \hat{\mathbf{n}}$ , and flexoelectric  $\mathbf{T}_{\text{flex}} = \frac{\delta \psi_{\text{flex}}}{\delta \hat{\mathbf{n}}} \times \hat{\mathbf{n}}$  torques exerted on the director  $\hat{\mathbf{n}}$ . Here  $\psi_{\text{el}} = -\frac{1}{2} \epsilon_0 \epsilon_a (\hat{\mathbf{n}} \cdot \mathbf{E})^2 =$  $-\frac{1}{2}\epsilon_0\epsilon_a(n_xE_x+n_zE_z)^2$  is the electric energy density,  $\psi_{\rm mg}^2 = -\frac{1}{2} \frac{\chi_a}{\mu_0} (\mathbf{\hat{n}} \cdot \mathbf{B})^2 = -\frac{1}{2} \frac{\chi_a}{\mu_0} (n_x B)^2$  is the magnetic energy density,  $\mathcal{R}^{\rm vis} = \gamma_1 \mathbf{N}^2 = \gamma_1 (n_{x,t}^2 + n_{z,t}^2)$  is the viscous dissipation function,  $\psi_{\text{elast}} = \frac{1}{2} [K_1 (\nabla \cdot \hat{\mathbf{n}})^2 + K_3 (\hat{\mathbf{n}} \times \nabla \times$  $\hat{\mathbf{n}}^2] = \frac{1}{2} [K_1 (n_{x,x} + n_{z,z})^2 + K_3 (n_{z,x} - n_{x,z})^2]$  is the elastic energy density, and  $\psi_{\text{flex}} = -\mathbf{P} \cdot \mathbf{E}$  is the flexoelectric energy density, respectively. The vector **N** is equal to  $\frac{\partial \hat{\mathbf{n}}}{\partial t} = \hat{\mathbf{n}}_{,t}$ , whereas the vector **P** is equal to  $e_1\hat{\mathbf{n}}(\nabla \cdot \hat{\mathbf{n}}) + e_3(\nabla \times \hat{\mathbf{n}}) \times \hat{\mathbf{n}}$ . It allows us to rewrite the torque contributions as  $T_{elast} =$  $\{n_{z} [K_{1}n_{x,xx} + K_{3}n_{x,zz} + (K_{1} - K_{3})n_{z,xz}] - n_{x} [K_{1}n_{z,zz} + (K_{1} - K_{3})n_{z,xz}] - n_{x} [K_{1}n_{z,zz} + (K_{1} - K_{3})n_{z,xz}] - n_{x} [K_{1}n_{z,zz} + (K_{1} - K_{3})n_{z,xz}] - n_{x} [K_{1}n_{z,xz} + (K_{1} - K_{3})n_{z,xz}] - n_{x} [K_{1}n_{x,x} + (K_{1} - K_{3})n_{z,xz}] - n_{x} [K_{1}n_{x,xx} + (K_{1} - K_{3})n_{x,xx}] - n_{x} [K_{1}n_{x,xx} + (K_{1$  $K_{3}n_{z,xx} + (K_{1} - K_{3})n_{x,xz}]$ **j**,  $\mathbf{T}_{vis} = \gamma_{1}[n_{x}n_{z,t} - n_{z}n_{x,t}]$ **j**,  $\mathbf{T}_{el} =$  $\epsilon_{0}\epsilon_{a}(n_{x}E_{x} + n_{z}E_{z})(n_{z}E_{x} - n_{x}E_{z})\mathbf{\hat{j}}, \mathbf{T}_{mg} = \frac{\chi_{a}}{\mu_{0}}n_{x}n_{z}B^{2}\mathbf{\hat{j}}, \text{ and} \mathbf{T}_{flex} = (e_{1} + e_{3})E_{,z}\sin\alpha n_{x}n_{z}\mathbf{\hat{j}}, \text{ where } n_{x,x} = \frac{\partial n_{x}}{\partial x} \text{ and } n_{x,xx} =$  $\frac{\partial^2 n_x}{\partial x^2}$ . The appropriate angle's forms for the torques are given below as  $-T_{elast}^y = (K_1 \sin^2 \theta + K_3 \cos^2 \theta)\theta_{,xx} +$  $(K_1\cos^2\theta + K_3\sin^2\theta)\theta_{,zz} + (K_3 - K_1)\sin 2\theta\theta_{,xz} + \frac{1}{2}(K_1 - K_3)$  $\begin{aligned} \sin 2\theta(\theta_{,x}^2 - \theta_{,z}^2) + (K_1 - K_3)\cos 2\theta\theta_{,x}\theta_{,z}, & T_{\text{vis}}^y = \gamma_1\theta_{,t}, \\ T_{\text{el}}^y &= -\frac{1}{2}\epsilon_0\epsilon_a(\frac{U}{2d})^2\sin 2(\alpha - \theta), & \text{and} & T_{\text{mg}}^y = \frac{1}{2}\frac{\chi_a}{\mu_0}B^2\sin 2\theta, \end{aligned}$  $T_{\text{flex}}^{y} = \frac{1}{2}(e_1 + e_3)E_{z,z}\sin\alpha\sin 2\theta.$ 

- R. Y. Dong, Nuclear Magnetic Resonance of Liquid Crystals, 2nd ed. (Springer-Verlag, New York, 1997).
- [2] A. Sugimura and G. R. Luckhurst, in *Nuclear Magnetic Resonance Spectroscopy of Liquid Crystals*, edited by R. Y. Dong (World Scientific, Singapore, 2009), Chap. 10.
- [3] G. R. Luckhurst, T. Miyamoto, A. Sugimura, and B. A. Timimi, J. Chem. Phys. 117, 5899 (2002).
- [4] G. R. Luckhurst, A. Sugimura, B. A. Timimi, and H. Zimmermann, Liq. Cryst. 32, 1389 (2005).
- [5] M. Cifelli, D. Frezzato, G. R. Luckhurst, G. J. Moro, A. Sugimura, and C. A. Veracini, Liq. Cryst. 37, 773 (2010).
- [6] A. F. Martins and A. Veron, Liq. Cryst. 37, 747 (2010).
- [7] A. Sugimura and A. V. Zakharov, Phys. Rev. E 84, 021703 (2011).

## A. A. VAKULENKO AND A. V. ZAKHAROV

- [8] A. Sugimura, A. A. Vakulenko, and A. V. Zakharov, Phys. Procedia 14, 102 (2011).
- [9] N. V. Madhusudana and R. Pratibha, Mol. Cryst. Liq. Cryst. 89, 249 (1982).
- [10] A. V. Zakharov and A. Maliniak, Eur. Phys. J. E 4, 435 (2001).
- [11] A. G. Chmielewski, Mol. Cryst. Liq. Cryst. 132, 339 (1986).
- [12] A. V. Zakharov and A. A. Vakulenko, Crystallogr. Rep. 48, 686 (2003).
- [13] G. Srajer, S. Fraden, and R. B. Meyer, Phys. Rev. A 39, 4828 (1989).
- [14] D. Hamasuna, G. R. Luckhurst, A. Sugimura, B. A. Timimi, K. Usami, and H. Zimmermann, Thin Solid Films 517, 1394 (2008).