



Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gmcl20>

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Version of record first published: 07 Jan 2010

To cite this article: K. R. MacKenzie & G. McKay (2004): DIRECTOR ORIENTATION IN NEMATIC LIQUID CRYSTALS UNDER ORTHOGONAL MAGNETIC AND ELECTRIC FIELDS, Molecular Crystals and Liquid Crystals, 413:1, 197-209

To link to this article: <http://dx.doi.org/10.1080/15421400490437150>

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DIRECTOR ORIENTATION IN NEMATIC LIQUID CRYSTALS UNDER ORTHOGONAL MAGNETIC AND ELECTRIC FIELDS

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The orientation of the director in nematic liquid crystals can be driven by an electric or a magnetic field or a crossed combination of both. The dynamic response of nematics to crossed fields has been studied experimentally by Faetti et al. [1] and others in an attempt to measure quantities such as the rotational viscosity coefficient. We investigate the director orientation of an incompressible nematic liquid crystal under the influence of tilted, mutually perpendicular, constant magnetic and electric fields. We assume that flow effects are negligible and employ an averaging method to derive an equation describing the dynamic response of the average molecular tilt angle. Travelling wave solutions are calculated and we discuss criteria for their stability. Finally, we investigate director response when both or either of the applied fields are turned off with a view to gaining information about the characteristic times of relaxation. These analytical characteristic times are shown to depend on the various material properties.

Keywords: crossed fields; nematics; relaxation times; travelling waves

INTRODUCTION

The response of nematics to crossed magnetic and electric fields has been studied experimentally by Faetti *et al.* [1] and others in an attempt to measure quantities such as the rotational viscosity coefficient. Both electric and magnetic fields are used for reasons pertaining to the experimental procedure; in particular, the dielectric and magnetic anisotropies can be measured in the same experiment. In these experiments the orientation of the director is driven by the two crossed fields. Stewart and Faulkner [2,3] studied a nematic which was assumed to have a twist wall in the

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y -direction when the crossed fields were the xz -plane (as in Fig. 1). Time-independent solutions in a semi-infinite sample and time-dependent solutions in an infinite sample were examined, where magnetic field was fixed but the angle between the fields was allowed to vary between 0 and $\pi/2$.

We consider an incompressible, homeotropic nematic liquid crystal under the influence of tilted, mutually perpendicular, constant magnetic and electric fields \mathbf{H} and \mathbf{E} . The sample is infinite in the xy -plane, but is constrained in the z -direction by two plates a distance d apart. The problem examined here is similar to that considered by Lam [4] with the addition of an electric field. However, here we assume that flow effects are negligible and employ a different method to derive soliton-like equations for the tilt angle. By fixing the angle between the fields at $\pi/2$, we ensure that the analysis closely mimics that for the single field case.

In our description we set

$$\mathbf{E} = E(\cos \epsilon, 0, \sin \epsilon), \quad \mathbf{H} = H(-\sin \epsilon, 0, \cos \epsilon),$$

where H is the magnitude of the magnetic field, E is the magnitude of the electric field and ϵ is the angle that the electric field makes with the x -axis (see Fig. 1). We may assume, using the symmetry of the system, that $\epsilon \in [-\pi/2, \pi/2]$. The average orientation of the molecules is represented by the director, \mathbf{n} , a unit vector which takes the form

$$\mathbf{n} = (\sin \theta, 0, \cos \theta), \quad \theta = \theta(y, z, t),$$

where θ is the molecular tilt angle with respect to the z -axis.

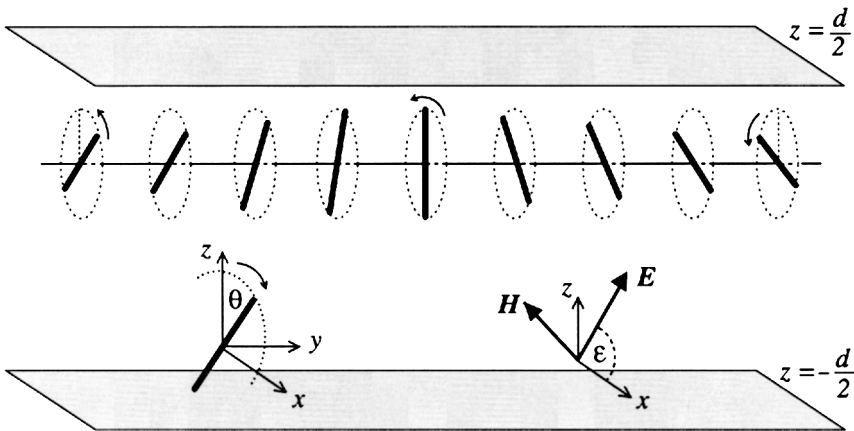


FIGURE 1 Schematic of the liquid crystal cell.

ERICKSEN-LESLIE EQUATIONS

Following the procedure detailed in Stewart and Faulkner [2], the Ericksen-Leslie equations [5] for nematic liquid crystals (in the absence of flow) reduce to

$$0 = K_2 \frac{\partial^2 \theta}{\partial y^2} + (K_1 \sin^2 \theta + K_3 \cos^2 \theta) \frac{\partial^2 \theta}{\partial z^2} + \frac{1}{2} (K_1 - K_3) (\sin 2\theta) \left(\frac{\partial \theta}{\partial z} \right)^2 + \delta^2 \sin 2(\theta + \epsilon) - \gamma_1 \frac{\partial \theta}{\partial t}, \quad (1)$$

where K_1, K_2 , and K_3 are the Frank elastic constants and γ_1 is the well-known (non-negative) twist viscosity coefficient. We have set $\delta^2 = (1/2)(\epsilon_a \epsilon_0 E^2 - \chi_a H^2)$, where the magnetic anisotropy, χ_a , and the dielectric anisotropy, ϵ_a , are assumed to be positive and the permittivity of free space is denoted by ϵ_0 . Parameter δ^2 is a measure of the relative strength of the two fields. In their study of nematics by microwave dielectrometry, Faetti *et al.* [1] overcome the drawbacks of fast switching of electric fields by assuming $E^2 \gg (\chi_a / \epsilon_a \epsilon_0) H^2$, i.e. $\delta^2 \gg 0$. We assume that δ^2 is positive. (The case where $\delta^2 = 0$ corresponds to the magnetic and electric fields “cancelling” each other out so that their net effect is negligible).

Employing the commonly used approximation $K_1 = K_3 = K$ in order to simplify the equations, we may rewrite (1) as

$$\gamma_1 \frac{\partial \theta}{\partial t} = K \frac{\partial^2 \theta}{\partial z^2} + K_2 \frac{\partial^2 \theta}{\partial y^2} + \delta^2 \sin 2(\theta + \epsilon). \quad (2)$$

Assuming strong homeotropic anchoring of the liquid crystal at the plates, we have the boundary conditions

$$\theta = 0 \quad \text{at } z = \pm \frac{d}{2}, \quad (3)$$

where d is the thickness of the cell. In order to satisfy (3) we employ the ansatz

$$\theta(y, z, t) = \theta_m(y, t) \cos \frac{\pi z}{d}. \quad (4)$$

After substituting (4) into (2), we derive

$$\gamma_1 \frac{\partial \theta_m}{\partial t} \cos \frac{\pi z}{d} = \left(K_2 \frac{\partial^2 \theta_m}{\partial y^2} - \frac{\pi^2 K}{d^2} \theta_m \right) \cos \frac{\pi z}{d} + \delta^2 \sin \left(2 \left(\epsilon + \theta_m \cos \frac{\pi z}{d} \right) \right). \quad (5)$$

AVERAGING

Equation (5) cannot be satisfied for all z , so there are two possible approaches to simplify the system. In Lam [4] only the central layer $z = 0$ is considered. However, since it is possible to integrate the last term of (5) exactly (see Gradshteyn and Ryzhik [6]), we average (5) over the thickness of the cell, integrating from $-d/2$ to $d/2$ with respect to z . This is a more general approach to the problem since it is possible that the behaviour of the cell at $z = 0$ does not accurately reflect the average response of the entire cell. The averaged form of (5) is

$$\gamma_1 \frac{\partial \theta_m}{\partial t} = K_2 \frac{\partial^2 \theta_m}{\partial y^2} - \frac{\pi^2 K}{d^2} \theta_m + \frac{\pi}{2} \delta^2 [\mathbf{H}_0(2\theta_m) \cos 2\epsilon + J_0(2\theta_m) \sin 2\epsilon], \quad (6)$$

where $\mathbf{H}_0(x)$ and $J_0(x)$ are the Struve [7] and Bessel functions of order zero, respectively.

In dimensionless form, (6) becomes

$$\frac{\partial \theta_m}{\partial T} = \frac{\partial^2 \theta_m}{\partial Y^2} - G(\theta_m), \quad (7)$$

where

$$G(\theta_m) = 2\beta\theta_m - \frac{\pi}{2} [\mathbf{H}_0(2\theta_m) \cos 2\epsilon + J_0(2\theta_m) \sin 2\epsilon], \quad (8)$$

and variables β, T and Y are defined via:

$$\beta = \frac{\pi^2 K}{2\delta^2 d^2} (>0), \quad T = \frac{\delta^2 t}{\gamma_1}, \quad Y = \frac{\delta y}{\sqrt{K_2}}.$$

Effectively we now have two parameters in our problem, field angle ϵ and β , a ratio of elastic and field effects.

CUBIC APPROXIMATION

In order to obtain solutions of (7) we introduce an approximation for $G(\theta_m)$. Adopting the approach of Lam [4], namely set $z = 0$ in (5) then expand the final term via a Taylor series, is restrictive as it assumes $|\theta_m + \epsilon| \ll 1$. Instead we introduce a cubic approximation for $G(\theta_m)$ (similar to Stewart and Faulkner [3]). This method makes no assumptions on the size of θ_m or ϵ .

In general, the equation

$$\frac{\partial \theta}{\partial T} = \frac{\partial^2 \theta}{\partial Y^2} - C(\theta), \quad (9)$$

where $C(\theta)$ is a polynomial of degree three, has soliton-like solutions only when $C(\theta)$ has at least two distinct real roots. When this is the case, we may write (9) in the form

$$\frac{\partial \theta}{\partial T} = \frac{\partial^2 \theta}{\partial Y^2} - (\theta - \theta_1)(\theta - \theta_2)(\theta - \theta_3), \quad (10)$$

where at most two of θ_1, θ_2 and θ_3 are equal, and we have rescaled to remove the coefficient of θ^3 . Travelling wave solutions of (10) are given in Stewart and Faulkner [2].

In order to apply this method to (7) we introduce a cubic approximation, $P(\theta_m)$, for the original function $G(\theta_m)$. We define $P(\theta_m)$ via

$$P(\theta_m) = A(\theta_m - \theta_1)(\theta_m - \theta_2)(\theta_m - \theta_3), \quad (11)$$

where A is a constant and θ_1, θ_2 , and θ_3 are the three real zeros of $G(\theta_m)$ which are closest to the origin. Since $G \rightarrow \pm\infty$ as $\theta_m \rightarrow \pm\infty$, $G(\theta_m)$ will always have an odd number of zeros, although these may not necessarily be distinct. If $G(\theta_m)$ has only one zero there will be no travelling wave solutions. Without loss of generality, we may take, as appropriate, either $\theta_1 \leq \theta_2 < \theta_3$ or $\theta_1 < \theta_2 \leq \theta_3$. Now for any constant A , $P(\theta_m)$ will share the same zeros as $G(\theta_m)$ in the closed interval bounded by θ_1 and θ_3 . The best fitting constant can be found by minimizing the integral

$$\int_{\theta_3}^{\theta_1} [G(\theta_m) - P(\theta_m)]^2 d\theta_m \quad (12)$$

over A .

We are interested only in the behaviour of $G(\theta_m)$ over the interval $[\theta_1, \theta_3]$, so the approximation of $G(\theta_m)$ by $P(\theta_m)$ will be an accurate one. The zeros of $G(\theta_m)$ cannot be found analytically, but can be obtained numerically for given values of ϵ and β . Thereafter the integral (12) can be calculated, and minimised to find the best fitting constant A . Figure 2 demonstrates the behaviour of both functions, $G(\theta_m)$ and $P(\theta_m)$, close to $\theta_m = 0$. Equation 7 can now be approximated by

$$\frac{\partial \theta_m}{\partial T} = \frac{\partial^2 \theta_m}{\partial Y^2} - P(\theta_m), \quad (13)$$

where $P(\theta_m)$ is given by (11) with A chosen to be the best fitting constant.

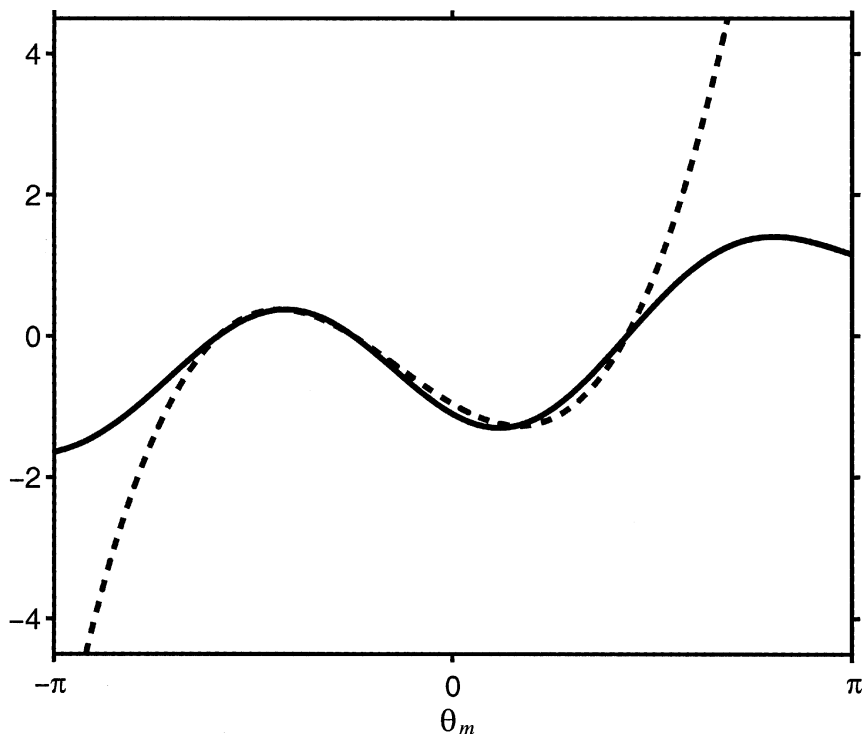


FIGURE 2 Comparison of $G(\theta_m)$ (—) and $P(\theta_m)$ (---), for $\epsilon = \pi/8$, $\beta = 0.2$.

It is possible to produce an approximate stability diagram for the soliton-like solutions as β and ϵ vary, but only if $G(\theta_m)$ is approximated by a cubic *Taylor series* polynomial which is not defined in terms of the zeros of $G(\theta_m)$. We cannot produce such a plot from the more accurate approximation, $P(\theta_m)$, since the zeros of $G(\theta_m)$ used to construct $P(\theta_m)$ are themselves dependent upon the parameters β and ϵ . Expanding $G(\theta_m)$ via a Taylor series, we derive (for small θ_m)

$$G(\theta_m) \approx \frac{8}{9}(\cos 2\epsilon)\theta_m^3 + \frac{\pi}{2}(\sin 2\epsilon)\theta_m^2 + 2(\beta - \cos 2\epsilon)\theta_m - \frac{\pi}{2}\sin 2\epsilon.$$

The cubic discriminant, Δ_G , of this approximation is found to be

$$\begin{aligned} \Delta_G(\epsilon, \beta) = & \left(\frac{3}{4}\beta \sec 2\epsilon - \frac{9}{256}\pi^2 \tan^2 2\epsilon - \frac{3}{4} \right)^3 \\ & + \left(\frac{9}{128}\pi \tan 2\epsilon + \frac{27}{128}\pi\beta \tan 2\epsilon \sec 2\epsilon - \frac{27}{4096}\pi^3 \tan^3 2\epsilon \right)^2. \end{aligned}$$

In Figure 3 the values of the parameters β and ϵ for which $\Delta_G = 0$ correspond to the situation where Taylor series has only two distinct real roots. For β and ϵ on the curve and to the left of it, soliton-like solutions exist. For values to the right of the curve, no travelling wave solutions can be found. However, this plot is valid only for small values of θ_m , and is intended only to give an indication of the influence β and ϵ have on the existence of soliton-like solutions. In particular we observe that for large β solutions will not exist unless angle ϵ is close to zero.

TRAVELLING WAVE SOLUTIONS

For convenience we first rescale (13) so that the constant A does not appear explicitly. By setting $\hat{\theta}_m = \sqrt{A}\theta_m$ and $\hat{\theta}_i = \sqrt{A}\theta_i$, where $i = 1, 2, 3$,

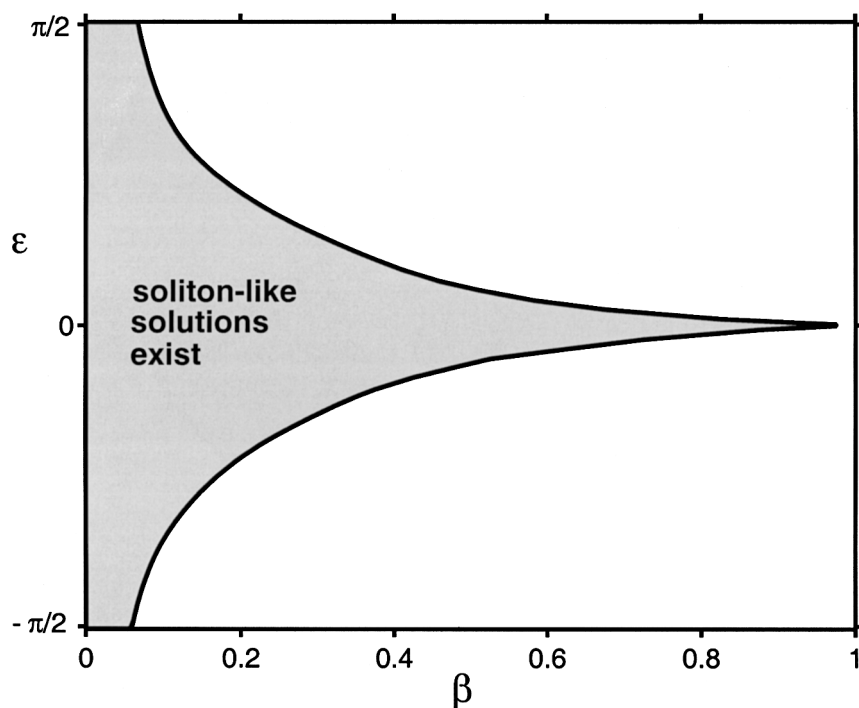


FIGURE 3 Region in (β, ϵ) space for which the Taylor series for $G(\theta_m)$ has at least three roots in the interval $(-\pi, \pi)$, and therefore a soliton-like solution of (7) exists.

we may rewrite (13) as

$$\frac{\partial \hat{\theta}_m}{\partial T} = \frac{\partial^2 \hat{\theta}_m}{\partial Y^2} - Q(\hat{\theta}_m), \quad (14)$$

with

$$Q(\hat{\theta}_m) = (\hat{\theta}_m - \hat{\theta}_1)(\hat{\theta}_m - \hat{\theta}_2)(\hat{\theta}_m - \hat{\theta}_3).$$

We now seek travelling wave solutions of (14) by introducing the variable

$$\xi = Y - cT + Y_0$$

where $c = c(\beta, \epsilon)$ is the wave speed and Y_0 is an arbitrary constant. Equation (14) may now be rewritten as

$$\frac{d^2 \hat{\theta}_m}{d\xi^2} = c \frac{d\hat{\theta}_m}{d\xi} = Q(\hat{\theta}_m). \quad (15)$$

Travelling wave solutions of (15) are of the form [2]:

$$\hat{\theta}_m = (\hat{\theta}_j - \hat{\theta}_i) \left\{ 1 + \exp \left[\frac{\alpha}{\sqrt{2}} (\hat{\theta}_j - \hat{\theta}_i) \xi \right] \right\}^{-1} + \hat{\theta}_i, \quad (16)$$

where $\alpha = \pm 1$ and is determined from the sign of the wave speed,

$$c = \frac{\alpha}{\sqrt{2}} (\hat{\theta}_j + \hat{\theta}_i - 2\hat{\theta}_k).$$

In the above, $i, j, k = 1, 2$ or 3 ; $\hat{\theta}_i \neq \hat{\theta}_j$; and $\hat{\theta}_k$ is the remaining zero of $Q(\hat{\theta}_m)$. Solution (16) corresponds to a wave travelling from $\hat{\theta}_j \rightarrow \hat{\theta}_i$ as $\xi \rightarrow \infty$.

MacKenzie and McKay [8] establish criteria for the stability of wavefront solutions (16) in terms of the wave speed and roots $\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3$. When $i = 2$, $j = 1$ and $k = 3$, $\alpha = +1$ and (in the terminology of Lam [4]) the solution is a type A wave. Type B waves correspond to the case in which $i = 2$, $j = 3$, $k = 1$, and $\alpha = -1$. Type C waves occur when $i = 3$, $j = 1$, $k = 2$, and $\alpha = +1$. To demonstrate, we have calculated $\hat{\theta}_1, \hat{\theta}_2$, and $\hat{\theta}_3$ when $\epsilon = \pi/8$ and $\beta = 0.2$. A type A wave is stable for these values [8] and its evolution is shown in Figure 4.

RELAXATION

We may now investigate the behaviour of system (6) when the applied fields are switched off, with a view to gaining information about the characteristic times for relaxation. Since the rescaled variables Y and T used

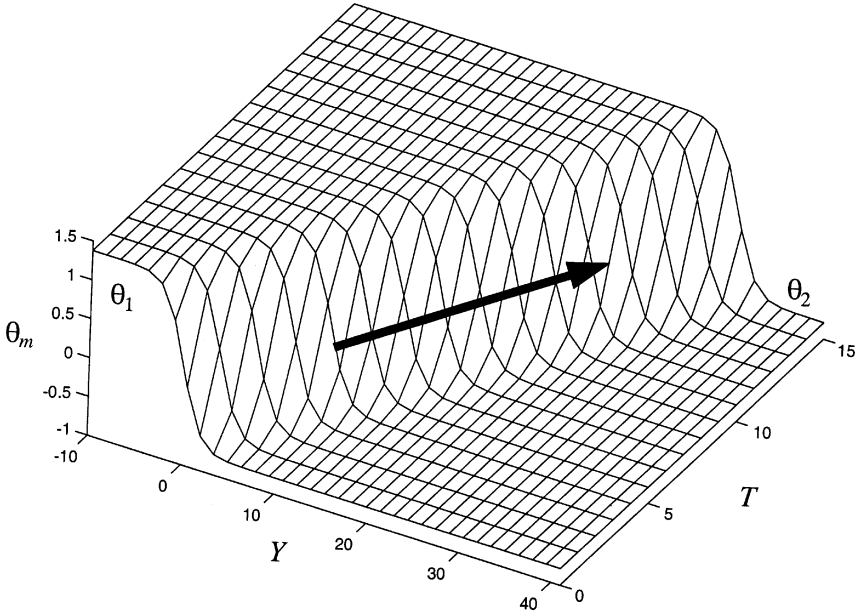


FIGURE 4 Plot of type A wave, for $\epsilon = \pi/8$, $\beta = 0.2$.

earlier depend upon the field parameter δ^2 , we now apply an alternative rescaling for (6). After setting $Y = y/\sqrt{K_2}$ and $T = t/\gamma_1$, we obtain a modified version of (6).

$$\frac{\partial \theta_m}{\partial T} = \frac{\partial^2 \theta_m}{\partial Y^2} - \mu \theta_m + \frac{\pi}{2} \delta^2 [\mathbf{H}_0(2\theta_m) \cos 2\epsilon + J_0(2\theta_m) \sin 2\epsilon], \quad (17)$$

where we define $\mu = \pi^2 K/d^2$.

We wish to calculate characteristic times for decay when the fields are switched off. Although our liquid crystal is infinite in the y -direction (and hence the Y -direction), we first assume that the sample is bounded, $Y \in [-L, L]$, for some constant $L(>0)$. For example, a type A wave travels from $\theta_1 \rightarrow \theta_2$ as $Y \rightarrow \infty$. For the finite system we assume that θ_1 and θ_2 are boundary conditions on the molecular tilt. This allows us to calculate an initial configuration prior to switching off the fields. Subsequently we can calculate characteristic times in terms of L . Decay times for the infinite sample are found by allowing $L \rightarrow \infty$.

In order to determine the configuration of the system immediately prior to switching off the fields, i.e. the initial profile for the relaxation problem,

we first derive an ‘equilibrium solution’, $\bar{\theta}_m(Y)$ of (17) for which $\partial\bar{\theta}_m/\partial T \equiv 0$. This solution therefore satisfies

$$\frac{d^2\bar{\theta}_m}{dY^2} - \mu\bar{\theta}_m + \frac{\pi}{2}\delta^2[H_0(2\bar{\theta}_m)\cos 2\epsilon + J_0(2\bar{\theta}_m)\sin 2\epsilon] = 0, \quad (18)$$

$$\bar{\theta}_m(-L) = \theta_1, \quad \bar{\theta}_m(L) = \theta_2,$$

where θ_1 and θ_2 are the roots of the function $G(\theta_m)$ defined in (8). These boundary conditions correspond to a stable type A wave. We could also examine cases involving type B or type C waves by changing the boundary conditions accordingly.

Given values for the parameters, (18) may be solved numerically. However the system does not possess a unique solution, as illustrated in Figure 5. Analysis of switching times when only one field is switched

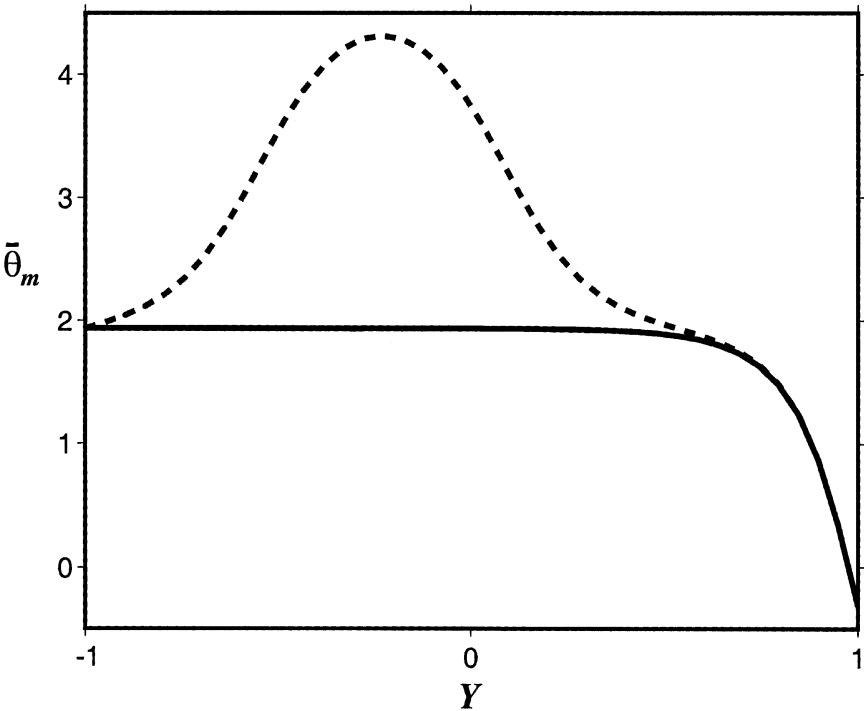


FIGURE 5 Equilibrium solutions of (18) for $\epsilon = 0.2$. Convex solution (—) is adopted in the relaxation analysis.

off [8] shows that the convex solutions give rise to longest decay time. In Figure 6 we concentrate on this type of profile for our initial condition. Furthermore, in Figure 5 and 6 we set the physical parameters as follows [9,10]: $K = 3 \times 10^{-7}$ dyne, $d = 2 \times 10^{-3}$ cm, $\chi_a = 1 \times 10^{-7}$, $H = 7.7 \times 10^3$ gauss and $\epsilon_a \epsilon_0 E^2 = 100$ (to ensure that $\epsilon_a \epsilon_0 E^2 \gg \chi_a H^2$). In addition, we have set $L = 1$.

Having found the initial profile $\bar{\theta}_m(Y)$, we may now ‘switch off’ the fields by setting $\delta^2 = 0$. System (17) becomes

$$\begin{aligned} \frac{\partial \theta_m}{\partial T} &= \frac{\partial^2 \theta_m}{\partial Y^2} - \mu \theta_m, \\ \theta_m(-L, T) &= \theta_1, \quad \theta_m(L, T) = \theta_2, \quad \theta_m(Y, 0) = \bar{\theta}_m(Y). \end{aligned} \quad (19)$$

Reducing the problem to one with homogeneous boundary conditions and employing separation of variables [8], we can obtain the full solution to (19),

$$\theta_m(Y, T) = u(Y, T) + \theta_e(Y),$$

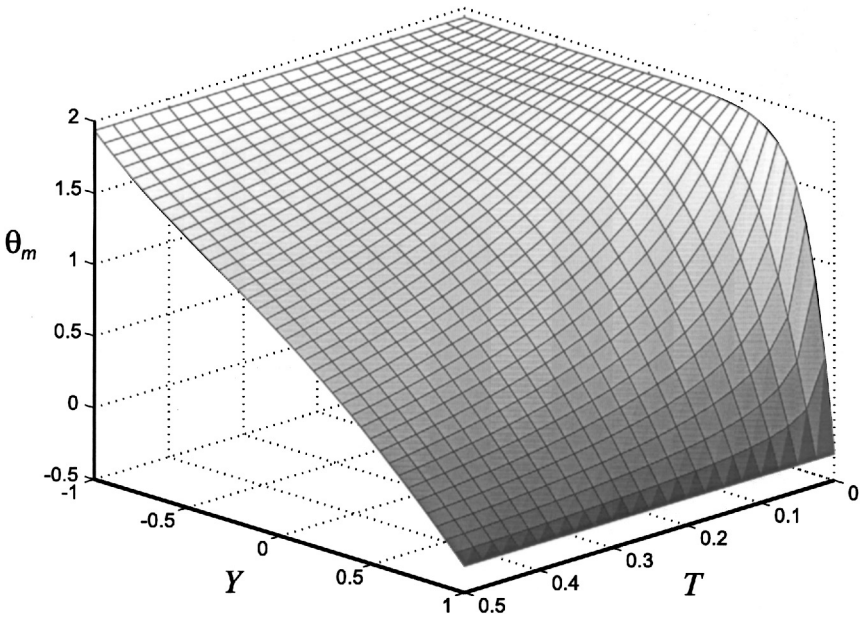


FIGURE 6 Relaxation of type A wave for $\epsilon = 0.2$. Characteristic time $\tau_1 \approx 0.31$ s for given material parameters.

where we have introduced

$$\begin{aligned}\theta_e(Y) &= \frac{(\theta_1 + \theta_2)}{2 \cosh(\sqrt{\mu}L)} \cosh(\sqrt{\mu}Y) + \frac{\theta_2 - \theta_1}{2 \sinh(\sqrt{\mu}L)} \sinh(\sqrt{\mu}Y), \\ u(Y, T) &= \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi(Y+L)}{2L}\right) \exp\left(-\left(\mu + \left(\frac{n\pi}{2L}\right)^2\right)T\right), \\ A_n &= \frac{1}{L} \int_{-L}^L [\bar{\theta}_m(Y) - \theta_e(Y)] \sin\left(\frac{n\pi(Y+L)}{2L}\right) dY.\end{aligned}\quad (20)$$

One acceptable measure for the characteristic time of relaxation, τ_n , is the reciprocal of the coefficient of t in (20),

$$\tau_n = \frac{\gamma_1}{\left(\mu + (n\pi/2L)^2\right)} = \frac{4\gamma_1 L^2 d^2}{\pi^2 (4L^2 K + n^2 d^2)}.$$

(Note: this is the reciprocal of the coefficient of t , not the rescaled variable T .) As the mode number n increases, τ_n decreases and so the first mode is the most influential one,

$$\tau_1 = \frac{4\gamma_1 L^2 d^2}{\pi^2 (4L^2 K + d^2)}. \quad (21)$$

By letting $L \rightarrow \infty$ in (21), we derive the characteristic relaxation time for the infinite region,

$$\tau_\infty = \frac{\gamma_1 d^2}{\pi^2 K}. \quad (22)$$

The relaxation of the molecular tilt is demonstrated in Figure 6, where we have restricted our solution to the first twenty terms in the series for $\theta_m(Y, T)$. MacKenzie and McKay [8] apply a more complicated analysis in order to calculate the relaxation times when only the electric field is switched off, as implemented experimentally in Faetti *et al* [1]. In this case it is found that the characteristic times depend on χ_a, H, ϵ and $\bar{\theta}_m$ in addition to the parameters which occur in (22).

SUMMARY

We have examined travelling waves in a nematic liquid crystal which is subject to tilted, mutually perpendicular magnetic and electric fields. Flow effects have been ignored and an averaging technique employed to remove

the z -dependence in the Ericksen-Leslie equations for our model without making assumptions on the size of the molecular tilt. The overall behavior of the system was found to be dependent upon two parameters, ϵ and β . In the case where θ_m is small, the effect of these parameters on the existence of soliton-like solutions can be determined from Figure 3.

We subsequently investigated relaxation of the system, solving the equation of motion corresponding to zero field strength. This was achieved using a numerical solution of the steady-state equation as the initial profile. The system eigenvalues provide information on the characteristic times of relaxation, which are found to depend upon the thickness of the cell in addition to the viscosity and elasticity of the liquid crystal. Any experimental testing of these predictions would be of great interest.

In addition to relaxation times when one or both fields are switched off, a similar analysis can be carried out for characteristic switch-on (reaction) times [8]. This can be further extended in order to examine the effects of fluid flow, e.g. kickback or backflow. However for the twist geometry examined here it is not anticipated that flow will have a significant influence on the effective rotational viscosity, especially when the field tilt angle is small.

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