Journal of Mathematical Analysis and Applications **255,** 391–403 (2001)
doi:10.1006/jmaa.2000.7129, available online at http://www.idealibrary.com on IDEAL®

On Instability of a Bend Fréedericksz Configuration in Nematic Liquid Crystals

D. Golovaty[1]

Department of Mathematics, The Pennsylvania State University, University Park, Pennsylvania 16802

L. K. Gross[2] and S. I. Hariharan[3]

Department of Mathematics and Computer Science, The University of Akron, Akron, Ohio 44325

and

E. C. Gartland, Jr.[4]

Department of Mathematics and Computer Science, Kent State University, Kent, Ohio 44242

Submitted by Maria Clara Nucci

Received April 8, 1999

In this paper we discuss the stability of a uniform Fréedericksz configuration in highly anisotropic thin nematic films. We show that the Fréedericksz transition in a bend geometry is at least two-dimensional, and it occurs at field strengths lower than the known classical threshold. © 2001 Academic Press

[1] E-mail: golovaty@math.psu.edu.
[2] E-mail: gross@math.uakron.edu; supported in part by the University of Akron Faculty Research Grant FRG 1400.
[3] E-mail: hari@math.uakron.edu; supported in part by the National Aeronautics and Space Administration Grant NCC-3-494.
[4] E-mail: gartland@mcs.kent.edu; supported in part by the National Science Foundation Grants DMR 89-20147 and DMS-9870420.

0022-247X/01 $35.00

1. INTRODUCTION

Liquid crystalline phases can be observed in substances consisting of molecules or groups of molecules that are anisotropic in shape. For example, a typical nematic liquid crystal (or, simply, nematic) consists of polarizable, rod-like molecules that tend to organize themselves in a parallel fashion, developing a local orientational order. The direction of molecular orientation can be influenced by external fields or by the presence of surfaces.

Let ω be a planar region occupied by a liquid crystal film of a thickness $2d$. Then the average orientation of the molecules near a point $\mathbf{x} \in \omega \times [-d, d]$ can be described by introducing a unit vector $\mathbf{n}(\mathbf{x})$, called the director. A continuum theory of nematic liquid crystals is based on the Oseen–Frank free energy functional $\mathscr{E}[\mathbf{n}]$ as introduced by Leslie [9] and Ericksen [4, 5]. In the presence of a (static) magnetic field,

$$\mathscr{E}[\mathbf{n}] := \tfrac{1}{2}\int_{\omega\times[-d,d]} \Big[K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + K_3|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 - \chi_a(\mathbf{H}_m\cdot\mathbf{n})^2 \Big]\, d\mathbf{x}, \qquad (1)$$

where $\mathbf{H}_m$ is the magnetic field, and K_1, K_2, and K_3 are the splay, twist, and bend elastic constants, respectively. The constant χ_a represents the anisotropy of the magnetic susceptibility and is taken to be positive for our system. The functional (1) can be written in a dimensionless form

$$\begin{aligned} E[\mathbf{n}] &:= \frac{2}{\pi^2}\int_{\Omega\times[-1,1]} e(\mathbf{x})\, d\mathbf{x} \\ &= \frac{2}{\pi^2}\int_{\Omega\times[-1,1]} \left[M(\operatorname{div}\mathbf{n})^2 + MN(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 - \left(\frac{\pi}{2}\right)^2 (\mathbf{H}\cdot\mathbf{n})^2 \right] d\mathbf{x}, \qquad (2) \end{aligned}$$

where $M = K_1/K_3$ and $N = K_2/K_1$, all lengths are in units of d, the field $\mathbf{H}$ is in units of $\pi\sqrt{K_3}/2d\sqrt{\chi_a}$, and the energy E is in units of $\pi^2 K_3 d/4$. Note also that the region Ω is ω rescaled by a factor of $\frac{1}{d}$.

Stable liquid crystal configurations are given by those configurations that minimize the bulk energy E subject to the constraint

$$|\mathbf{n}(\mathbf{x})| = 1, \qquad \mathbf{x} \in \Omega \times [-1, 1]. \tag{3}$$

If we define the class of admissible director fields C by imposing the appropriate boundary conditions and the constraint (3), then a stable director configuration $\mathbf{n}$ should satisfy

$$E[\mathbf{n}] = \inf_{\mathbf{m} \in C} E[\mathbf{m}]. \tag{4}$$

By placing further restrictions on the admissible class C (for example, by assuming $\mathbf{n}$ is independent of some of the spatial coordinates) and solving the Euler–Lagrange equations corresponding to (4), one may obtain candidates for minimizers of E. One of the complicating features of (2) is that the type of minimizing configuration depends on the strength of the applied magnetic field and the material characteristics of the liquid crystal. Moreover, in certain cases, the corresponding structural changes cannot be captured unless the admissible class C is extended to a wider class of functions $\hat{C}$.

Consider, for example, a sufficiently anisotropic nematic, subjected to a magnetic field. Liquid crystals of this type exhibit visible periodic spatial patterns, [8, 10], different from uniform director configurations, commonly observed in weakly anisotropic materials. Therefore, a minimizer of E over the set C of uniform configurations may have a higher energy than a minimizer of E over a larger set $\hat{C}$, containing periodic director configurations. As a consequence, the minimizer of E over C would be unstable under certain perturbations from $\hat{C}$. In the present paper, we investigate how stability issues determine configurational changes in nematics. Our analysis applies to materials with a bend geometry, i.e. the particular combination of anchoring (boundary) conditions and direction of applied magnetic field.

We consider a nematic film confined between two square plates (Fig. 1). Suppose that the film is subject to strong anchoring conditions on the plates so that

$$\mathbf{n}|_{\Omega \times \{-1, 1\}} = \mathbf{e}_1 \tag{5}$$

and that the magnetic field $\mathbf{H}$ is parallel to the z-axis. Here $\mathbf{e}_1$ is a unit vector in the direction of the x-axis which is perpendicular to the plates

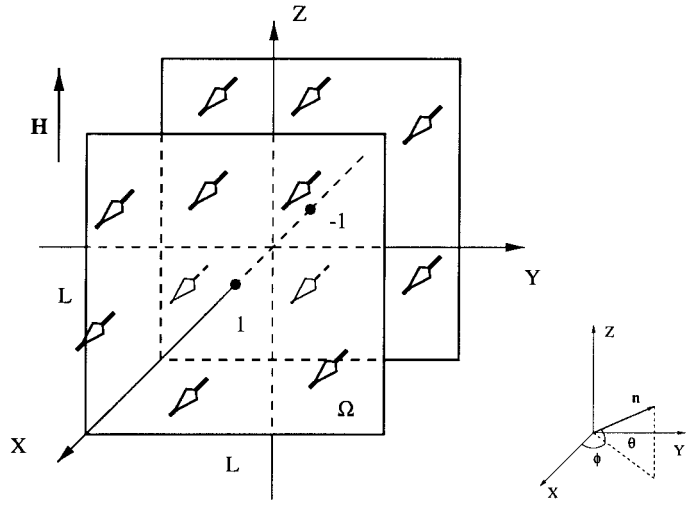


FIG. 1. Liquid crystal film confined between two plates with director field **n** perpendicular to the plates. The magnetic field **H** points in the z-direction.

and

$$\Omega := \{(y, z) \in \mathbf{R}^2 : -L/2 \le y \le L/2, -L/2 \le z \le L/2\},$$

where $L \gg 1$.

If the magnetic field is absent, then the director field is constant throughout the crystal; that is, $\mathbf{n}(\mathbf{x}) = \mathbf{e}_1$ for every $\mathbf{x} \in \Omega \times [-1, 1]$ since this configuration minimizes the energy (2) when $\mathbf{H} = \mathbf{0}$. In the presence of the field, however, the molecules inside the crystal will favor orientation in the direction of the field **H**, and the new minimizing configuration will arise through the competition between elastic inner forces and surface anchoring forces.

In the classical approach (see, for example, Virga [13]), it is customary to assume that the director field $\mathbf{n} = \langle n_1, n_2, n_3 \rangle$ is uniform in the y- and z-directions, while $n_2 \equiv 0$. Under these assumptions, (2) takes the form

$$E[\mathbf{n}] = \frac{1}{2}\int_{-1}^{1}\left[\left(\frac{2}{\pi}\right)^2 M n_{1x}^2 + \left(\frac{2}{\pi}\right)^2 n_{3x}^2 - h^2 n_3^2\right] dx, \qquad (6)$$

where $h = |\mathbf{H}|$. To analyze this functional, we need the following Poincaré's inequality [12]: *If ω is a strip of width a, then the inequality*

$$\int_\omega u^2\,dx \le \left(\frac{a}{\pi}\right)^2 \int_\omega |\operatorname{grad} u|^2\,dx \tag{7}$$

holds for every $u \in H^1(\omega)$ such that $u = 0$ on the sides of the strip.

Since the liquid crystal is included in the strip of width 2, while $n_3|_{x=\pm 1} = 0$, and the term involving n_1 in (6) is strictly positive, we conclude that

$$E[\mathbf{n}] \ge 0 \tag{8}$$

whenever $h < 1$. The equality in (8) can only hold when $n_3 \equiv 0$. Hence the initial configuration remains the unique global minimizer of the energy functional (6) for every $h < 1$, and the presence of the field has no effect on the crystal. In fact, $h = 1$ is a threshold in magnetic field strength, since for $h > 1$ the nontrivial minimizer with a negative energy can be obtained by solving the Euler–Lagrange equation associated with (6).

In the case of small M, however, the experiments [8] have shown that a different, nonuniform configuration, called the stripe phase, appears in a sufficiently strong magnetic field. In this configuration, the director field is still independent of the z-variable but is periodic in y.

A simple stability analysis shows the minimizer corresponding to the stripe phase cannot bifurcate off the trivial solution branch. This situation is in direct contrast with the splay Fréedericksz geometry, studied by Lonberg and Meyer [10], Cohen and Luskin [3], and others. The main difference between the two models is in the type of boundary conditions—the splay geometry is characterized by a parallel, rather than orthogonal, anchoring of the director to the plates. Although the stripe phase is observed in both cases, the stability analysis is significantly less complicated for the splay geometry, as the solution branch corresponding to the periodic configuration bifurcates from the trivial solution branch.

The stability of the uniform Fréedericksz solution for the bend geometry was studied numerically by Allender et al. in [2]. They established the existence of a new threshold value $\hat{h}$, slightly above the classical threshold $h = 1$, such that the periodic perturbations of the uniform solution have a lower energy whenever the magnetic field exceeds $\hat{h}$. Further numerical simulations were performed by Gartland et al. [7], Gartland [6], and Allender and Gartland [1] who showed that the stripe phase exists even for $h < 1$.

Here we present an analytical verification of the global instability of the trivial solution branch for $h < 1$ and M small, confirming the computational result of [6]. Our method does not require numerical calculations and is significantly simpler than the procedure in [2]. In particular, we show that it is sufficient to study the stability of solutions in the case when $h = 1$ and $M = 0$. Then the stability results can be extended to nonzero M and $h < 1$ by the continuity of (2) in M and h.

2. STABILITY ANALYSIS

The stripe phase can be observed when the elastic constants of the liquid crystal are sufficiently anisotropic, in particular, when M is small. As is noted above, we will assume throughout this section that $M = 0$. Although this assumption appears to be physically unreasonable, the corresponding analysis can be easily extended to $M > 0$ by using a simple continuity argument. Following [6] we set

$$\frac{\partial \mathbf{n}}{\partial z} = 0.$$

Then using (6) we obtain that

$$E[\mathbf{n}] = \frac{1}{2}\int_{-1}^{1}\left[\left(\frac{2}{\pi}\right)^2 n_{3x}^2 - h^2 n_3^2\right] dx.$$

The Euler–Lagrange equation corresponding to the functional E is

$$\left(\frac{2}{\pi}\right)^2 n_{3xx} + h^2 n_3 = 0, \tag{9}$$

where n_3 is subject to the boundary conditions

$$n_3|_{x=\pm 1} = 0. \tag{10}$$

Now let $h = 1$. The general solution of (9), (10) is given by

$$n_3(x) = \alpha \cos\left(\frac{\pi x}{2}\right), \tag{11}$$

where $\alpha \in [-1, 1]$. By Poincaré's inequality (7), the energy E corresponding to (11) is nonnegative for every α and is, in fact, equal to zero. Our goal is to show that there exist two-dimensional perturbations of the primary states (11) such that the energy of the perturbed director configuration is negative.

Assume for simplicity that $\alpha = 1$:

$$n_3(x) = \cos\left(\frac{\pi x}{2}\right). \tag{12}$$

To simplify some of our computations we introduce the spherical coordinates

$$n_1 = \cos\theta\cos\phi, \qquad n_2 = \cos\theta\sin\phi, \qquad n_3 = \sin\theta,$$

as shown on Fig. 1. Then we can express the solution (12) by

$$\theta(x) = \frac{\pi}{2}(1 - |x|), \qquad \phi = 0. \tag{13}$$

Next consider the perturbations of the primary state (13),

$$\theta(x, y) = \frac{\pi}{2}(1 - |x|) - \epsilon\Psi(x, y),$$
$$\phi(x, y) = \epsilon\Phi(x, y),$$

where ϵ is small. We shall require that Φ, Ψ, and their gradients be square integrable over the region $R = [-1, 1] \times [-L/2, L/2]$. In seeking a configuration with negative energy, we will assume that

- Both Φ and Ψ are periodic in y with a period $2l$ and $\frac{L}{2l} \in \mathbf{N}$.
- Within each period, the field Φ is odd with respect to both variables x and y.
- Within each period, the field Ψ is even with respect to both variables x and y.

The same properties of minimizers of (2) are suggested by numerical simulations (Fig. 2).

Under these assumptions, one can easily show that

$$E[\mathbf{n}] = \frac{L}{l}\int_0^1\int_0^l\left[\left(\frac{2}{\pi}\right)^2|\mathbf{n} \times \operatorname{curl}\mathbf{n}|^2 - n_3^2\right]dy\,dx,$$

and in the spherical representation

$$E[\mathbf{n}] = \frac{L}{l}\int_0^1\int_0^l(A^2\cos^2\theta + B^2\cos^4\theta - \sin^2\theta)\,dy\,dx, \tag{14}$$

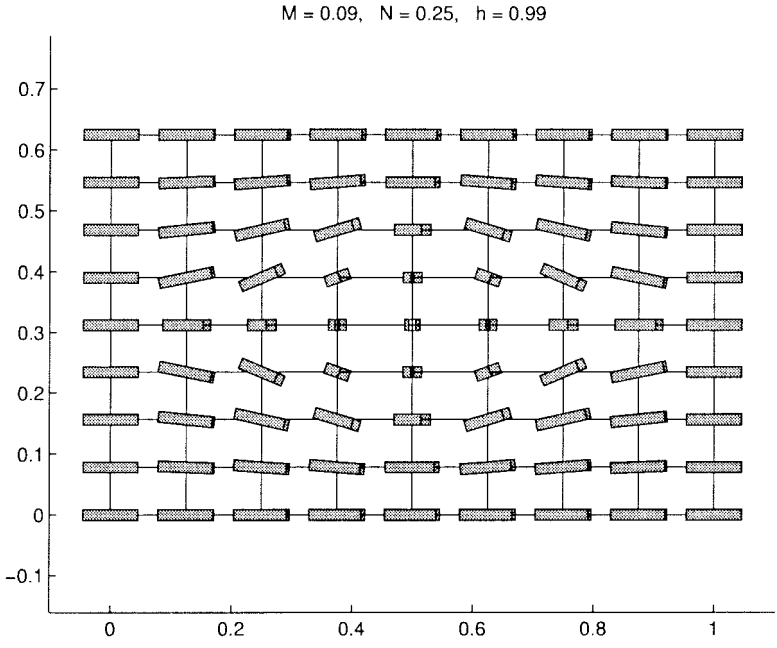


FIG. 2. A single period of the stripe phase as viewed from the direction of the magnetic field. The director field is periodic in the vertical direction and the glass plates bound the crystal from the right and from the left [6].

where

$$A = \frac{2}{\pi}\big(\theta_x \cos\phi + \theta_y \sin\phi\big),$$

$$B = \frac{2}{\pi}\big(\phi_x \cos\phi + \phi_y \sin\phi\big).$$

In addition, the symmetry of Φ and Ψ, along with (5), yields the boundary conditions

$$\Psi|_{x=1} = 0, \qquad \Phi|_{x=0,1} = \Phi|_{y=0,l} = 0. \tag{15}$$

Expanding (14) in powers of ϵ we obtain

$$E[\mathbf{n}] = \frac{L}{l}\int_0^1\int_0^l \big[e_0(x) + \epsilon e_1(x,y) + \epsilon^2 e_2(x,y)\big]\,dy\,dx + o(\epsilon^2), \tag{16}$$

where

$$
\begin{aligned}
e_0(x) &= \sin^2\left(\frac{\pi x}{2}\right) - \cos^2\left(\frac{\pi x}{2}\right),\\
e_1(x,y) &= \frac{4}{\pi}\left(\Psi(x,y)\sin^2\left(\frac{\pi x}{2}\right)\right)_x,\\
e_2(x,y) &= \frac{4}{\pi^2}\left\{\sin^2\left(\frac{\pi x}{2}\right)\left[\Psi_x^2(x,y) - \left(\frac{\pi}{2}\right)^2\Phi^2(x,y)\right.\right.\\
&\qquad \left.+\pi\Phi(x,y)\Psi_y(x,y)\right]\\
&\qquad\left. + \Phi_x^2(x,y)\sin^4\left(\frac{\pi x}{2}\right) + \frac{\pi}{2}\left(\Psi^2(x,y)\sin(\pi x)\right)_x\right\}.
\end{aligned}
\tag{17}
$$

By integrating $e_0(x)$ and $e_1(x,y)$ in (16) and using boundary conditions (15), the functional $E[\mathbf{n}]$ can be reduced to

$$
E[\mathbf{n}] = \frac{4L\epsilon^2}{\pi^2 l}\int_0^1\int_0^l\left[\left(\Psi_x^2 - \left(\frac{\pi}{2}\right)^2\Phi^2 + \pi\Phi\Psi_y\right)\sin^2\left(\frac{\pi x}{2}\right)\right.
$$
$$
\left. + \Phi_x^2\sin^4\left(\frac{\pi x}{2}\right)\right] dy\,dx + o(\epsilon^2). \tag{18}
$$

Suppose that

$$
\Phi(x,y) = \Phi_0\left(x,\frac{y}{l}\right), \qquad \Psi(x,y) = \Psi_0\left(x,\frac{y}{l}\right),
$$

and set $u = \frac{y}{l}$. Then (18) can be rewritten as

$$
E[\mathbf{n}] = \frac{4L\epsilon^2}{\pi^2}\int_0^1\int_0^1\left[\left(\Psi_{0x}^2 - \left(\frac{\pi}{2}\right)^2\Phi_0^2 + \frac{\pi}{l}\Phi_0\Psi_{0u}\right)\sin^2\left(\frac{\pi x}{2}\right)\right.
$$
$$
\left. + \Phi_{0x}^2\sin^4\left(\frac{\pi x}{2}\right)\right] du\,dx + o(\epsilon^2).
$$

This integral can be made negative if $\Phi_0(x,u) < 0$ and $\Psi_{0u}(x,u) > 0$ for every $(x,u) \in (0,1)\times(0,1)$ and if l is sufficiently small. For example,

$$
\begin{aligned}
\Phi_0(x,u) &= -\sin(\pi x)\sin(\pi u),\\
\Psi_0(x,u) &= -\frac{1}{2}(1+\cos(\pi x))\cos(\pi u).
\end{aligned}
\tag{19}
$$

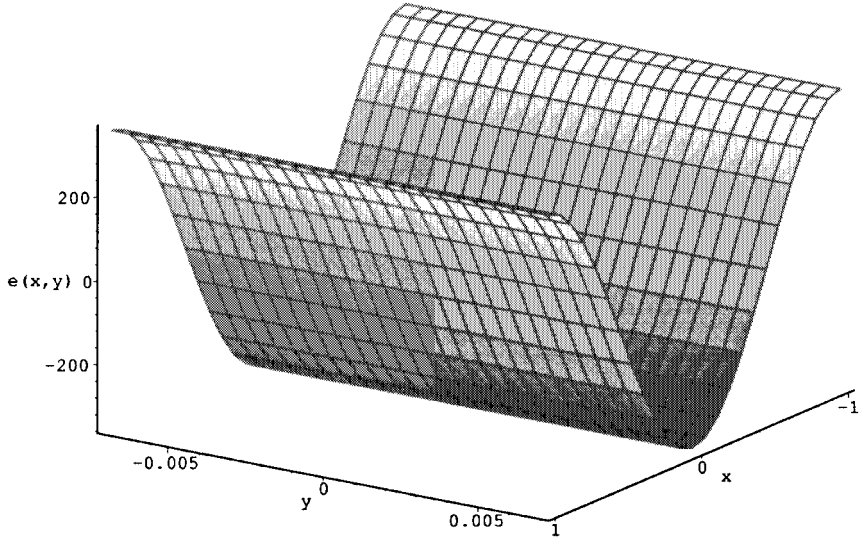
From this we conclude that when $M = 0$ and $h = 1$, the primary state (13) is unstable under two-dimensional perturbations, and there exist director configurations with negative energy. Further, since the functional (2) is linear with respect to both M and h, there exist $M > 0$, director field $\mathbf{n}$, and $h < 1$ such that $E[\mathbf{n}] < 0$. Under these conditions the trivial configuration is only metastable, since the energy of the solution $\theta(x, y) = \phi(x, y) \equiv 0$ is equal to zero. Therefore, for small M, the critical value of h is below the classical threshold value $h = 1$. In addition, the smallness of l is consistent with the numerical observations that indicate that the period of the stripes tends to zero as $M \to 0$.

To verify our conclusions we used particular perturbations of the director field (13) to compute the full energy $E[\mathbf{n}]$ in (2). Assuming that $\Phi_0(x, u)$ and $\Psi_0(x, u)$ are given by (19) and $\mathbf{n} = \langle n_1, n_2, n_3 \rangle$, we have that

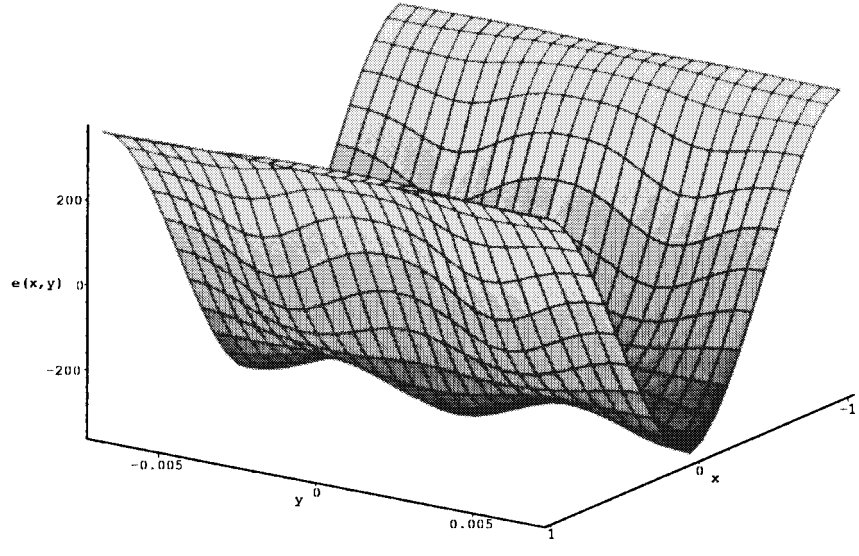
$$\begin{aligned} n_1(x, y) &= \cos\left(\frac{\pi}{2}(1 - |x|) - \epsilon\Psi_0\left(x, \frac{y}{l}\right)\right)\cos\left(\epsilon\Phi_0\left(x, \frac{y}{l}\right)\right), \\ n_2(x, y) &= \cos\left(\frac{\pi}{2}(1 - |x|) - \epsilon\Psi_0\left(x, \frac{y}{l}\right)\right)\sin\left(\epsilon\Phi_0\left(x, \frac{y}{l}\right)\right), \\ n_3(x, y) &= \sin\left(\frac{\pi}{2}(1 - |x|) - \epsilon\Psi_0\left(x, \frac{y}{l}\right)\right). \end{aligned} \tag{20}$$

The stripes were observed by Gooden et al. [8] in nematics when two elastic constants, K_2 and K_3, diverge, while the third, K_1, remains bounded as the temperature of the material approaches the temperature of the nematic-to-smectic-A transition. In accordance with the rates of convergence for K_1, K_2, and K_3 determined in [8], both M and MN are small, while N is large near the transition point. Hence we require that our choice of the dimensionless elastic constants conforms to convergence results of [8], but only qualitatively since the perturbation (20) might be quite far from the minimizing configuration. In particular, it is not unreasonable to set $M = 0.0001$ and $N = 10$.

Assuming in addition that $l = 0.007$, $\epsilon = 0.05$, and $h = 0.99$, we used a simple quadrature rule as well as the Maple computer algebra system [11] to evaluate $E[\mathbf{n}]$. In both cases we found that the energy is indeed negative with $E[\mathbf{n}] \approx -0.076$. In Maple, this result can be illustrated by comparing the graphs of the energy density $e(x, y)$ in (2), for the unperturbed (13), and perturbed (20) director configurations. The corresponding surfaces are shown on Fig. 3. Also, Fig. 4 demonstrates the distribution of the director within a single period of the director field (20). Although not a minimizer of the energy, this configuration resembles the periodic director field for a numerically obtained minimizer of (2), shown on Fig. 2.



(a)



(b)

FIG. 3. The energy density $e(x, y)$ for a single period of the stripe phase corresponding to (a) the Fréedericksz solution (13) and positive total energy, (b) the perturbation (20) of the Fréedericksz solution and negative total energy.

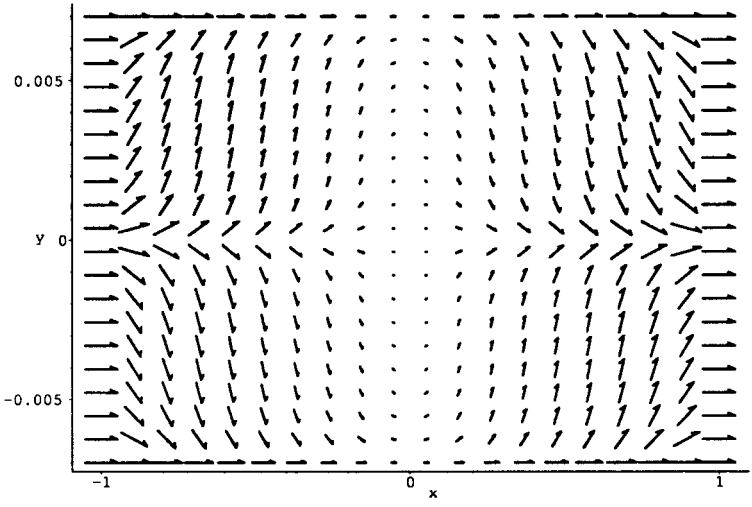


FIG. 4. A single period of a perturbation (20) of the Fréedericksz solution as viewed from the direction of the magnetic field.

Thus, in a bend geometry nematic, if the splay and twist elastic constants are sufficiently small compared to bend, there is a transition from the trivial to the periodic director configuration (or "stripe phase"). This transition occurs at a field strength below the classical threshold for the uniform Fréedericksz transition.

REFERENCES

1. D. W. Allender and E. C. Gartland Jr., Numerical modeling of the stripe phase in bend-Fréedericksz-geometry films, in preparation.
2. D. W. Allender, R. M. Hornreich, and D. L. Johnson, Theory of the stripe phase in bend-Fréedericksz-geometry nematic films, *Phys. Rev. Lett.* **59** (1987), 2654–2657.
3. R. Cohen and M. Luskin, Field induced instabilities in nematic liquid crystals, *in* "Nematics, Mathematical and Physical Aspects" (J.-M. Coron, J.-M. Ghidaglia, and F. Hélein, Eds.), pp. 261–278, Kluwer Academic, Dordrecht, 1991.
4. J. L. Ericksen, Conservation laws for liquid crystals, *Trans. Soc. Reol.* **5** (1961), 23–34.
5. J. L. Ericksen, Anisotropic fluids, *Arch. Rational Mech. Anal.* **4** (1960), 231–237.
6. E. C. Gartland Jr., "Structures and Structural Phase Transitions in Confined Liquid Crystal Systems," Technical report ICM-199511-03, Institute for Computational Mathematics, Department of Mathematics and Computer Science, Kent State University, 1995.
7. E. C. Gartland Jr., D. W. Allender, and R. M. Hornreich, Numerical simulation of the stripe phase in bend-Fréedericksz-geometry films, *in* "Technical Reports, ALCOM Symposium on Stabilized and Modified Liquid Crystals," Kent State University, Kent, OH, 1991, pp. 170–174.

8. C. Gooden, R. Mahmood, D. Brisbin, A. Baldwin, D. L. Johnson, and M. E. Neubert, Simultaneous magnetic deformation and light-scattering study of bend and twist elastic constant divergence at the neumatic-smectic-A phase transition, *Phys. Rev. Lett.* **54** (1985), 1035–1038.
9. F. M. Leslie, Some constitutive equations for liquid crystals, *Arch. Rational Mech. Anal.* **28** (1968), 265–283.
10. F. Lonberg and R. B. Meyer, New ground state for the splay-Fréedericksz transition in a polymer nematic liquid crystal, *Phys. Rev. Lett.* **55** (1985), 718–721.
11. Maple V, Release 4, Waterloo Maple Inc., Waterloo, Ontario, Canada, 1996.
12. L. Tartar, "Lecture Notes on PDE's," Carnegie–Mellon Univ., unpublished, 1990.
13. E. G. Virga, "Variational Theories for Liquid Crystals," Chapman & Hall, London, 1994.