Rendiconti di Matematica, Serie VII
Volume 14, Roma (1994), 291-307

Special solutions in a generalized theory of nematics

G. CAPRIZ – P. BISCARI

In memoria di Aldo Ghizzetti, maestro e guida di scienza e di vita

RIASSUNTO: *Usando un modello di cristallo liquido nematico che generalizza quello di Ericksen e permette stati biassiali, trattiamo due semplici problemi per una cella nematica tra due piani paralleli in condizioni di ancoraggio forte alla frontiera. Facciamo vedere che, mentre i modelli di Frank ed Ericksen conducono a prevedere una transizione del primo ordine tra due tipi di soluzione quando l'angolo di ancoraggio varia, la transizione è del secondo ordine nel nuovo modello, ancorché la soluzione di transizione sia ora del tipo a scaglione.*

ABSTRACT: *Using a model of a nematic liquid crystal which extends Ericksen's and allows for biaxiality, we solve two simple problems for a slab of a nematic with strong anchoring conditions on the boundary planes. We show that, as the anchoring angle changes, a first-order transition between two solution types would be predicted on the basis of the Frank's and Ericksen's models, whereas, when biaxiality is allowed, the transition predicted is second-order, but with a non-smooth transition mode of the chevron type.*

KEY WORDS AND PHRASES: *Nematic liquid crystals – Biaxiality – First and second order transition*

A.M.S. CLASSIFICATION: 76A15 (82D30)

This research was supported by the Gruppo Nazionale di Fisica Matematica and by the Istituto Nazionale di Alta Matematica "Francesco Severi".

1 – Introduction

In three recent papers [1 – 3] we have considered a model of a nematic liquid crystal, which allows for optic biaxiality. Briefly, the model arises as follows: the single molecule of the nematic is imagined as a thin stick with the direction of a unit vector $\mathbf{n}$: a 'material element' (in the macroscopic understanding of the term) is supposed to contain very many molecules. The macroscopic model should deal with fields (of directions in the present instance) with a value at point x which is in some sense the mesoscopic average, over the 'element around x', of the microscopic values on the molecules.

When, as in the present instance, the order parameter takes values on a manifold which is not a linear space, the most elementary way to secure averages is to seek first an embedding of the manifold (here of dimension 2) in a linear space of higher dimension (here of dimension 5). The existence of such an embedding is assured in general by Withney theorem; notice, however, that the embedding need not to be unique, and so may even appear to be an artificial, if convenient, tool. Nevertheless, in our case the following embedding seems very natural.

The direction of $\mathbf{n}$ is in one-to-one correspondence with the tensor $\mathbf{n}\otimes\mathbf{n}$, or with the tensor $\mathbf{N} := \mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}$ ($\mathbf{I}$, identity tensor) belonging to the algebraic manifold $\mathcal{N}$ of symmetric tensors with principal invariants having respectively the values 0, $-\frac{1}{3}$, and $\frac{2}{27}$. The latter tensor can be accepted as the value at each molecule in lieu of $\mathbf{n}$ and, as $\mathcal{N}$ is a subset of the linear space $\mathcal{S}ym_0$ with dimension 5 of the symmetric traceless tensors, averages can be taken in that space for each element x without hindrance and each average $\mathbf{Q}(x)$ will also belong to $\mathcal{S}ym_0$ although, of course, not necessarily to $\mathcal{N}$. Precisely, these values will belong to the convex hull $\mathcal{Q}$ of the set $\mathcal{N}$; second and third invariant of $\mathbf{Q}$ (or those of $\mathbf{M} := \mathbf{Q} + \frac{1}{3}\mathbf{I}$) give additional useful information on the distribution of $\mathbf{n}$ within the element and in particular on the possible emergence of optic biaxiality, though, as we have shown in [3], optic biaxiality does not correspond exactly to lack of rotational symmetry of the ellipsoid generated by the tensor $\mathbf{M}$. Thus, strictly, the adjectives uniaxial or triaxial are meant below with reference to properties of that ellipsoid, even when degenerate.

Because of the importance in our developments of the tensor $\mathbf{M}$ and also to fall in line with earlier notation, we refer often below to the manifold $\mathcal{M}$

$$\mathcal{M} := \left\{ \mathbf{M} \;\middle|\; \mathbf{M} = \mathbf{Q} + \frac{1}{3}\mathbf{I},\ \mathbf{Q} \in \mathcal{Q} \right\}. \tag{1.1}$$

In papers [1] and [2] we have considered situations which might be reproduced in careful experiments with nematic cells, so as to test the appropriateness of the model. But knowledge of other simple mathematical consequences might also contribute to its assessment. Some immediate corollaries, valid for homogeneous fields, were already drawn in [3]. Here we continue the exploration and imagine converse cases, where the effects of direction gradients prevail (i.e. the characteristic length associated to the internal potential is very large); we show that, within a significant class of problems, bend, splay, and twist in the field of principal directions inevitably entail triaxiality of $\mathbf{M}$.

2 – General remarks

We have introduced already elsewhere two parameters, convenient in the process of singling out a member $\mathbf{M}$ of $\mathcal{M}$: the degree of prolation s, and of triaxiality β:

$$\begin{aligned} s &:= \frac{1}{2}\left[\prod_{i=1}^{3}(3\lambda_i - 1)\right]^{1/3}, \\ \beta &:= \left[6\sqrt{3}\prod_{i=1}^{3}|\lambda_i - \lambda_{i+1}|\right]^{1/3}, \end{aligned} \tag{2.1}$$

where λ_i (i=1,2,3) are the eigenvalues of $\mathbf{M}$ and indices are modulo 3. Note that s and β are symmetric functions of the eigenvalues of $\mathbf{M}$, so that any internal potential for the nematic can be written in terms of them.

Any member of $\mathcal{M}$ is completely identified when s and β are assigned together with at most two orthogonal directions. When $\mathbf{M}$ is such that $\beta > 0$ (and thus the three eigenvalues are distinct), the directions need be exactly two: for instance, those of the eigenvectors associated respectively with the largest and the smallest eigenvalue of $\mathbf{M}$. When $\beta = 0$, but $s \neq 0$, the direction that needs be assigned is only one: when $s > 0$ ($s < 0$) it could be that of the eigenvector associated with the largest (smallest) eigenvalue. No preferred direction exists when β and s vanish together.

Thus $\mathcal{M}$ is the union of three disjoint manifolds $\mathcal{M}^{(i)}$ $(i = 1, 2, 3)$, the last one a singleton; their topological properties are of the essence to decide on the possible existence of defects, where the liquid crystal may 'melt' partially or totally.

We recall that, in general, whereas s may take any value in $[-\frac{1}{2}, 1]$ and β any value in $[0, 1]$, not all the couples (s, β) in the rectangle $[-\frac{1}{2}, 1] \times [0, 1]$ are accesible, but only those which satisfy the inequality

$$\beta^6 \leq \frac{16}{27} \left(s^3 - 1\right)^2 \left(8s^3 + 1\right). \tag{2.2}$$

For elements of $\mathcal{M}^{(1)}$, the value of β is greater than zero; for elements of $\mathcal{M}^{(2)}$, $\beta = 0$ but $s \neq 0$; for the singleton $\mathcal{M}^{(3)}$ both s and β vanish.

We leave a general study of $\mathcal{M}$ for a later paper but, to appreciate at least some relevant aspects of the matter, we consider in this paper the submanifold $\mathcal{C}_{\mathbf{c}}$ of tensors $\mathbf{M}$ for which one of the principal directions is assigned (as the direction of a unit vector $\mathbf{c}$). To describe a member of the class $\mathcal{C}_{\mathbf{c}}$, knowledge of the parameters s and β is insufficient, of course: $\mathcal{C}_{\mathbf{c}}$ itself is not orthogonally invariant.

In an orthogonal reference with the third axis parallel to $\mathbf{c}$, any member $\mathbf{M}$ of $\mathcal{C}_{\mathbf{c}}$ takes the form

$$\mathbf{M} = \begin{pmatrix} \alpha_1 & \alpha_2 & 0 \\ \alpha_2 & 1 - \alpha_1 - \lambda_c & 0 \\ 0 & 0 & \lambda_c \end{pmatrix}, \tag{2.3}$$

where λ_c is the eigenvalue which corresponds to the eigenvector $\mathbf{c}$, whereas α_1, α_2 are related with the other two eigenvalues λ_+, λ_- by

$$\lambda_\pm = \frac{1}{2}(1 - \lambda_c \pm \zeta), \tag{2.4}$$

where

$$\zeta := \left(4\alpha_2^2 + (\lambda_c - 1 + 2\alpha_1)^2\right)^{1/2}, \tag{2.5}$$

and to the parameters β and s by

$$\beta = \left[\frac{3\sqrt{3}}{2}\zeta \left|(3\lambda_c - 1)^2 - \zeta^2\right|\right]^{1/3}, \tag{2.6}$$
$$s = \frac{1}{2}\left[(3\lambda_c - 1)\left((3\lambda_c - 1)^2 - 9\zeta^2\right)\right]^{1/3}.$$

The angle ψ between the first reference axis and the eigenvector which corresponds to λ_+ satisfies the relations

$$\sin 2\psi = \frac{2\alpha_2}{\zeta}, \qquad \cos 2\psi = \frac{2\alpha_1 - 1 + \lambda_c}{\zeta}, \tag{2.7}$$

provided that $\zeta \neq 0$. 2ψ is thus determined mod 2π and ψ is determined mod π; this is exactly what is required from a physical point of view, because the orientation is irrelevant. When $\zeta = 0$, the eigenvalues λ_+ and λ_- coincide; the second principal direction is arbitrary among directions orthogonal to $\mathbf{c}$.

Each tensor $\mathbf{M}$ can be represented by a point in $\mathbb{R}^3$, using α_1, α_2, and λ_c as coordinates; then the image of $\mathcal{C}_{\mathbf{c}}$ is a full cone (see [1]). The vertex has coordinates (0,0,1); the base belongs to the plane $\lambda_c = 0$ and is a disk of radius $\frac{1}{2}$ and centre at the point $(\frac{1}{2}, 0, 0)$. For values of α_1, α_2, λ_c which are coordinates of points in the boundary of the cone, the ellipsoid connected with $\mathbf{M}$ reduces to an ellipse or, in the extreme, to a segment at the vertex. Uniaxial states belong to the lateral surface $\mathcal{S}$ of a double cone (with vertex in $(\frac{1}{3}, 0, \frac{1}{3})$), embellished with the axis of the cone. Another double cone, again with vertex in $(\frac{1}{3}, 0, \frac{1}{3})$ but smaller aperture, plus the disk at $\lambda_c = \frac{1}{3}$, separate points which represent prolate and oblate ellipsoids.

Frank's model considers only cases of perfect local ordering, when $\beta = 0$ and $s = 1$; then $\mathbf{M}$ either coincides trivially with $\mathbf{c} \otimes \mathbf{c}$ (the vertex of our cone) or with $\mathbf{d} \otimes \mathbf{d}$, where $\mathbf{d}$ is any unit vector orthogonal to $\mathbf{c}$ (and the corresponding states fall on the base circle of the cone).

3 – Fields with values within the class $\mathcal{C}_c$

For the density σ of the elastic energy of orientation, the simplest expression $K\|\Delta\mathbf{M}\|^2$ (K, a positive constant) will be accepted, although, within Frank's model, also the fuller expression with three constants will be considered:

$$\sigma = K_1(\operatorname{div}\mathbf{d})^2 + K_2(\mathbf{d}\cdot\operatorname{rot}\mathbf{d})^2 + K_3(\mathbf{d}\times\operatorname{rot}\mathbf{d})^2. \tag{3.1}$$

As announced in the introduction, terms not involving derivatives of $\mathbf{M}$ ($\overline{\sigma}$ in the notation of [3]) will be disregarded. We will be concerned with static fields of $\mathbf{M}$ with values in $\mathcal{C}_\mathbf{c}$ and depending on one space variable z only. The 'nematic cell' considered is a slab within which z takes values in the interval $[0,\delta]$ ($\delta > 0$).

As can be checked easily, the density of elastic energy reduces to

$$\sigma = \frac{K}{2}\left(3\lambda_c'^2 + \zeta'^2 + 4\zeta^2\psi'^2\right), \tag{3.2}$$

where a prime denotes derivation with respect to the space variable.

For the uniaxial model, when $\mathbf{d}$ is in the plane orthogonal to $\mathbf{c}$, there is a further simplification

$$\sigma_{\text{uni}} = 2K\left(\frac{1}{3}\,\zeta'^2 + \zeta^2\psi'^2\right) \tag{3.3}$$

and ζ coincides with Ericksen's degree of orientation.

For Frank's model, $\zeta^2 = 1$ and

$$\sigma_{\text{F}} = 2K\psi'^2 \tag{3.4}$$

or, more completely, with three constants, in Problem 1 (see below: bend and splay of the orientation field)

$$\sigma_{\text{F}1} = 2\left(K_1\cos^2\psi + K_3\sin^2\psi\right)\psi'^2 \tag{3.5}$$

and, in Problem 2 (twist),

$$\sigma_{\text{F}2} = 2K_2\psi'^2. \tag{3.6}$$

In all cases the solution is sought as the field that satisfies certain boundary conditions and minimizes the functional

$$\mathcal{F} := \int_0^\delta \sigma \, \mathrm{d}z, \tag{3.7}$$

which measures the energy stored in a cell of unit cross-section within the slab.

Strong anchoring conditions are presumed to prevail at the boundary. Also, to allow direct comparison of results obtained within different models (Frank's, uniaxial and fully biaxial), the anchoring will be assumed perfect, *i.e.*

$$\beta(0) = \beta(\delta) = 0; \qquad s(0) = s(\delta) = 1. \tag{3.8}$$

In the whole slab, ψ is measured from the direction of an axis of reference in the plates, say the x-axes, and is counted positive anticlockwise. On each plate, its absolute value is equal to $\overline{\psi}$. Thus, $\psi = \overline{\psi}$ (and, for convenience, $0 \leq \overline{\psi} \leq \frac{\pi}{2}$) at $z = 0$ and $\psi = -\overline{\psi}$ (mod π) at $z = \delta$.

More precisely, in Problem 1 the imposed direction at each plate is supposed to lie in the plane (x, z), while in Problem 2 the direction is supposed to be in the plane of the plate.

4 – Problem 1: splay and bend

We accept without direct proof that the boundary conditions imply the property that the minimizer of $\mathcal{F}$ belongs to the class $\mathcal{C}_{\mathbf{e_y}}$. From the anchoring conditions follows also that λ_c vanishes and $\zeta = 1$ for $z = 0$, $z = \delta$; finally, $\psi = \overline{\psi}$ for $z = 0$, whereas ψ must differ from $-\psi$ by a multiple of π for $z = \delta$: we will consider as relevant only the two choices $\psi = -\overline{\psi}$ or $\psi = \pi - \overline{\psi}$ (and recall that $\overline{\psi}$ falls in the interval $[0, \frac{\pi}{2}]$).

Problem 1a: Frank's model

λ_c and ζ are constant in the whole cell. From the expression (3.5) of the energy density the following Euler equation ensues

$$(K_1 \cos^2\psi + K_3 \sin^2\psi)\, \psi'' = (K_3 - K_1) \sin\psi \, \cos\psi \, \psi'^2. \tag{4.1}$$

This equation has two distinct solutions, depending on the condition that we impose on the upper plate (either $\psi = -\overline{\psi}$, or $\psi = \pi - \overline{\psi}$); they are:

$$
\begin{aligned}
\psi_s(z) &= \mathcal{E}\left(E(\overline{\psi},\xi)\left(1-\frac{2z}{\delta}\right)\ ,\ \xi\right),\\
\psi_b(z) &= \mathcal{E}\left(\frac{2z}{\delta}\,\mathrm{E}(\xi)+E(\overline{\psi},\xi)\left(1-\frac{2z}{\delta}\right)\ ,\ \xi\right).
\end{aligned}
\tag{4.2}
$$

Here

$$
\xi := \frac{K_3-K_1}{K_1},
\tag{4.3}
$$

whereas

$$
E(\vartheta,\xi) := \int_0^{\vartheta}\sqrt{1+\xi\ \sin^2\varphi}\,\mathrm{d}\varphi
\tag{4.4}
$$

is the elliptic integral of the second kind; $\mathrm{E}(\xi) := E(\frac{\pi}{2},\xi)$ is the complete elliptic integral of the second kind, and $\mathcal{E}(\varphi,\xi)$ is the inverse function of $E(\vartheta,\xi)$ with respect to its first argument.

The values of the energy relative to the two solutions are respectively

$$
\begin{aligned}
\mathcal{F}[\psi_s] &= \frac{8K_1}{\delta}\ E(\overline{\psi},\xi)^2, \qquad \text{and}\\
\mathcal{F}[\psi_b] &= \frac{8K_1}{\delta}\ \Big(\mathrm{E}(\xi)-E(\overline{\psi},\xi)\Big)^2.
\end{aligned}
\tag{4.5}
$$

Notice that both solutions exist for every value of $\overline{\psi} \in (0,\frac{\pi}{2})$, but the first one is the absolute minimizer if

$$
\overline{\psi} \le \overline{\psi}_{\mathrm{cr}}(\xi) := \mathcal{E}\left(\frac{\mathrm{E}(\xi)}{2},\xi\right),
\tag{4.6}
$$

whereas the second one is the minimizer for $\overline{\psi}$ above $\overline{\psi}_{\mathrm{cr}}(\xi)$. If $\overline{\psi} = \overline{\psi}_{\mathrm{cr}}(\xi)$ the two solutions are distinct but lead to the same energy. Thus, when $\overline{\psi}$ increases from 0 to $\frac{\pi}{2}$ a first order transtion is encountered from a splay-type to a bend-type solution.

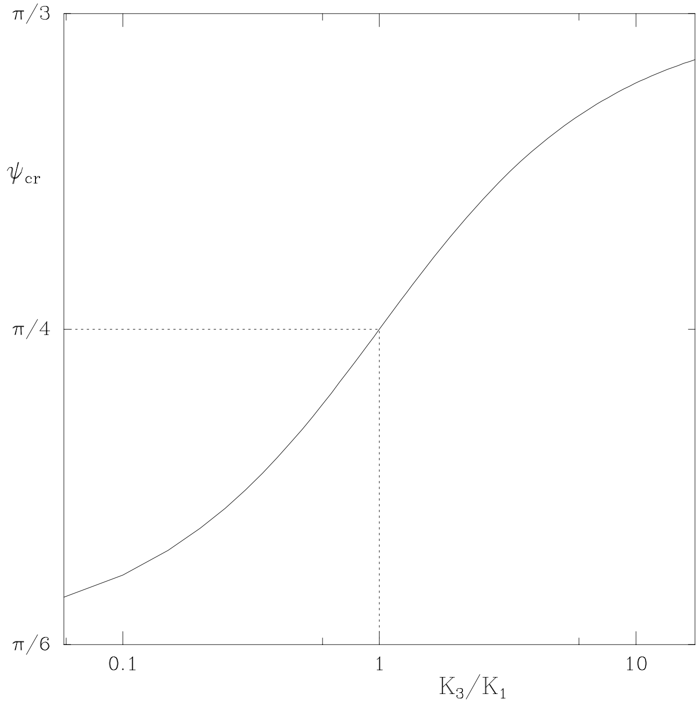

Figure 1

Figure 1 shows the dependence of $\overline{\psi}_{\rm cr}(\xi)$ on ξ: the values are always between $\frac{\pi}{6}$ and $\frac{\pi}{3}$; $\overline{\psi}_{\rm cr}$ becomes equal to $\frac{\pi}{4}$ when $K_1 = K_3 = K$.

Figures 2 and 3 show one field line of ψ_s and ψ_b respectively for each different choice of $\overline{\psi}$ when $K_1 = K_3$: the bold line represents the critical solution obtained for $\overline{\psi} = \frac{\pi}{4}$.

To allow an easy comparison of the results just obtained we note that, when $K_1 = K_3$, the energy associated with the solutions becomes simply

$$\mathcal{F}[\psi_s] = \frac{8K_1}{\delta}\,\overline{\psi}^2, \qquad \text{and}$$

(4.7)

$$\mathcal{F}[\psi_b] = \frac{8K_1}{\delta}\,\left(\frac{\pi}{2} - \overline{\psi}\right)^2.$$

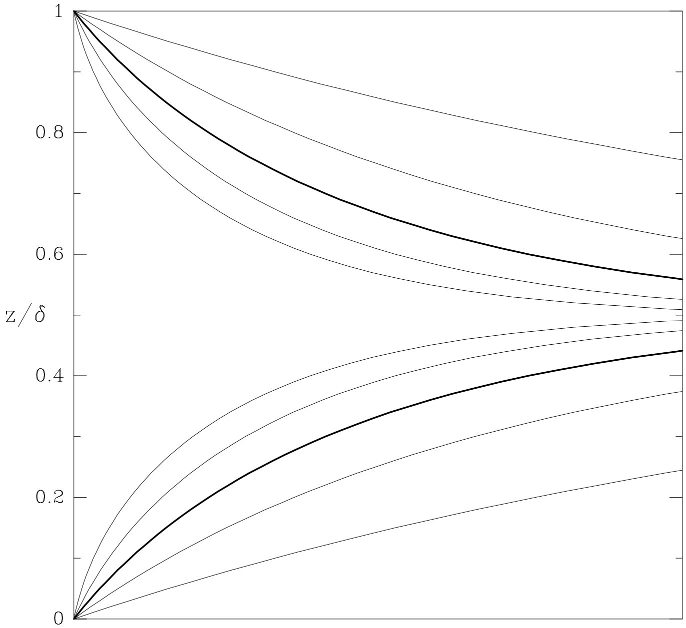

Figure 2

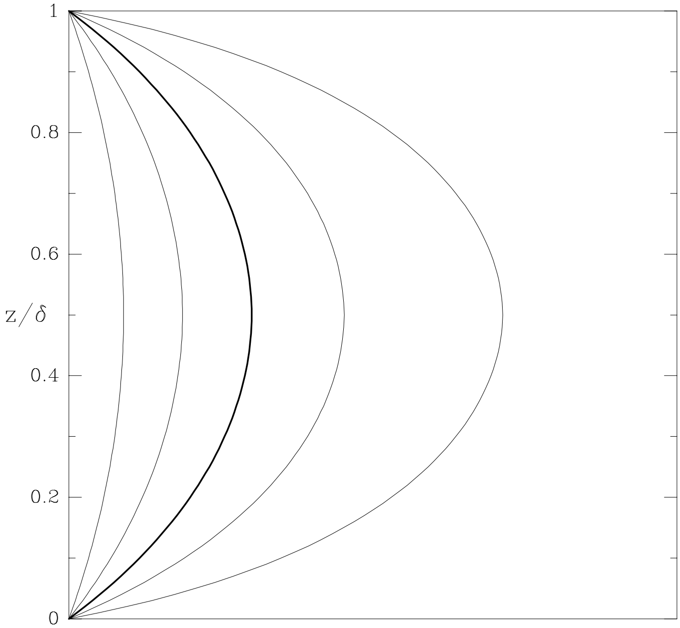

Figure 3

PROBLEM 1B: ERICKSEN'S MODEL

In the uniaxial case, the situation becomes slightly different: the Euler equations following from the choice (3.3) of the energy density can be integrated once and put in the form

$$\begin{cases} \zeta^2\psi' = \text{const.} \\ \dfrac{\zeta'^2}{3} + \zeta^2\,\psi'^2 = \text{const.} \end{cases} \tag{4.8}$$

There are still two solutions of these equations, but they do not both exist for every value of $\overline{\psi}$:

$$\begin{cases} \psi_s(z) = \dfrac{1}{\sqrt{3}}\operatorname{arctg}\left[\operatorname{tg}\left(\sqrt{3}\,\overline{\psi}\right)\left(1-\dfrac{2z}{\delta}\right)\right], \\ \zeta_s(z) = \sqrt{\cos^2\left(\sqrt{3}\,\overline{\psi}\right) + \sin^2\left(\sqrt{3}\,\overline{\psi}\right)\left(1-\dfrac{2z}{\delta}\right)^2}, \end{cases} \tag{4.9}$$

if $\overline{\psi} \in \left[0, \dfrac{\pi}{2\sqrt{3}}\right)$, and

$$\begin{cases} \psi_s(z) = \begin{cases} \overline{\psi} & \text{if } 0 \le z < \delta/2, \\ -\overline{\psi} & \text{if } \delta/2 < z \le \delta, \end{cases} \\ \zeta_s(z) = \left|1-\dfrac{2z}{\delta}\right|, \end{cases} \tag{4.10}$$

in the singular case $\overline{\psi} = \dfrac{\pi}{2\sqrt{3}}$, are the splay-type solutions;

$$\begin{cases} \psi_b(z) = \dfrac{\pi}{2} - \dfrac{1}{\sqrt{3}}\operatorname{arctg}\left[\operatorname{tg}\left(\sqrt{3}\left(\dfrac{\pi}{2}-\overline{\psi}\right)\right)\left(1-\dfrac{2z}{\delta}\right)\right], \\ \zeta_b(z) = \sqrt{\cos^2\left(\sqrt{3}\left(\dfrac{\pi}{2}-\overline{\psi}\right)\right) + \sin^2\left(\sqrt{3}\left(\dfrac{\pi}{2}-\overline{\psi}\right)\right)\left(1-\dfrac{2z}{\delta}\right)^2}, \end{cases} \tag{4.11}$$

if $\overline{\psi} \in \left(\dfrac{\pi}{2}\dfrac{\sqrt{3}-1}{\sqrt{3}}, \dfrac{\pi}{2}\right]$, and

$$\begin{cases} \psi_b(z) = \begin{cases} \overline{\psi} & \text{if } 0 \le z < \delta/2, \\ \pi-\overline{\psi} & \text{if } \delta/2 < z \le \delta, \end{cases} \\ \zeta_b(z) = \left|1-\dfrac{2z}{\delta}\right|, \end{cases} \tag{4.12}$$

in the singular case $\overline{\psi} = \frac{\pi}{2}\frac{\sqrt{3}-1}{\sqrt{3}}$, are the bend-type solutions.

The values of the energy are, respectively,

$$\mathcal{F}[\psi_s, \zeta_s] = \frac{8K}{3\delta}\sin^2\left(\sqrt{3}\,\overline{\psi}\right), \tag{4.13}$$

and

$$\mathcal{F}[\psi_b, \zeta_b] = \frac{8K}{3\delta}\sin^2\left(\sqrt{3}\left(\frac{\pi}{2}-\overline{\psi}\right)\right) : \tag{4.14}$$

both values are lower than the energies corresponding to Frank's solutions in the appropriate ranges.

The first solution is the absolute minimizer of $\overline{\psi} \in [0, \frac{\pi}{4}]$; it is a relative minimum if $\overline{\psi} \in (\frac{\pi}{4}, \frac{\pi}{2\sqrt{3}})$, becomes singular when $\overline{\psi} = \frac{\pi}{2\sqrt{3}}$ and does not exist for $\overline{\psi} > \frac{\pi}{2\sqrt{3}}$. Figure 4 illustrates some of the splay solutions obtained with different values of $\overline{\psi}$; the bold lines correspond to the critical value $\overline{\psi} = \frac{\pi}{4}$. The direction of the lines is determined by $\psi(z)$, while their lenght is proportional to $\zeta(z)$. Sets of lines at the left of the bold set correspond to absolute minimizers, while those at the right (obtained with greater vaules of $\overline{\psi}$) correspond to extremals.

The second solution is the absolute minimizer of $\overline{\psi} \in [\frac{\pi}{4}, \frac{\pi}{2}]$, a relative minimum if $\overline{\psi} \in (\frac{\pi}{2}\frac{\sqrt{3}-1}{\sqrt{3}}, \frac{\pi}{4})$; it is singular when $\overline{\psi} = \frac{\pi}{2}\frac{\sqrt{3}-1}{\sqrt{3}}$ and does not exist for $\overline{\psi} < \frac{\pi}{2}\frac{\sqrt{3}-1}{\sqrt{3}}$. Figure 5 shows some of the bend solutions obtained with different values of $\overline{\psi}$; the meaning of the set of bold lines, as well as the direction and the length of the lines are the same as in figure 4. Absolute minimizers are now at the right of the critical solution.

Note that, although singular relative minimizers exist, the absolute minimizer is always smooth. Furthermore, a first order transition from splay-type to bend-type minimizers occurs again.

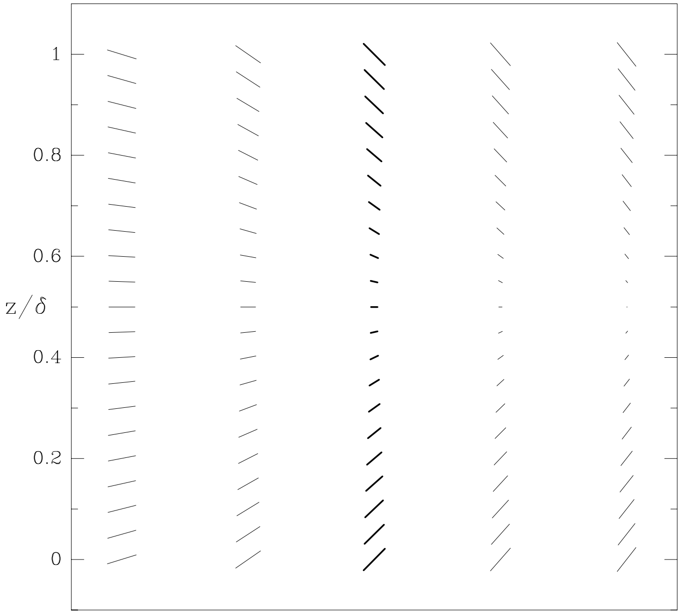

Figure 4

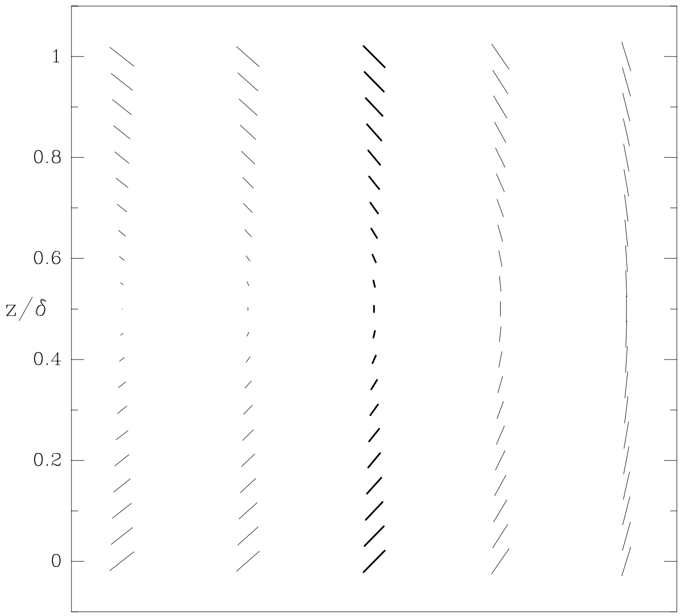

Figure 5

Problem 1c: Biaxial model

The Euler equations ensuing from the choice (3.2) of the energy density can be written:

$$\begin{cases} \lambda_c' = \text{const.} \\ 3\lambda_c'^2 + \zeta'^2 + 4\zeta^2\psi'^2 = \text{const.} \\ \zeta^2\psi' = \text{const.} \end{cases} \tag{4.15}$$

They can be integrated and admit only one solution for each choice of $\overline{\psi}$:

$$\begin{cases} \psi(z) = \dfrac{1}{2}\,\text{arctg}\left[\text{tg}\, 2\overline{\psi}\left(1 - \dfrac{2z}{\delta}\right)\right], \\[2ex] \zeta(z) = \sqrt{\cos^2 2\overline{\psi} + \sin^2 2\overline{\psi}\left(1 - \dfrac{2z}{\delta}\right)^2}, \\[2ex] \lambda_c(z) = 0, \end{cases} \tag{4.16}$$

if $\overline{\psi} \in \left[0, \dfrac{\pi}{4}\right)$;

$$\begin{cases} \psi(z) = \begin{cases} \overline{\psi} & \text{if } 0 \le z < \delta/2, \\ -\overline{\psi} & \text{if } \delta/2 < z \le \delta, \end{cases} \\[2ex] \zeta(z) = \left|1 - \dfrac{2z}{\delta}\right|, \\[2ex] \lambda_c = 0, \end{cases} \tag{4.17}$$

if $\overline{\psi} = \dfrac{\pi}{4}$; and

$$\begin{cases} \psi(z) = \dfrac{\pi}{2} - \dfrac{1}{2}\,\text{arctg}\left[\text{tg}\,(\pi - 2\overline{\psi})\left(1 - \dfrac{2z}{\delta}\right)\right], \\[2ex] \zeta(z) = \sqrt{\cos^2(\pi - 2\overline{\psi}) + \sin^2(\pi - 2\overline{\psi})\left(1 - \dfrac{2z}{\delta}\right)^2}, \\[2ex] \lambda_c(z) = 0, \end{cases} \tag{4.18}$$

if $\overline{\psi} \in \left(\dfrac{\pi}{4}, \dfrac{\pi}{2}\right]$.

The transition from one type of solution to the other is now continuous, and the absolute minimizer becomes singular when $\overline{\psi} = \dfrac{\pi}{4}$. Figure 6 shows the behaviour of the biaxial minimizers: when $\overline{\psi} = \dfrac{\pi}{4}$ a sudden jump in ψ happens at $z = \delta/2$, where ζ is zero.

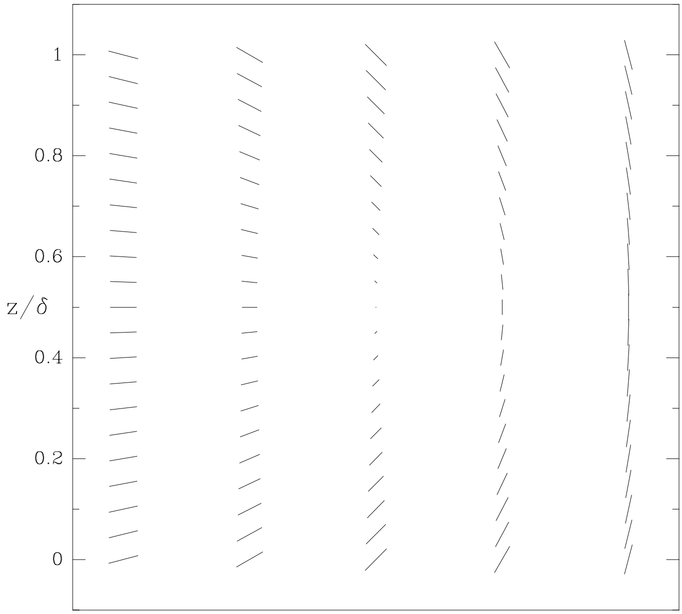

Figure 6

The values of the energy at these solutions are even lower:

$$\mathcal{F}[\psi,\zeta,\lambda_c] = \begin{cases} \dfrac{2K}{\delta}\ \sin^2 2\overline{\psi}, & \text{if } \overline{\psi} \in \left[0, \dfrac{\pi}{4}\right], \\[2ex] \dfrac{2K}{\delta}\ \sin^2\left(\pi - 2\overline{\psi}\right), & \text{if } \overline{\psi} \in \left[\dfrac{\pi}{4}, \dfrac{\pi}{2}\right]. \end{cases} \tag{4.19}$$

Thus, if biaxiality is allowed, it will prevail within the slab, except at the boundary (where uniaxiality is arbitrarily imposed), and at $z = \delta/2$ in the singular case $\overline{\psi} = \dfrac{\pi}{4}$, when the nematic 'melts' with an uniaxial defect in a biaxial field.

5 – Problem 2: twist

The preceding analytical results can be very easily reinterpreted to describe the biaxiality arising in a case of pure twist. It is only necessary to think of the class $\mathcal{C}_{\mathbf{e_z}}$ and of ψ as an angle in the (x, y)-plane. No other change is necessary and we leave to the reader to adapt the statements so that they apply to the new situation. Notice in particular that the transitions lead now from an anticlockwise to a clockwise twist.

6 – Conclusions

Within the Frank's or the uniaxial models two extremals exist; the one which is the absolute minimizer is always smooth; a first order transition occurs at a critical value of the angle imposed at the boundary.

Within the model that allows biaxiality the solution of the Euler equation is unique, gives $\mathcal{F}$ the minimum value and is smooth with one exception corresponding to the value $\dfrac{\pi}{4}$ of the angle $\overline{\psi}$ (when the solution is of chevron type and the jump in orientation from one plate to the other is exactly $\dfrac{\pi}{2}$), where a second order transition between the two solutions occurs.

These results are partially at variance with some obtained by Ambrosio and Virga in [5]. They have studied the functional

$$\mathcal{F}_k := \int_0^\delta \left(k\, \zeta'^2 + \zeta^2\, \psi'^2\right), \qquad k > 0, \tag{6.1}$$

which reduces to the one examined here in the uniaxial case if $k = \dfrac{1}{3}$. They have sought minimizers $\psi(z)$, as uniquely determined mod 2π (rather than mod π, as we have done here). This choice explains the differences in results, in particular as to the existence (excluded here) of singular minimizers.

REFERENCES

[1] P. Biscari – G. Capriz – E.G. Virga: *On Surface Biaxiality*, to appear in Liquid Crystals (1994).

[2] P. Biscari – G. Capriz – E.G. Virga: *Biaxial Nematic Liquid Crystals*, in "Boundary-Value Problems for Partial Differential Equations and Applications", ed. Masson (Paris), (1993), 331.

[3] P. Biscari – G. Capriz: *Optical and statistical anisotropy in nematics*, Rend. Mat. ed Appl. Acc. Lincei, **4**, 4 (1993), 307.

[4] J.L. Ericksen: *Liquid Crystals with Variable Degree of Orientation*, Arch. Rat. Mech. Anal., **113** (1991) 97.

[5] L. Ambrosio – E.G. Virga: *A Boundary-Value Problem for Nematic Liquid Crystals with a Variable Degree of Orientation*, Arch. Rat. Mech. Anal., **114** (1991) 335.

Lavoro pervenuto alla redazione il 29 gennaio 1994

Indirizzo degli Autori:

Paolo Biscari e Gianfranco Capriz – Dipartimento di Matematica Università di Pisa – Via Buonarroti, 2 – 56127 Pisa, Italy