AXIS-SYMMETRIC BOUNDARY-VALUE PROBLEMS FOR NEMATIC LIQUID CRYSTALS WITH VARIABLE DEGREE OF ORIENTATION

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AXIS-SYMMETRIC BOUNDARY-VALUE PROBLEMS FOR NEMATIC LIQUID CRYSTALS WITH VARIABLE DEGREE OF ORIENTATION

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Abstract. We employ a special class of orientations for the optical axis to minimize an energy functional for nematic liquid crystals whose degree of orientation varies in space. When the boundary data possess a certain symmetry with respect to an axis, we prove that the energy minimizers share that symmetry, and we establish a criterion to decide about uniqueness of minimizers within the class we employ here.

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1. Introduction. Liquid crystals are oriented materials whose microscopic state is described at a macroscopic scale by the *optical axis*. The regions in space where the optical axis suffers discontinuities are called *defects*. ERICKSEN [1] has recently proposed a new mathematical model to describe defects in liquid crystals. ERICKSEN's model differs from OSEEN and FRANK's classical model [2,3] in that it allows the *degree of orientation* of liquid crystals to vary in space.

The interpretation of both the optical axis and the degree of orientation in terms of microscopic parameters can be found in Section 2 of [1]. Here we regard both as macroscopic, phenomenological quantities.

We represent the optical axis by a unit vector $\mathbf{n}$ and the degree of orientation by a scalar s that ranges in the interval $[-1/2, 1]$. A liquid crystal becomes isotropic wherever s vanishes: there $\mathbf{n}$ cannot be defined.

Let $\mathcal{B}$ be the region in space occupied by a liquid crystal. The subset of $\mathcal{B}$ defined by

$$\mathcal{S}(s) := \{p \in \mathcal{B} | s(p) = 0\} \tag{1.1}$$

is called *singular set*, because there $\mathbf{n}$ may exhibit defects.

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In ERICKSEN's model the free energy of a nematic liquid crystal is a functional $\mathcal{F}$ that depends on both s and $\mathbf{n}$. A simple formula for $\mathcal{F}$ compatible with ERICKSEN's general formula is

$$\mathcal{F}[s,\mathbf{n}] := \kappa \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2 + \sigma_0(s)\} \ , \tag{1.2}$$

where κ and k are both positive constants and σ_0 is a given positive function (cf. Section 5 of [1]). The fields s and $\mathbf{n}$ in (1.2) are defined thus:

$$s : \mathcal{B} \rightarrow [-1/2, 1] \quad , \quad \mathbf{n} : \mathcal{B}\backslash\mathcal{S}(s) \rightarrow \mathbb{S}^2 \ ,$$

where $\mathbb{S}^2$ is the unit sphere of $\mathcal{V}$, the translation space of the three-dimensional space.

If $\mathcal{B}$ is an open bounded set with Lipschitzian boundary and if both s and $\mathbf{n}$ are prescribed on the whole of $\partial\mathcal{B}$ or on an open subset of $\partial\mathcal{B}$, say $\mathcal{D}$, $\mathcal{F}$ attains its minimum in the following class of admissible functions:

$$\mathcal{A} := \{(s,\mathbf{n})|s \in W^{1,2}(\mathcal{B};[-1/2,1])\,, \mathbf{u} \in W^{1,2}(\mathcal{B};\mathcal{V}), \mathbf{u} := s\mathbf{n}\} \ . \tag{1.3}$$

If the boundary data are prescribed on the whole of $\partial\mathcal{B}$, this result is proven in [4] (cf. also [5]); essentially the same arguments apply if the boundary data are prescribed only on $\mathcal{D}$. For all members of $\mathcal{A}$ we agree to set $\mathbf{u} = 0$ in $\mathcal{S}(s)$.

The regularity of the minimizers of $\mathcal{F}$ has been examined in [6] and [7]: in particular, we know that any pair that minimizes $\mathcal{F}$ is such that s is continuous on the whole of $\mathcal{B}$ and, if σ_0 is of class C^m with m an integer, both s and $\mathbf{n}$ are of class $C^{m,\alpha}$, for all $\alpha < 1$, away from the singular set $\mathcal{S}(s)$. Furthermore, reasoning as in Section 5 of [7], one sees that if $\mathcal{D}$ is a surface of class $C^{1,\gamma}$, with $\gamma > 0$, and if both s and $\mathbf{n}$ are prescribed on $\mathcal{D}$ as Lipschitzian functions, then for all minimizers of $\mathcal{F}$ both s and $\mathbf{u}$ are Hölder continuous in $\mathcal{B}$ up to $\mathcal{D}$. As to the singular set of a minimizing pair, another theorem of [7] (cf. Section 6) shows that its Hausdorff dimension is at most 2 for all $k \leq 1$, while it is at most 1 for all $k > 1$.

Also the uniqueness of the minimizers of $\mathcal{F}$ has been addressed in [7]. In particular, if $\sigma_0 = 0$ and $k \in]0,1[$, we know that there is only one pair $(s,\mathbf{n})$ that minimizes $\mathcal{F}$. If $k \geq 1$, this conclusion may in general be false.

Several boundary-value problems for $\mathcal{F}$ have been solved so far; a review can be found in [8]. In some of these problems both the region $\mathcal{B}$ and the data prescribed on its boundary are axis-symmetric (see [9], for example). Thus, the solution is assumed to share the same symmetry. Though this is quite natural, an explanation still wants. In this paper we get closer to such an explanation.

In Section 2 we introduce the class $\mathcal{R}$ of all fields $\mathbf{n}$ whose longitude on $\mathbb{S}^2$ can be defined as a smooth function on the whole of $\mathcal{B}\backslash\mathcal{S}(s)$, except where $\mathbf{n}$ is directed along the polar axis of $\mathcal{S}^2$. A subclass of $\mathcal{R}$ plays a special rôle in our work: its members have the same longitude on all planes through a given axis; we call $\mathcal{R}_0$ this class not *longitudinal* orientations its members. Assuming no special symmetry for $\mathcal{B}$, we show that when the boundary data for $\mathbf{n}$ are longitudinal, the minimum of $\mathcal{F}$ in $\mathcal{R}$ is the same as the minimum in $\mathcal{R}_0$, though the minimizers need not be all in $\mathcal{R}_0$. Furthermore, we give a criterion to decide whether all minimizers of $\mathcal{F}$ in $\mathcal{R}$ belong indeed to $\mathcal{R}_0$. Of course, when the minimizer of $\mathcal{F}$ happens to be unique in $\mathcal{R}_0$, and our criterion applies, we get uniqueness in the whole of $\mathcal{R}$.

In Section 3 we take $\mathcal{B}$ as a circular cylinder and we prescribe $\mathbf{n}$ on the lateral boundary of $\mathcal{B}$ so as to be constant on all the generatrices of $\mathcal{B}$ and symmetric about its axis. We also prescribe s on the lateral boundary of $\mathcal{B}$ as a positive constant. In [9] the minimizers of $\mathcal{F}$ subject to these conditions have been studied within the class $\mathcal{R}_0$ relative to the axis of $\mathcal{B}$. Here we prove that the variational problem studied in [9] has a unique minimizer in $\mathcal{R}$, *modulo* a reflection. We think that for this problem each minimizer of $\mathcal{F}$ belongs indeed to $\mathcal{R}$, and so there would be only one minimizer among all admissible orientations.

2. Longitudinal minimizers and uniqueness. Let $\mathcal{B}$ have Lipschitzian boundary and let $\mathcal{D}$, an open subset of $\partial\mathcal{B}$, be a connected surface of class $C^{1,\gamma}$, for some $\gamma > 0$. Let 0 be a point of the three-dimensional space. We call $\mathfrak{b}$ the axis through 0 in the direction of a given unit vector $\mathbf{e}_z$:

$$\mathfrak{b} := \{0 + z\mathbf{e}_z | z \in \mathbb{R}\} . \tag{2.1}$$

We call *longitudinal plane of* $\mathcal{B}$ each plane containing $\mathfrak{b}$ that intersects $\mathcal{B}$. The axis $\mathfrak{b}$ itself may or may not intersect $\mathcal{B}$. In either case we can represent $\mathcal{B}$ in the cylindrical co-ordinates (r, θ, z) whose axis is $\mathfrak{b}$. Away from $\mathfrak{b}$ we employ the local orthonormal frame $\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_z\}$, where $\mathbf{e}_r$ is the radial unit vector.

Let a pair $(s, \mathbf{n})$ be given in $C(\mathcal{B}; [-1/2, 1]) \times C^1(\mathcal{B}\backslash\mathcal{S}(s); \mathcal{S}^2)$. W define a closed subset of $\mathcal{B}$ by

$$\mathcal{B}_0 := \{p \in \mathcal{B}\backslash\mathcal{S}(s) | (\mathbf{n} \cdot \mathbf{e}_z)^2 = 1\} \cup \mathcal{S}(s) . \tag{2.2}$$

DEFINITION. We say that $\mathbf{n}$ belongs to the class $\mathcal{R}$ if there are two functions of class C^1 , $\alpha : \mathcal{B}\backslash(\mathcal{B}_0 \cup \mathfrak{b}) \to \mathbb{R}$ and $\beta : \mathcal{B}\backslash\mathcal{S}(s) \to [0, \pi]$, such that in $\mathcal{B}\backslash(\mathcal{B}_0 \cup \mathfrak{b})$ $\mathbf{n}$ can be represented by the following formula

$$\mathbf{n} = \sin\beta\cos\alpha\mathbf{e}_r + \sin\beta\cos\alpha\mathbf{e}_\theta + \cos\beta\mathbf{e}_z . \tag{2.3}$$

We say that $\mathbf{n}$ belongs to $\mathcal{R}_0$, if it belongs to $\mathcal{R}$ and $\alpha = 0$ in (2.3).

REMARK 1. Locally, each field $\mathbf{n}$ that minimizes $\mathcal{F}$ in $\mathcal{A}$ is represented by (2.3). Nevertheless, while β is well defined in the whole of $\mathcal{B}\backslash\mathcal{S}(s)$ for all smooth fields $\mathbf{n}$, this is not the case for α, whose determination need not be unique along all closed curves in $\mathcal{B}\backslash\mathcal{B}_0$, though it is well defined on all simply connected subset of $\mathcal{B}\backslash\mathcal{B}_0$.

We assume that $\mathcal{F}$ attains minimum in $\mathcal{R}$.

In our opinion this is not a severe assumption. We think that the existence of a minimizer of $\mathcal{F}$ in $\mathcal{R}$ is to be proved along the same lines of though pursued in [4]. Here, as is made plain by (2.6) below, $\sin\beta$ is to be treated the same way as s and $\mathcal{B}_0$ is to play the same rôle as $\mathcal{S}(s)$ in the existence theorem of [4]. In so doing, one should achieve a weak existence result in a suitable subclass of $\mathcal{A}$. Then, a regularity result for α, β, and s, away from $\mathcal{B}_0$, should be at hand. We think so since both α and β are locally determined in terms of $\mathbf{n}$, to within an additive constant.

THEOREM. *Let σ_0 be a function of class C^1. If both s and $\mathbf{n}$ are prescribed on $\mathcal{D}$ as Lipschitz continuous functions such that*

$$s|_{\mathcal{D}} \geq s_0 > 0\ ,\ \ \mathbf{n}\cdot\mathbf{e}_r|_{\mathcal{D}\backslash\mathfrak{b}} > 0\ ,\ \ \mathbf{n}\cdot\mathbf{e}_\theta|_{\mathcal{D}\backslash\mathfrak{b}} = 0\ , \tag{2.4}$$

then the minimum of $\mathcal{F}$ in $\mathcal{R}$ is the same as the minimum in $\mathcal{R}_0$. Furthermore, if the set $\mathcal{B}\backslash\mathcal{B}_0$ is connected for all minimizers of $\mathcal{F}$ in R_0, then there is no other minimizer of $\mathcal{F}$ in $\mathcal{R}$.

Proof. Let the pair $(s, \mathbf{n})$, with s a continuous function and $\mathbf{n}$ in $\mathcal{R}$, be a minimizer of $\mathcal{F}$. It follows from (2.3) that

$$\int\limits_{\mathcal{B}\backslash\mathcal{B}_0} s^2|\nabla\mathbf{n}|^2 = \int\limits_{\mathcal{B}\backslash\mathcal{B}_0} s^2\{\beta_r^2 + \sin^2\beta\alpha_r^2 + \frac{1}{r^2}(\beta_\theta^2 + \sin^2\beta(\alpha_\theta+1)^2) + \beta_z^2 + \sin^2\beta\alpha_z^2\}r\,dr\,d\theta\,dz =: \mathcal{G}[\alpha,\beta]\ , \tag{2.5}$$

where partial derivatives with respect to co-ordinates are denoted by subscripts. If the pair $(s, \mathbf{u})$ minimizes $\mathcal{F}$ subject to (2.4), then the pair (α, β) minimizes $\mathcal{G}$ subject to

$$\alpha|_{\mathcal{D}\backslash\mathfrak{b}} = 0 \tag{2.6}$$

and to the approximate boundary condition for β on $\mathcal{D}\backslash\mathfrak{b}$. In particular, the function $g : \mathsf{R}^+ \to \mathsf{R}^+$ defined by

$$g(\lambda) := \mathcal{G}[\lambda\alpha, \beta] \tag{2.7}$$

attains its minimum at $\lambda = 1$. It is easily seen that

$$g(\lambda) = a\lambda^2 + b\lambda + c\ , \tag{2.8}$$

where

$$(2.9) \qquad a := \int_{\mathcal{B}\setminus\mathcal{B}_0} s^2 \sin^2\beta |\nabla\alpha|^2 \ , \ b := 2 \int_{\mathcal{B}\setminus\mathcal{B}_0} \frac{s^2}{r^2} \sin^2\beta\alpha_\theta \ , \ c := \int_{\mathcal{B}\setminus\mathcal{B}_0} |\nabla\beta|^2 \ .$$

We show now that $g(1)$ is the minimum of g only if both a and b vanish. We see from $(2.9)_1$ that $a \geq 0$, and so $b \leq 0$, otherwise we would have $g(\lambda) < g(1)$ for all $\lambda \in [0,1[$. Were $a > 0$, the minimum of g would be $g\left(-\frac{b}{2a}\right)$; since

$$g\left(-\frac{b}{2a}\right) - g(1) = -\frac{(b+2a)^2}{4a^2} < 0 \ ,$$

we conclude that $a = 0$. Thus, g is a linear function, which attains minimum at $\lambda = 1$ only if it is constant. Likewise, α minimizes $\mathcal{G}$ only if it is constant in $\mathcal{B}\setminus\mathcal{B}_0$. Furthermore, the value of α does not affect the value of $\mathcal{G}$, and so the minimum of $\mathcal{F}$ in $\mathcal{R}$ is the same as in $\mathcal{R}_0$ where $\alpha \equiv 0$.

If a pair $(s, \mathbf{n}_0)$, with $\mathbf{n}_0 \in \mathcal{R}_0$, minimizes $\mathcal{F}$ and the set $\mathcal{B}\setminus\mathcal{B}_0$ corresponding to $\mathbf{n}_0$ is not connected, then infinitely many minimizers of $\mathcal{F}$ in $\mathcal{R}$ can be produced by merely rotating $\mathbf{n}_0$ about $\mathbf{e}_z$ in each component of $\mathcal{B}\setminus\mathcal{B}_0$ whose boundary does not include $\mathcal{D}$. If, on the contrary, the set $\mathcal{B}\setminus\mathcal{B}_0$ is connected for all minimizers of $\mathcal{F}$ in R_0, there is no other orientation of $\mathcal{R}$ with constant α that minimizes $\mathcal{F}$. □

The following Corollary is an immediate consequence of the Theorem.

COROLLARY. *If $\mathbf{n}_0$ is the only minimizer of $\mathcal{F}$ in $\mathcal{R}_0$ and the set $\mathcal{B}\setminus\mathcal{B}_0$ is connected, then $\mathbf{n}_0$ is the only minimizer of $\mathcal{F}$ in $\mathcal{R}$.*

REMARK 2. It is easily seen that the Theorem above holds also if $\mathbf{n}\cdot\mathbf{e}_r|_{\mathcal{D}\setminus\mathfrak{b}} < 0$, but if $\mathbf{n}\cdot\mathbf{e}_r$ has not the same sign on $\mathcal{D}\setminus\mathfrak{b}$, explicit counterexamples have been constructed in [10].

REMARK 3. At each point of $\mathcal{B}$ away from $\mathfrak{b}$ all fields of $\mathcal{R}_0$ lie in a longitudinal plane of $\mathcal{B}$. Thus, the Theorem tells us that $\mathcal{F}$ possess in $\mathcal{R}$ a *longitudinal minimizer*. Then, the uniqueness criterion established in the Corollary can be rephrased as follows: If there is only one longitudinal minimizer of $\mathcal{F}$ and for it $\mathcal{B}\setminus\mathcal{B}_0$ is connected, then the longitudinal minimizer of $\mathcal{F}$ is its unique minimizer in the whole of $\mathcal{R}$.

3. An example. In this section we apply the Theorem proved in Section 2 to the special case in which $\mathcal{B}$ is a circular cylinder:

$$(3.1) \qquad \mathcal{B} = \{0 + r\mathbf{e}_r + z\mathbf{e}_z | z \in]0, H[\ , \ r \in [0, R[, \ \vartheta \in [0, 2\pi[\} \ .$$

We denote by $\partial_R\mathcal{B}$ the lateral boundary of $\mathcal{B}$. Here, of course, $\mathfrak{b}$ intersects $\mathcal{B}$.

THEOREM. *Let σ_0 be of class C^1. If*

$$\mathbf{n}|_{\partial_R \mathcal{B}} = \cos\varphi_0 \mathbf{e}_r + \sin\varphi_0 \mathbf{e}_z \quad \text{and} \quad s|_{\partial_R \mathcal{B}} = s_0 \ , \tag{3.2}$$

where $\varphi_0 \in]-\frac{\pi}{2}, \frac{\pi}{2}[$ and $s_0 > 0$ are given constants, then all minimizers of $\mathcal{F}$ in $\mathcal{R}_0$ have the form

$$\mathbf{n} = \cos\varphi(r)\mathbf{e}_r + \sin\varphi(r)\mathbf{e}_z \tag{3.3}$$

and all minimizing s depend only on r.

Proof. Away from $\mathcal{S}(s) \cup \mathfrak{b}$ any field of $\mathcal{R}_0$ can be represented as follows

$$\mathbf{n} = \cos\varphi(r,\vartheta,z)\mathbf{e}_r + \sin\varphi(r,\vartheta,z)\mathbf{e}_z \ , \tag{3.4}$$

where φ is a function of class C^1 into $]-\frac{\pi}{2}, \frac{\pi}{2}[$. To prove (3.3) it remains to see that φ is indeed a function of r only. If $\mathbf{n}$ is as in (3.4), an easy computation shows that

$$\begin{aligned}\mathcal{F}[s,\mathbf{n}] = \kappa \int_0^{2\pi} d\theta \int_0^H dz \int_0^R dr\ r\Big\{ & k\left(s_r^2 + s_z^2 + \frac{s_\theta^2}{r^2}\right) + \\ & + s^2\left(\varphi_r^2 + \varphi_z^2 + \frac{\cos^2\varphi + \varphi_\theta^2}{r^2}\right) + \sigma_0(s)\Big\} \ .\end{aligned} \tag{3.5}$$

Thus,

$$\mathcal{F}[s,\mathbf{n}] \geq 2\pi H \kappa \inf_A F[t,\psi] \tag{3.6}$$

where

$$F[t,\psi] := \int_0^R dr\ r\left\{kt'^2 + t^2\left(\psi'^2 + \frac{\cos^2\psi}{r^2}\right) + \sigma_0(t)\right\} \tag{3.7}$$

and

$$A := \{(t,\psi) | t \in AC(0,R), \psi \in AC_{\text{loc}}(]0,R[\backslash S(t)) : t(R) = s_0, \psi(R) = \varphi_0\} \ . \tag{3.8}$$

In (3.7) a prime denotes differentiation with respect to r. In (3.8) the set $S(t)$ is defined as

$$S(t) := \{r \in [0,R] | t(r) = 0\} \ . \tag{3.9}$$

In (3.6) the equality holds if, and only if, both s and φ depend only on r and there is a pair $(t_0, \psi_0) \in A$ such that

$$F[t_0,\psi_0] = \inf_A F[t,\psi] \ . \tag{3.10}$$

Since the infimum of F is indeed attained in A, as one sees in Section 4 of [11], the proof of the Theorem is complete. □

REMARK 1. The problem of finding the longitudinal minimizers of $\mathcal{F}$ has been solved in [9] under the assumption that $\varphi_0 = 0$. Apart from the reflection that changes φ into $-\varphi$, there is only one longitudinal minimizer of $\mathcal{F}$ for all $k > 0$. Furthermore, $\mathcal{B}_0 = \mathcal{B} \cap \mathfrak{b}$ for all $k > 0$, and so the longitudinal minimizer is the only minimizer of $\mathcal{F}$ in $\mathcal{R}$, *modulo* a reflection.

REMARK 2. We conjecture that if $\mathcal{B}$ is axis-symmetric and both s and $\mathbf{n}$ are prescribed on the lateral boundary of $\mathcal{B}$ as in (3.2), then all orientations that minimize $\mathcal{F}$ belong to $\mathcal{R}$, and so the uniqueness criterion stated in Section 2 holds indeed among all admissible fields.

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