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A Boundary-Value Problem for Nematic Liquid Crystals with a Variable Degree of Orientation

LUIGI AMBROSIO & EPIFANIO G. VIRGA

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1. Introduction

In a recent paper [1] ERICKSEN proposed a theory for liquid crystals that aims to overcome the difficulties that arise within the classical theory of OSEEN, ZÖCHER, and FRANK when the orientation field exhibits defects other than isolated points. Though the new theory also generalizes the dynamical theory of LESLIE and ERICKSEN, in this paper we confine attention to statics.

In [1] ERICKSEN gives a mathematical formulation of an idea that in recent years has been variously expressed in the literature on defects. Roughly speaking, in the vicinity of a defect, the energy per unit volume becomes so large as to affect the degree of microscopic order which underlies the very definition of orientation. If the degree of microscopic order somehow enters into the energy density, the concentration of energy around the defects should "relax". One would expect the liquid crystal to undergo a phase transition that makes it an isotropic fluid just where the discontinuities of the orientation field occur. Thus defects should correspond to regions with the least degree of microscopic order.

In this paper we do not take over ERICKSEN's new theory in its full generality. Rather, we employ an energy functional that is consistent with ERICKSEN's (*cf.*, in particular, equation (7.3) of [1]), but is much simpler. Functionals of the same sort have been recently considered by HARDT [2] and LIN [3]. Following ERICKSEN, we represent the degree of microscopic order through a scalar-valued function, the *degree of orientation*, which vanishes where the fluid becomes isotropic.

In Section 2 we set up a variational problem in which both the orientation and the degree of orientation are prescribed on the boundary of the container filled with the liquid crystal. We deduce a qualitative feature of the solution from the general setting of the problem. Then we switch to a simpler version of the problem, which we can solve completely. Thus in Section 3 we assume that the container is bounded by two parallel plates and that the orientation lies everywhere in the same plane, which is generally not the plane of the plates. Both the orientation and the degree of orientation are taken as functions of the space variable orthogonal to the plates, which ranges in the interval $[0, l]$. We provide an exhaustive justification of these assumptions in the closing Section 9, where we show how a true three-dimensional problem reduces to the one-dimensional problem set up in Section 3.

In Section 4 we prove that minimizers of the one-dimensional variational problem exist in a class of functions smooth everywhere except in a subset of $[0, l]$, the *singular set*, where the degree of orientation vanishes. In Section 5 the analysis of the Euler equations leads us to conclude that the minimizers are actually far more regular than expected outside the singular set. Furthermore, we prove that the singular set must be either a singleton or the empty set (see Section 6). In the former case the orientation field actually possesses a plane of discontinuity. Two distinct solutions of the Euler equations correspond to the two possible singular sets: their energy is evaluated in Section 7. A bifurcation with exchange of stability arises for a critical value of the material modulus entering the energy functional. Since one minimizer is smooth while the other is not, we examine in Section 8 whether the *Lavrentiev phenomenon* can occur; we prove that it does not.

2. The variational problem

Let $\mathscr{B}$ be the region of the three-dimensional Euclidean space $\mathscr{E}$ occupied by a nematic liquid crystal. The orientation of the liquid crystal is the vector-valued function $n: \mathscr{B} \to \mathscr{S}^2$, where $\mathscr{S}^2$ is the unit sphere of $\mathscr{V}$, the translation space of $\mathscr{E}$. The degree of orientation is the scalar-valued function $s: \mathscr{B} \to]-\frac{1}{2}, 1[$ (*cf.* Section 2 of [1]). When $s = 0$ there is no microscopic order, that is, the molecules do not lie along any preferred direction: *defects* of n arise. Different values of s correspond to different degrees of microscopic order.

We take the following functional as the free energy of the liquid crystal:

$$\mathscr{F}[\mathscr{B}; s, n] := \int_{\mathscr{B}} (k\, |\nabla s|^2 + s^2\, |\nabla n|^2), \tag{2.1}$$

where k is a positive material modulus. ERICKSEN's energy is far more general than (2.1) (*cf.* Section 5 of [1]). In particular, it possesses a term which depends on s and $\mathscr{B}$ only:

$$\int_{\mathscr{B}} \psi(s). \tag{2.2}$$

We have omitted (2.2) for simplicity. The qualitative features of $\mathscr{F}$ are not greatly affected by it, as is shown in [4] by examples. Apart from this omission, when $k = 2$, equation (2.1) yields formula (3.12) of [3]. If we take s as constant, $\mathscr{F}$ reduces to the so-called "one-constant approximation" of FRANK's energy functional (see, *e.g.*, [5], p. 239).

For any mapping φ of a region $\mathscr{D} \subset \mathscr{E}$ into $\boldsymbol{R}$ we define the set

$$\mathscr{S}(\varphi) := \{p \in \mathscr{D} \mid \varphi(p) = 0\}. \tag{2.3}$$

The pairs (s, n) admissible for $\mathscr{F}$ belong to the class

$$\mathscr{C} := \{(s, n) \mid s : \mathscr{B} \to]-\tfrac{1}{2}, 1[,\ n : \mathscr{B} \to \mathscr{S}^2,\ s \in C^0(\overline{\mathscr{B}}) \cap C^1(\overline{\mathscr{B}} \setminus \mathscr{S}(s)),$$
$$n \in C^1(\overline{\mathscr{B}} \setminus \mathscr{S}(s))\}.$$

Problem. *Let the functions* $s_0 : \partial\mathscr{B} \to]-\tfrac{1}{2}, 1[$ *and* $n_0 : \partial\mathscr{B} \to \mathscr{S}^2$ *be given in the classes* $C^0(\partial\mathscr{B}) \cap C^1(\partial\mathscr{B} \setminus \mathscr{S}(s_0))$ *and* $C^1(\partial\mathscr{B} \setminus \mathscr{S}(s_0))$, *respectively. Find* $(s, n) \in \mathscr{C}$ *that minimizes* $\mathscr{F}[\mathscr{B}; \cdot, \cdot]$ *subject to*

$$s|_{\partial\mathscr{B}} = s_0, \qquad n|_{\partial\mathscr{B} \setminus \mathscr{S}(s_0)} = n_0.$$

We are not able to solve this problem, yet we know a qualitative property of its solutions.

Proposition 1. *Let the function* s_0 *be such that*

$$s_0(p) \geqq 0 \quad \text{for all } p \in \partial\mathscr{B}.$$

If $(s, n) \in \mathscr{C}$ *is a solution of the Problem, then*

$$s(p) \geqq 0 \quad \text{for all } p \in \mathscr{B}.$$

This proposition is easily proved by evaluating $\mathscr{F}[\mathscr{B}; \hat{s}, n]$, where

$$\hat{s}(p) := \begin{cases} s(p) & \text{if } s(p) \geqq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Essentially the same argument leads also to the following conclusion:

Proposition 2. *If* $s_0(p) \leqq 0$ *for all* $p \in \partial\mathscr{B}$, *then every solution* $(s, n) \in \mathscr{C}$ *of the Problem satisfies*

$$s(p) \leqq 0 \quad \text{for all } p \in \mathscr{B}.$$

Remark. The same assertions as in Propositions 1 and 2 also hold when the pairs of functions admissible for $\mathscr{F}$ are merely absolutely continuous. The proof relies essentially upon Lemma 7.6 of [6].

3. The one-dimensional problem

We take $\mathscr{B}$ as the set

$$\mathscr{B} := \{p \in \mathscr{E} \mid 0 < (p - O) \cdot e < l\},$$

where $O \in \mathscr{E}$ and $e \in \mathscr{S}^2$. Let e_1 and e_2 be orthogonal unit vectors. We assume that

$$n(p) = \cos\alpha(x)\, e_1 + \sin\alpha(x)\, e_2 \quad \text{for all } p \in \mathscr{B}, \tag{3.1}$$

where $x := (p - O) \cdot e$ and $\alpha :]0, l[\to]0, \pi[$. Furthermore, we assume that the function $s : \mathscr{B} \to]-\frac{1}{2}, 1[$ depends only on x, and we define the function $\sigma :]0, l[\to]-\frac{1}{2}, 1[$ through

$$\sigma(x) := s(p), \quad \text{where } x = (p - O) \cdot e. \tag{3.2}$$

Let $e_\perp, e^\perp \in \mathscr{S}^2$ both be orthogonal to e, and let $e_\perp \cdot e^\perp = 0$. Thus the energy of the cell

$$\mathscr{P} := \{p \in \mathscr{B} \mid 0 < (p - O) \cdot e_\perp < l_\perp, 0 < (p - O) \cdot e^\perp < l^\perp\}$$

is given by

$$\mathscr{F}[\mathscr{P}; s, n] = l_\perp l^\perp F[\sigma, \alpha],$$

where

$$F[\sigma, \alpha] := \int_0^l [k(\sigma')^2 + \sigma^2(\alpha')^2]. \tag{3.3}$$

Here a prime $'$ denotes differentiation with respect to x.

Assumptions (3.1) and (3.2) have been introduced with no justification other than their simplicity. However, we shall see in Section 9 that the minimizers of $\mathscr{F}[\mathscr{P}, \cdot, \cdot]$ in a suitable class of functions that depend on all the coordinates of p do indeed obey (3.1) and (3.2).

We assume that σ and α satisfy the boundary conditions

$$\sigma(0) = \sigma(l) = \sigma_0, \tag{3.4}$$

$$\alpha(0) = 0, \quad \alpha(l) = \alpha_0, \tag{3.5}$$

where $\sigma_0 > 0$ and $0 < \alpha_0 \leqq \pi$. We could easily consider boundary conditions less restrictive than (3.4), allowing, for example, different values of σ at $x = 0$ and $x = l$. Despite a slight gain in generality, the analysis would become clumsier without providing any new qualitative feature (*cf.* the Remark in Section 7 below).

In the next section we shall prove that there exist minimizers of F subject to (3.4) and (3.5). To open the way to this conclusion we now seek a suitable class of admissible pairs (σ, α) for F. The presence of $(\sigma')^2$ in (3.3) leads us to assume that σ belong to $AC(]0, l[,]-\frac{1}{2}, 1[)$, the class of all absolutely continuous functions of $]0, l[$ into $]-\frac{1}{2}, 1[$. Let $\sigma \in AC(]0, l[,]-\frac{1}{2}, 1[)$ be given. In accord with (2.3) we define

$$\mathscr{S}(\sigma) := \{x \in]0, l[\mid \sigma(x) = 0\}. \tag{3.6}$$

For any open set K that is relatively compact in $]0, l[\setminus \mathscr{S}(\sigma)$, *i.e.*, such that $\overline{K} \subset]0, l[\setminus \mathscr{S}(\sigma)$, we have

$$F[\sigma, \alpha] \geqq \inf_K \sigma^2 \int_K (\alpha')^2. \tag{3.7}$$

Thus we are led to assume that α belongs to $AC_{loc}(]0, l[\setminus \mathscr{S}(\sigma),]0, \pi[)$, the class of all locally absolutely continuous functions of $]0, l[\setminus \mathscr{S}(\sigma)$ into $]0, \pi[$. We define the class

$$A := \{(\sigma, \alpha) \in AC(]0, l[,]-\tfrac{1}{2}, 1[) \times AC_{loc}(]0, l[\setminus \mathscr{S}(\sigma),]0, \pi[)\}.$$

If $(\sigma, \alpha) \in A$, the function α need not even be continuous in $]0, l[$. In particular, F is not defined on the whole of A. We extend F to the whole of A by setting

$$\sigma^2(\alpha')^2 = 0 \quad \text{in } \mathscr{S}(\sigma). \tag{3.8}$$

We shall see in Section 8 that this assumption is indeed well justified.

It is easy to see that if $(\sigma, \alpha) \in A$ is such that $F[\sigma, \alpha] < \infty$ and $\sigma(0) = \sigma(l) = \sigma_0$, then α takes definite values at the endpoints of the interval $[0, l]$. Thus we may define the admissible class of F as follows:

$$\mathscr{A} := \{(\sigma, \alpha) \in A \mid F[\sigma, \alpha] < \infty, \quad (3.4) \text{ and } (3.5) \text{ hold}\}. \tag{3.9}$$

4. Existence of minimizers

In this section we prove that minimizers of F do exist in $\mathscr{A}$.

Lemma 1. *Let a sequence $\{(\sigma_h, \alpha_h)\}_{h\in N}$ of elements of $\mathscr{A}$ be such that $F[\sigma_h, \alpha_h] < C$ for all $h \in N$ and for some $C > 0$. Then there are a pair $(\sigma, \alpha) \in \mathscr{A}$ and a subsequence $\{(\sigma_{h_k}, \alpha_{h_k})\}_{k\in N}$ such that*

(i) $\sigma_{h_k} \to \sigma$ *uniformly in* $[0, l]$,

(ii) $\alpha_{h_k} \to \alpha$ *uniformly in every compact subset of* $[0, l] \setminus \mathscr{S}(\sigma)$.

Proof. To prove (i) it suffices to observe that

$$\sup_{h\in N} \int_0^l (\sigma_h')^2 < \infty$$

and then recall a classical theorem (*e.g.*, Theorem VIII.7 of [7]).

For any given open subset K of $]0, l[$ that is relatively compact in $[0, l] \setminus \mathscr{S}(\sigma)$ we have

$$\sup_{h\in N} \left(\inf_K \sigma_h^2 \int_K (\alpha_h')^2\right) < \infty \tag{4.1}$$

(*cf.* (3.7) above). Thus we may find an absolutely continuous function $\alpha^K : \overline{K} \to]0, \pi[$ such that a subsequence $\{\alpha_{h_k}\}_{k\in N}$ converges to α^K uniformly in $\overline{K}$. For all $j \in N \setminus \{0\}$ let $K_j := \{x \in [0, l] \mid \operatorname{dist}(x, \mathscr{S}(\sigma)) > 1/j\}$. We denote by $\{\alpha_h^{(j)}\}_{h\in N}$ the sequence converging uniformly in $\overline{K_j}$ to α^{K_j}. Letting $\{\alpha_h^{(j+1)}\}_{h\in N}$ agree in K_j with a subsequence of $\{\alpha_h^{(j)}\}_{h\in N}$ for all j, we easily see that $\{\alpha_h^{(h)}\}_{h\in N}$ converges uniformly to $\alpha \in AC_{\text{loc}}([0, l] \setminus \mathscr{S}(\sigma),]0, \pi[)$ in every compact subset of $]0, l[\setminus \mathscr{S}(\sigma)$. This completes the proof of the lemma. □

Lemma 2. *Let $\{(\sigma_h, \alpha_h)\}_{h\in N}$ be a sequence of elements of $\mathscr{A}$ and (σ, α) an element of $\mathscr{A}$ such that* (i) *and* (ii) *of Lemma 1 apply. Then*

$$F[\sigma, \alpha] \leq \liminf_{h\to\infty} F[\sigma_h, \alpha_h]. \tag{4.2}$$

Proof. Let an open subset K of $]0, l[$ that is relatively compact in $]0, l[\setminus \mathscr{S}(\sigma)$ be given. Since the sequence $\{\sigma_h\}_{h\in N}$ converges to σ uniformly in K, well-known theorems of semiconitnuity (*e.g.*, Theorem 4.1.1 of [8]) ensure that

$$\int_K [k(\sigma')^2 + \sigma^2(\alpha')^2] \leqq \liminf_{h\to\infty} \int_K [k(\sigma_h')^2 + \sigma^2(\alpha_h')^2]$$
$$\leqq \liminf_{h\to\infty} \int_K [k(\sigma_h')^2 + \sigma_h^2(\alpha_h')^2]$$
$$+ \limsup_{h\to\infty} \|\sigma^2 - \sigma_h^2\|_{L^\infty(K)} \int_K (\alpha_h')^2.$$

Since $\inf_K \sigma_h^2 \geqq C_K$, where C_K is a positive constant depending on K only, we get from (4.1) that

$$\sup_{h\in N}\left(\int_K (\alpha_h')^2\right) < \infty.$$

Thus

$$\int_K [k(\sigma')^2 + \sigma^2(\alpha')^2] \leqq \liminf_{h\to\infty} \int_K [k(\sigma_h')^2 + \sigma_h^2(\alpha_h')^2]$$
$$\leqq \liminf_{h\to\infty} \int_0^l [k(\sigma_h')^2 + \sigma_h^2(\alpha_h')^2].$$

Taking K closer and closer to $]0, l[\setminus \mathscr{S}(\sigma)$, we then arrive at (4.2) because $\sigma' = 0$ a.e. in $\mathscr{S}(\sigma)$ (*cf.* Lemma 7.7 of [6]). □

Combining Lemmata 1 and 2 we reach the following conclusion:

Theorem. *F attains a minimum in $\mathscr{A}$.*

5. Euler Equations

Let (σ, α) be a member of $\mathscr{A}$. For every $\hat{\sigma} \in C^1(]0, l[\setminus \mathscr{S}(\sigma))$ and for every $\hat{\alpha} \in C^1(]0, l[\setminus \mathscr{S}(\sigma))$ having compact support there is an $\varepsilon_0 > 0$ such that $(\sigma + \varepsilon\hat{\sigma}, \alpha + \varepsilon\hat{\alpha})$ also belongs to $\mathscr{A}$ for all $\varepsilon \in [0, \varepsilon_0]$. If (σ, α) is a minimizer of F in $\mathscr{A}$, then

$$\liminf_{\varepsilon\to 0} \frac{F[\sigma + \varepsilon\hat{\sigma}, \alpha + \varepsilon\hat{\alpha}] - F[\sigma, \alpha]}{|\varepsilon|} \geqq 0 \tag{5.1}$$

for all $\hat{\sigma} \in C_0^1(]0, l[\setminus \mathscr{S}(\sigma))$ and all $\hat{\alpha} \in C_0^1(]0, l[\setminus \mathscr{S}(\sigma))$. One easily sees that (5.1) is satisfied if and only if

$$\begin{aligned} (k\sigma')' &= \sigma(\alpha')^2 \\ (\sigma^2\alpha')' &= 0 \end{aligned} \quad \text{in }]0, l[\setminus \mathscr{S}(\sigma), \tag{5.2}$$

where a prime now denotes differentiation in the sense of distributions.

It follows from $(5.2)_2$ that the function $\sigma^2\alpha'$ is locally constant in $]0, l[\setminus \mathscr{S}(\sigma)$. This implies that $\alpha \in C^1(]0, l[\setminus \mathscr{S}(\sigma),]0, \pi[)$. Then, by $(5.2)_1$, we see that

$\sigma' \in C^1(]0, l[\setminus \mathcal{S}(\sigma))$. Hence $\sigma \in C^2(]0, l[\setminus \mathcal{S}(\sigma),]-\frac{1}{2}, 1[)$. By repeatedly applying this argument, we prove that every minimizer (σ, α) of F in $\mathcal{A}$ is such that $\sigma \in C^\infty(]0, l[\setminus \mathcal{S}(\sigma),]-\frac{1}{2}, 1[)$ and $\alpha \in C^\infty(]0, l[\setminus \mathcal{S}(\sigma),]0, \pi[)$. Thus (5.2) holds in the classical sense and

$$\min \{F[\sigma, \alpha] \mid (\sigma, \alpha) \in \mathcal{A}\} = \min \{F[\sigma, \alpha] \mid (\sigma, \alpha) \in \mathcal{A}^\infty\}, \tag{5.3}$$

where

$$\mathcal{A}^\infty := \{(\sigma, \alpha) \in \mathcal{A} \mid \sigma \in C^\infty(]0, l[\setminus \mathcal{S}(\sigma),]-\tfrac{1}{2}, 1[), \ \ \alpha \in C^\infty(]0, l[\setminus \mathcal{S}(\sigma),]0, \pi[)\}.$$

6. The singular set

So far we have learned nothing about the set $\mathcal{S}(\sigma)$ when (σ, α) minimizes F in $\mathcal{A}$. In this section we show that it must be either a singleton or the empty set.

Proposition 1. *If* $(\sigma, \alpha) \in \mathcal{A}$ *minimizes* F, *then* $\mathcal{S}(\sigma)$ *is connected.*

Proof. Since σ is continuous, $\mathcal{S}(\sigma)$ is a closed subset of $]0, l[$. Let $m_\sigma := \min \mathcal{S}(\sigma)$ and $M_\sigma := \max \mathcal{S}(\sigma)$. We suppose for contradiction that the set $\{x \in [m_\sigma, M_\sigma] \mid \sigma(x) \neq 0\}$ is not empty. We define the function $\tilde{\sigma} :]0, l[\to]-\frac{1}{2}, 1[$ as

$$\tilde{\sigma}(x) := \begin{cases} \sigma(x) & \text{if } x \in]0, l[\setminus [m_\sigma, M_\sigma], \\ 0 & \text{otherwise}. \end{cases} \tag{6.1}$$

An easy computation shows that

$$F[\sigma, \alpha] > F[\tilde{\sigma}, \alpha]. \tag{6.2}$$

Thus (σ, α) does not minimize F, which is a contradiction. □

Proposition 2. *If* $(\sigma, \alpha) \in \mathcal{A}$ *minimizes* F, *then* $\mathcal{S}(\sigma)$ *cannot be an interval.*

Proof. Let $\mathcal{S}(\sigma) = [m_\sigma, M_\sigma]$ with $m_\sigma < M_\sigma$. We define a piecewise linear function $\lambda: [0, l] \to [0, l]$ such that $\lambda^{-1}([m_\sigma, M_\sigma]) = [m'_\sigma, M'_\sigma]$ with $m'_\sigma > m_\sigma$ and $M'_\sigma < M_\sigma$. The first derivative of λ is the piecewise constant function defined by

$$\lambda'(x) := \begin{cases} \lambda_1 & \text{if } x \in [0, m'_\sigma[, \\ \lambda_2 & \text{if } x \in]m'_\sigma, M'_\sigma[, \\ \lambda_3 & \text{if } x \in]M'_\sigma, l]. \end{cases} \tag{6.3}$$

where $\lambda_1, \lambda_3 < 1$ and $\lambda_2 > 1$. It is plain that the pair $(\sigma \circ \lambda, \alpha \circ \lambda)$ belongs to $\mathcal{A}$ and that $\mathcal{S}(\sigma \circ \lambda) = [m'_\sigma, M'_\sigma]$. It is easily seen that

$$\begin{aligned} F[\sigma \circ \lambda, \alpha \circ \lambda] &= \lambda_1 \int_0^{m_\sigma} [k(\sigma')^2 + \sigma^2(\alpha')^2] \\ &\quad + \lambda_3 \int_{M_\sigma}^{l} [k(\sigma')^2 + \sigma^2(\alpha')^2] < F[\sigma, \alpha]. \end{aligned} \tag{6.4}$$

Thus (σ, α) is not a minimizer of F in $\mathscr{A}$, unless $m_\sigma = M_\sigma$. □

Corollary. *If* $(\sigma, \alpha) \in \mathscr{A}$ *minimizes* F *and if* $\mathscr{S}(\sigma) \neq \emptyset$, *then* $\mathscr{S}(\sigma) = \{x_0\}$ *with* $x_0 \in\,]0, l[$.

7. Minimizers

In this section we determine the minimizers of F in $\mathscr{A}$. We first seek pairs $(\sigma, \alpha) \in \mathscr{A}^\infty$ that satisfy equations (5.2) and are such that $\mathscr{S}(\sigma) = \emptyset$. It follows from $(5.2)_2$ that there is a constant c such that

$$\alpha' = \frac{c}{\sigma^2}. \tag{7.1}$$

By inserting (7.1) into $(5.2)_1$, we arrive at

$$k\sigma'' - \frac{c^2}{\sigma^3} = 0. \tag{7.2}$$

Hence σ is convex (*cf.* Proposition 1 of Section 2). Equation (7.2) implies that

$$k(\sigma')^2 = a - \frac{c^2}{\sigma^2}, \tag{7.3}$$

where a is a positive constant. It is easy to see that the only convex solution of (7.3) in $]0, l[$ that satisfies (3.4) is

$$\sigma(x) = \sqrt{\sigma_0^2 + \frac{a}{k}\, x(x - l)} \qquad \text{for all } x \in [0, l], \tag{7.4}$$

where we have set

$$c := \sqrt{a\left(\sigma_0^2 - \frac{al^2}{4k}\right)} \tag{7.5}$$

and a is constrained by

$$\sigma_0^2 - \frac{al^2}{4k} > 0. \tag{7.6}$$

Making use of (7.4) and (7.5) in (7.1), we get

$$\alpha(x) = \sqrt{k}\, \operatorname{arctg}\left(\frac{\sqrt{\frac{a}{k}}\left(x - \frac{l}{2}\right)}{\sqrt{\sigma_0^2 - \frac{al^2}{4k}}}\right) + b, \tag{7.7}$$

where b is an arbitrary constant. The constants a and b are determined by (3.5): A simple computation yields

$$b = \frac{\alpha_0}{2}, \tag{7.8}$$

$$\operatorname{arctg}\left(\frac{\sqrt{\frac{a}{k}}\,\frac{l}{2}}{\sqrt{\sigma_0^2 - \frac{al^2}{4k}}}\right) = \frac{\alpha_0}{2\sqrt{k}}. \tag{7.9}$$

There is precisely one solution of (7.9) satisfying (7.6), provided that

$$\sqrt{k} > \frac{\alpha_0}{\pi}. \tag{7.10}$$

If this is the case, then (7.1) and (7.3) imply that

$$\min\{F[\sigma,\alpha] \mid (\sigma,\alpha) \in \mathscr{A}\} = al, \tag{7.11}$$

whenever there is a minimizer of F such that $\mathscr{S}(\sigma) = \emptyset$, where a is the solution of (7.9). If (7.10) is not satisfied, then there is no minimizer of F in $\mathscr{A}$ such that $\mathscr{S}(\sigma) = \emptyset$.

We now seek minimizers of F in $\mathscr{A}^\infty$ such that $\mathscr{S}(\sigma) = \{x_0\}$ with $x_0 \in \,]0, l[$. Let σ be given with $\sigma(x_0) = 0$. The function α that minimizes $\int_0^l \sigma^2(\alpha')^2$ is constant in both the intervals $[0, x_0[$ and $]x_0, l]$. Then $(5.2)_1$ implies that σ is piecewise linear. Hence the boundary conditions (3.4) and (3.5) determine the solution:

$$\sigma(x) = \begin{cases} -\dfrac{\sigma_0(x - x_0)}{x_0} & \text{if } x \in [0, x_0], \\ \dfrac{\sigma_0(x - x_0)}{l - x_0} & \text{if } x \in [x_0, l], \end{cases} \tag{7.12}$$

$$\alpha(x) = \begin{cases} 0 & \text{if } x \in [0, x_0[, \\ \alpha_0 & \text{if } x \in\,]x_0, l]. \end{cases} \tag{7.13}$$

If we evaluate F on this pair, we get

$$F[\sigma,\alpha] = \frac{k\sigma_0^2 l}{x_0(l - x_0)}, \tag{7.14}$$

which is minimized when $x_0 = l/2$. Hence, if there is any minimizer of F such that $\mathscr{S}(\sigma) \neq \emptyset$, then

$$\min\{F[\sigma,\alpha] \mid (\sigma,\alpha) \in \mathscr{A}\} = \frac{4\sigma_0^2 k}{l}. \tag{7.15}$$

Comparing (7.15) and (7.11), and using (6.5) we conclude that if (7.10) is satisfied, then

$$\min\{F[\sigma,\alpha] \mid (\sigma,\alpha) \in \mathscr{A}\} = \min\{F[\sigma,\alpha] \mid (\sigma,\alpha) \in \mathscr{A},\ \mathscr{S}(\sigma) = \emptyset\}.$$

If (7.10) is not satisfied, then

$$\min\{F[\sigma,\alpha] \mid (\sigma,\alpha)\in\mathscr{A}\} = \min\{F[\sigma,\alpha] \mid (\sigma,\alpha)\in\mathscr{A},\ \mathscr{S}(\sigma)\neq\emptyset\}.$$

Thus for $k = k_c := \left(\frac{\alpha_0}{\pi}\right)^2$ a bifurcation occurs: The orientation field that minimizes the energy possesses a plane disclination at $x_0 = \frac{l}{2}$ when $k \leqq k_c$, while it is smooth everywhere when $k > k_c$.

Remark. Had we allowed σ to take different values at the endpoints of the interval $[0, l]$, we should have found different minimizers of F with the same qualitative features illustrated in this section and *just the same value of* k_c.

8. The Lavrentiev phenomenon

We have pointed out in the preceding section that when $k \leqq k_c$ the minimizers of F in $\mathscr{A}$ are not of class C^1 in $[0, l]$. Let

$$\mathscr{W} := \{(\sigma,\alpha)\in\mathscr{A} \mid \sigma,\ \alpha\in C^1([0,l])\}. \tag{8.1}$$

It is easy to see that $\mathscr{W}$ is dense in $\mathscr{A}$ with respect to the convergence specified in Lemma 1 of Section 4. We raise the question: Does

$$\min\{F[\sigma,\alpha] \mid (\sigma,\alpha)\in\mathscr{A}\} = \inf\{F[\sigma,\alpha] \mid (\sigma,\alpha)\in\mathscr{W}\}? \tag{8.2}$$

We show in this section that the answer is *yes*. In other words, the Lavrentiev phenomenon (*cf.*, *e.g.*, Ch. 18 of [9]) does not occur in the problem we have studied here.

If $k > k_c$, equality (8.2) is obviously satisfied. We assume that $k \leqq k_c$ and seek a sequence $\{(\sigma_h,\alpha_h)\}_{h\in N}$ of members of $\mathscr{W}$ such that (σ_h,α_h) converges to the minimizer (σ,α) of F in $\mathscr{A}$ in the sense of Lemma 1 of Section 4, and such that

$$\lim_{h\to\infty} F[\sigma_h,\alpha_h] = \frac{4k\sigma_0^2}{l} \tag{8.3}$$

(*cf.* equation (7.15) above). For all $\varepsilon\in\left]0,\frac{l}{2}\right[$ we define the function $\alpha_\varepsilon :=[0,l]\to[0,\pi]$ as follows:

$$\alpha_\varepsilon(x) := \begin{cases} 0 & \text{if } x\in\left[0,\frac{l}{2}-\varepsilon\right], \\ \left(x-\frac{l}{2}+\varepsilon\right)\frac{\alpha_0}{2\varepsilon} & \text{if } x\in\left[\frac{l}{2}-\varepsilon,\frac{l}{2}+\varepsilon\right], \\ \alpha_0 & \text{if } x\in\left[\frac{l}{2}+\varepsilon, l\right]. \end{cases} \tag{8.4}$$

An easy computation shows that

(8.5)
$$F[\bar{\sigma}, \alpha_\varepsilon] = \int_0^l k(\bar{\sigma}')^2 + \frac{\alpha_0^2}{4\varepsilon^2} \int_{\frac{l}{2}-\varepsilon}^{\frac{l}{2}+\varepsilon} \bar{\sigma}^2$$

for any $\bar{\sigma} \in C^1(]0, l[,]-\frac{1}{2}, 1[)$. If σ is given by (7.12) with $x_0 = \frac{l}{2}$, then

(8.6)
$$\int_0^l k(\sigma')^2 = \frac{4k\sigma_0^2}{l}, \qquad \int_{\frac{l}{2}-\varepsilon}^{\frac{l}{2}+\varepsilon} \sigma^2 = \frac{8\sigma_0^2\varepsilon^3}{3l^2}.$$

Thus for all $\varepsilon \in]0, \frac{l}{2}[$ there is a $\sigma_\varepsilon \in C^1(]0, l[,]-\frac{1}{2}, 1[)$ such that

(8.7)
$$\|\sigma_\varepsilon - \sigma\|_\infty < \varepsilon$$

and

(8.8)
$$\int_0^l k(\sigma_\varepsilon')^2 < \frac{4k\sigma_0^2}{l} + \varepsilon, \qquad \int_{\frac{l}{2}-\varepsilon}^{\frac{l}{2}+\varepsilon} \sigma_\varepsilon^2 < \frac{9\sigma_0^2\varepsilon^3}{3l^2}.$$

Combining (8.8) and (8.5), we get

(8.9)
$$F[\sigma_\varepsilon, \alpha_\varepsilon] < \frac{4k\sigma_0^2}{l} + \varepsilon + \frac{9\sigma_0^2\alpha_0^2\varepsilon}{4l^2} \quad \text{for all } \varepsilon \in]0, \frac{l}{2}[.$$

Taking the limit as $\varepsilon \to 0$, we see from (8.9) that

(8.10)
$$\min\{F[\sigma, \alpha] \mid (\sigma, \alpha) \in \mathscr{A}\} = \inf\{F[\sigma, \alpha] \mid (\sigma, \alpha) \in \mathscr{L}\},$$

where

(8.11)
$$\mathscr{L} := \{(\sigma, \alpha) \in \mathscr{A} \mid \sigma \text{ is of class } C^1 \text{ and } \alpha \text{ is Lipschitzian}\}.$$

By mollifying the members of $\mathscr{L}$ that do not belong to $\mathscr{W}$, as illustrated in Theorem VIII.6 of [7], we prove that

(8.12)
$$\inf\{F[\sigma, \alpha] \mid (\sigma, \alpha) \in \mathscr{L}\} = \inf\{F[\sigma, \alpha] \mid (\sigma, \alpha) \in \mathscr{W}\}.$$

Then from (8.10) and (8.12) we deduce the desired conclusion (8.2).

9. Justification of the one-dimensional problem

Let the region $\mathscr{P}$ and the unit vector e be defined as in Section 3. Let the functional

(9.1)
$$\mathscr{F}[\mathscr{P}; s, n] := \int_{\mathscr{P}} (k\,|\nabla s|^2 + s^2\,|\nabla n|^2)$$

be subject to the boundary conditions

(9.2) $$s|_{\mathscr{S}_1} = s|_{\mathscr{S}_2} = s_0,$$

(9.3) $$n|_{\mathscr{S}_1} = n_1, \quad n|_{\mathscr{S}_2} = n_2,$$

where $\mathscr{S}_1$ and $\mathscr{S}_2$ are the faces of $\partial\mathscr{P}$ orthogonal to e, s_0 is a positive constant, and n_1, n_2 are constant unit vectors not pointing in opposite directions. We show that all the minimizers of (9.1) in a suitable class of functions satisfying (9.2) and (9.3) are such that (3.1) and (3.2) hold.

Let the class $\mathscr{G}$ be defined as follows:

(9.4) $$\mathscr{G} := \{(s, n) \mid s \in H^{1,2}(\mathscr{P}), sn \in H^{1,2}(\mathscr{P}), s(\mathscr{P}) \subset]-\tfrac{1}{2}, 1[, n(\mathscr{P}) \subset \mathscr{S}^2\}.$$

It is shown in [10] (*cf.* also Section 3 of [3]) that (9.1) attains a minimum in $\mathscr{G}$ even when boundary conditions more general that (9.2) and (9.3) apply. In [11] and [12] the regularity of minimizers is explored from different perspectives. Furthermore, given a pair (s, n) in $\mathscr{G}$ that satisfies (9.2) and (9.3), the restriction of s and n to almost every segment of $\mathscr{P}$ parallel to e gives rise to pairs (t, v) such that

(9.5) $$t \in AC(]0, l[,]-\tfrac{1}{2}, 1[), \quad t(0) = t(l) = s_0,$$

(9.6) $$v \in AC_{\mathrm{loc}}(]0, l[\setminus \mathscr{S}(t), \mathscr{S}^2), \quad v(0) = n_1, v(l) = n_2.$$

Thus, defining

(9.7) $$L := \inf\left\{\int_0^l [k(t')^2 + t^2(v')^2] \mid t, v \text{ satisfy (9.5) and (9.6)}\right\},$$

we easily find that

(9.8) $$\mathscr{F}[\mathscr{P}; s, n] \geqq l_\perp l^\perp L,$$

where $l_\perp$ and $l^\perp$ are defined as in Section 3. In (9.8) the equality sign holds if and only if both s and n depend on p only through $x := (p - O) \cdot e$, and the functions t, s defined by $t(x) = s(p)$, $v(x) = n(p)$ are such that

$$\int_0^l [k(t')^2 + t^2(v')^2] = L.$$

Again applying the method illustrated in Section 4, we can show that L is indeed attained. Let (t, v) be a minimizer. The same dichotomy as in Section 6 applies now to $\mathscr{S}(t)$. Furthermore, if $\mathscr{S}(t) = \{x_0\}$, then $x_0 = \dfrac{l}{2}$, $L = \dfrac{4ks_0^2}{l}$, and v is piecewise constant; hence (3.1) obviously holds. If, on the contrary, $\mathscr{S}(t) = \emptyset$, then by using the change of variables

(9.9) $$\eta(y) := \int_0^y t^{-2}(x)\, dx$$

we easily prove that

$$\int_0^l t^2(z')^2 = \int_0^{\eta(l)} (w')^2, \tag{9.10}$$

for all $z \in AC(]0, l[, \mathcal{S}^2)$, where $w := z \circ \eta^{-1}$. Equality (9.10) shows that $v \circ \eta^{-1}$ is a geodesic on $\mathcal{S}^2$ connecting n_1 to n_2. Hence $v(x)$ lies in the plane defined by n_1 and n_2 for all $x \in [0, l]$.

Remark. LIN has proved in [3] (*cf.* Theorem 3.5) that when $k = 2$, the Hausdorff dimension of the singular set $\mathcal{S}(s)$ is at most 1 for the minimizers of $\mathcal{F}$. We have shown here that when k is sufficiently small, the dimension of the singular set may well be 2.

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Dipartimento di Matematica
Università di Roma II — Tor Vergata

and

Dipartimento di Matematica
Università di Pavia, Strada Nuova 65
27100 Pavia, Italy

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