A VARIATIONAL PROBLEM FOR NEMATIC LIQUID CRYSTALS WITH VARIABLE DEGREE OF ORIENTATION

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1. Introduction. In his seminal paper [1] FRANK proposed a model to describe the equilibrium of nematic liquid crystals that is now regarded as a classic. In FRANK's model the local microstructure of nematic liquid crystals is described by a unit vector $\mathbf{n}$ that represents the *optical axis*: only one vector is needed, for these materials are *uniaxial*.

Generally, the optical axis changes in space; it can exhibit singularities, which are called *defects*. *Disclinations* are those defects located along lines.

FRANK proved in [1] (for work of Oseen see [15]) that disclinations actually occur in some solutions of his model. Here we devote special attention to one of FRANK's disclinations: We examine its rôle within the classical model and discuss a puzzle it provided; we also recall the resolution of that puzzle by CLADIS & KLEMAN in [2]. Finally, we show how FRANK'S disclination also arises in a model proposed by ERICKSEN in [3] to accommodate all defects in a unified theory.

To illustrate this subject we employ neither FRANK's model nor ERICKSEN's in their full generality. In particular, we employ the *one constant approximation* of FRANK's energy functional (see e.g. [4] for both the general expression of the energy and its approximation). Accordingly, when we come to ERICKSEN's energy functional, we employ an approximation which somehow parallels the aforesaid approximation to FRANK's functional (cf. MADDOCKS [14] for a different approach.

Let $\mathcal{B}$ be the open region of the three-dimensional Euclidean space occupied by a nematic liquid crystal. The *orientation* of the crystal is a vector field $\mathbf{n}$ of class C^1 that maps the whole of $\mathcal{B}$, except possibly a closed set $\mathcal{S} \subset \mathcal{B}$, into the unit sphere $\mathcal{S}^2$. An orientation delivers the optical axis of the crystal at all points of $\mathcal{B}$ where it is defined.

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The energy associated to an orientation in the simplified setting of FRANK's model that we employ here is

$$\mathfrak{F}_F[\mathbf{n}] := \kappa_F \int_{\mathcal{B}} |\nabla \mathbf{n}|^2 \ , \tag{1.1}$$

where κ_F is a positive constant. We subject $\mathfrak{F}_F$ to the boundary condition

$$\mathbf{n}|_{\mathcal{S}_0} = \mathbf{n}_0 \ , \tag{1.2}$$

where $\mathcal{S}_0$ is a given part of $\partial\mathcal{B}$, possibly all of it, and $\mathbf{n}_0 : \mathcal{S}_0 \to \mathcal{S}^2$ is a prescribed map of class C^1. Equation (2) differs from the ***strong anchoring condition*** in that $\mathcal{S}_0$ need not coincide with the whole of $\partial\mathcal{B}$.

Now we turn our attention to disclinations.

Suppose that $\mathcal{B}$ is a circular cylinder of radius R and height H: in cylindrical co-ordinates it has the form

$$\mathcal{B} := \{p = 0 + r\mathbf{e}_r + z\mathbf{e}_z | r \in]0, R[, \ z \in]0, H[\} \ , \tag{1.3}$$

where 0 is the center of one base of the cylinder. Furthermore, suppose that $\mathcal{S}_0$ is the lateral surface of $\mathcal{B}$ and that $\mathbf{n}_0$ coincides with the outward unit normal to $\mathcal{S}_0$. Of course, the radial field

$$\mathbf{n} = \mathbf{e}_r \tag{1.4}$$

obeys the boundary condition (2); it possesses a line of discontinuity along the axis of $\mathcal{B}$, namely it possesses a disclination. FRANK proved that (4) indeed solves the Euler equation associated with (1). Moreover, (4) looks likes the orientation often observed by physicists in capillary tubes filled with nematic liquid crystals.

What is wrong with (4) is that its energy, as given by (1), is not finite. This presents the previously announced puzzle: ***Why does the orientation one would guess to be the minimizer of the energy not even make it finite?***

The answer was found by CLADIS and KLÉMAN in [2]. They sought for minimizers of (1) in the class of all axisymmetric fields

$$\mathbf{n} = \cos\varphi \mathbf{e}_r + \sin\varphi \mathbf{e}_z \ , \tag{1.5}$$

where φ is a real-valued function of class C^1 that depends only on the radial co-ordinate r and obeys the boundary condition

$$\varphi(R) = 0 \ . \tag{1.6}$$

In this class of orientations the energy functional (1) reads

$$\mathfrak{F}_F[\mathbf{n}] = 2\pi H \kappa_F \; F[\varphi] \,, \tag{1.7}$$

where

$$F[\varphi] := \int_0^R \left(\varphi'^2 + \frac{\cos^2\varphi}{r^2} \right) r\,dr \,, \tag{1.8}$$

a prime denoting differentiation with respect to r. CLADIS and KLÉMAN proved that the minimizer of F subject to (6) is

$$\varphi_{CK}(r) := \frac{\pi}{2} - 2\arctan\left(\frac{r}{R}\right) \;; \tag{1.9}$$

an easy computation shows that

$$F\,[\varphi_{CK}] = 2 \,. \tag{1.10}$$

The function φ_{CK} decreases from $\frac{\pi}{2}$ to 0 as r ranges from 0 to R. The orientation that corresponds to φ_{CK} through equation (5) is a field of class C^1 in the whole of $\mathcal{B}$, it coincides with the planar field $\mathbf{e}_r$ only on $\mathcal{S}_0$: this is the reason why CLADIS and KLEMAN's solution is sometimes referred to as the solution "escaping to the third dimension".

Recently, a new model for the mathematical theory of liquid crystals came on the scene; it is ERICKSEN's [3]. Besides $\mathbf{n}$, a scalar now describes the local microstructure of liquid crystals: it is s, the *degree of orientation*, which specifies the degree of microscopic order that legitimizes the definition of $\mathbf{n}$ as a statistical average of the axis of the molecules.

In ERICKSEN's model s ranges in the interval $\left[-\frac{1}{2}, 1\right]$. The values $-\frac{1}{2}$ and 1 correspond to the extreme situations in which all molecules in a macroscopic site lie parallel to a plane or along a direction, respectively. Where s vanishes the liquid crystal becomes isotropic: the molecules do not lie in any preferred direction and $\mathbf{n}$ is undefined. Defects may possibly coincide with the regions, of any space dimension, where s vanishes.

If a liquid crystal occupies the region $\mathcal{B}$, the degree of orientation s is delivered by a map of $\mathcal{B}$ into $\left[-\frac{1}{2}, 1\right]$ that is continuous on $\mathcal{B}$ and of class C^1 away from the *singular set*

$$\mathcal{S}(s) := \{p \in \mathcal{B} |\; s(p) = 0\} \,. \tag{1.11}$$

If $\mathcal{S}(s)$ is not empty, defects may arise there. Thus, the orientation $\mathbf{n}$ is a map of class C^1 defined on $\mathcal{B}\backslash\mathcal{S}(s)$.

The energy per unit volume depends on s and ∇s, besides $\mathbf{n}$ and $\nabla\mathbf{n}$. We refer to Section 5 of [3] for the general form of the energy functional. Here we employ a special form of it that resembles (1):

$$\mathcal{F}_E[s,\mathbf{n}] := \kappa_E \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2|\nabla\mathbf{n}|^2 + \sigma_0(s)\} \,, \tag{1.12}$$

where κ_E and k are positive constants and σ_0 is a smooth function whose main features are illustrated e.g. in Section 2 of [5]. When s is taken as constant in (12), $\mathcal{F}_E$ reduces to $\mathcal{F}_F$, *modulo* inessential constants.

Together with (2), we impose on $\mathcal{F}_E$ the boundary condition

$$s|_{\mathcal{S}_0} = s_0 \,, \tag{1.13}$$

where $s_0 : \mathcal{S}_0 \to \left[-\frac{1}{2}, 1\right]$ is a continuous function.

When s_0 is constant and different from zero, a heuristic argument discussed in [6] leads us to neglect σ_0 in (12). Apart from this argument, the strongest reason in favour of such an approximation that we are aware of is its simplicity. Thus, we write $\mathcal{F}_E$ as

$$\mathcal{F}[s,\mathbf{n}] = \kappa_E \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2|\nabla\mathbf{n}|^2\} \tag{1.14}$$

and we subject it to (2) and (13), with s_0 a *positive* constant.

Although the region $\mathcal{B}$ may in general be arbitrary, here it is to be the cylinder (3). If, as above, we take $\mathcal{S}_0$ as the lateral surface of $\mathcal{B}$ and $\mathbf{n}_0$ as the outward unit normal to $\mathcal{S}_0$, in the new setting the field (4) becomes a legitimate candidate to minimize $\mathcal{F}$, as soon as it is associated with a suitable field s that vanishes along the axis of $\mathcal{B}$.

Thus, it is conceivable that the singularity of (4) can be *tamed* so as to make it the minimizer of the energy functional. As mentioned above, we will prove that this is indeed the case. In fact, the critical value will be shown to be $k_c = 1$, so that the orientation field (4) together with a suitable field s minimizes $\mathcal{F}$ when $k < 1$, while when $k \geq 1$ the orientation that minimizes $\mathcal{F}$ shares many features of CLADIS and KLEMAN's solution, but is not quite the same.

The plan of the paper is as follows. In Section 2 we recall a few theorems, proven elsewhere, that are relevant to our development and we state the variational problem we solve in this paper.

In Section 3 we deduce those qualitative features of minimizers that follow by direct arguments. In particular, we pay attention to the admissible shapes of the singular set.

In Section 4 we derive the Euler equations. From them we deduce both a dichotomy concerning the singular set and the du Bois–Reymond equation. The latter leads to a first integral whose rôle will be made clear later in Section 5.

In Section 5 we apply the Hamilton–Jacobi method, also known as dynamic programming in the theory of optimal control. We also derive the Hamilton–Jacobi equation suitable to our problem and we state in precise terms the main theorem of the paper. A crucial rôle is played there by two special properties of $\mathcal{F}$, both of which fail to hold if we do not neglect σ_0 in (12).

Finally, Section 6 is devoted to the proof of a key ingredient of the main theorem, which relies on a phase plane analysis of the Hamilton–Jacobi equation.

2. Variational problem. The energy functional $\mathcal{F}_E$ in (1.12) has been extensively examined in recent times.

For $k = 2$, LIN proved in [7] that a unique minimizer $(s, \mathbf{n})$ of $\mathcal{F}_E$ subject to (1.2) and (1.13) exists in a suitable class of mappings. Later AMBROSIO proved in [8] that minimizers of $\mathcal{F}_E$ actually exist for all values of k.

The regularity of minimizers has been addressed from different perspectives by both AMBROSIO [9] and LIN [10]. Bringing together the results of their analyses, we learn that for all $k > 0$ any pair $(s, \mathbf{n})$ that minimizes $\mathcal{F}_E$ subject to (1.2) and (1.13) is such that s is continuous on the whole of $\mathcal{B}$ and, if σ_0 is of class C^1, both s and $\mathbf{n}$ are of class $C^{1,\alpha}$, for all $\alpha < 1$, away from the singular set $\mathcal{S}(s)$ where s vanishes. Furthermore, both s and $\mathbf{u} := s\mathbf{n}$ are Hölder continuous on the whole of $\overline{\mathcal{B}}$ for all $k > 0$, while they are Lipschitz continuous when $0 < k < 1$.

Of course, these results apply also to the functional $\mathcal{F}$ in (1.14). Moreover, since there $\sigma_0 \equiv 0$, a recursive argument shows that the minimizers of $\mathcal{F}$ are at least of class C^∞ away from the singular set; actually, they are even analytic (cf. again [9] and [10]).

Here the region $\mathcal{B}$ is the circular cylinder defined by (1.3) and $\mathcal{F}$ is subject to (1.2) and (1.13), where we take $\mathcal{S}_0$ as the lateral surface of $\mathcal{B}, \mathbf{n}_0$ as the outward normal to $\mathcal{S}_0$, and s_0 as a positive constant. Thus, the boundary conditions imposed on $\mathcal{F}$ share the axisymmetry of $\mathcal{B}$. Hence, as is proven in [11], the minimizers of $\mathcal{F}$ are axisymmetric too: specifically, *s depends only on r, the radial co-ordinate, and $\mathbf{n}$ takes the form* (1.5).

In the class of pairs with the same symmetry as the minimizers, $\mathcal{F}$ can be reduced to a simpler functional:

$$\mathcal{F}[s, \mathbf{n}] = 2\pi H \kappa_E \, F[s, \varphi] \; , \tag{2.1}$$

where

$$F[s, \varphi] := \int_0^R \left\{ k s'^2 + s^2 \left(\varphi'^2 + \frac{\cos^2 \varphi}{r^2} \right) \right\} r dr \; . \tag{2.2}$$

When s is a constant different from zero, F is proportional to the functional in (1.8). As in (1.8), a prime denotes differentiation with respect to r and φ is a real–valued function defined in [0,R]. Like the functional in (1.8), here F is subject to (1.6), but also to

$$s(R) = s_0 \ . \tag{2.3}$$

The singular set defined in (1.11) is generated here by a subset of $[0, R]$:

$$\mathcal{S}(s) = \{p = 0 + r\mathbf{e}_r + z\mathbf{e}_z | r \in S(s) \ , \ z \in [0, H]\} \ , \tag{2.4}$$

where

$$S(s) := \{r \in [0, R] \mid s(r) = 0\} \ . \tag{2.5}$$

With a slight abuse of language, we also call $S(s)$ the *singular set.*

The regularity result for the minimizers of $\mathcal{F}$ can easily be reformulated for the minimizers of F. Thus s will be Lipschitz continuous on $[0, R]$ for $0 < k < 1$ and just Hölder continuous for $k \geq 1$, while both s and φ are analytic away from the singular set $S(s)$.

Keeping these features in mind, we state the following

Variational Problem (VP). *Find the minimizers of F in the class*

$$\mathcal{C} := \{(s, \varphi) | s \in AC(0, R), \varphi \in AC_{\mathrm{loc}}]0, R[: s(R) = s_0 > 0, \varphi(R) = 0\}. \tag{2.6}$$

3. Qualitative features of minimizers. In this section we derive, by direct inspection of the functional F, a few qualitative features of the pairs that solve (VP).

REMARK. If (s, φ) is a solution of (VP) $(s, -\varphi)$ is one also. Henceforth we resolve this ambiguity by restricting the range of φ to the positive real line.

LEMMA 3.1. *If the pair (s, φ) solves* (VP) *then*

$$\begin{array}{llll} \text{(a)} \ \ s(r) \geq 0 & , \ \text{(b)} \ \ \varphi(r) \leq \frac{\pi}{2} & \textit{for all} & r \in [0, R] \ ; \\ \text{(c)} \ \ s'(r) \geq 0 & , \ \text{(d)} \ \ \varphi'(r) \leq 0 & \textit{for almost all} & r \in [0, R] \ . \end{array}$$

Proof. To prove (a) we simply show that a function s which is negative somewhere cannot minimize F. In fact, if we replace such an s by a function that vanishes wherever s is negative, we lower the value of F. To prove (c), we employ a similar argument. If s is a decreasing function of r somewhere, we replace it by a continuous function that is constant wherever s decreases. In so doing we again lower the value of F.

The proof of (b) and (d) parallels closely that of (a) and (c), respectively. □

LEMMA 3.2. *If (s,φ) solves* (VP) *then either $S(s)=\emptyset$ or $S(s)=[0,r_0]$ with $r_0\geq 0$.*

Proof. If $S(s)\neq\emptyset$ and $r_0:=\max\{r\in[0,R]|s(r)=0\}$, then on replacing s by a function that vanishes in $[0,r_0]$, we lower the value of F. □

In the next section, building upon the Euler equations of F, we derive other features of the singular set.

4. Euler equations. The regularity of minimizers recalled in Section 2 guarantees that all the pairs that solve (VP) obey the Euler equations away from the singular set. The Euler equations for F in $[0,R]\backslash S(s)$ are

$$k(rs')'=sr\left(\varphi'^2+\frac{\cos^2\varphi}{r^2}\right)\ , \tag{4.1}$$

$$(rs^2\varphi')'=-\frac{s^2}{r}\ \cos\varphi\sin\varphi\ , \tag{4.2}$$

subject to (1.6) and (2.3).

From equation (1) we arrive at a sharp dichotomy for the singular set.

LEMMA 4.1. *If (s,φ) solves* (VP) *then either $S(s)=\emptyset$ or $S(s)=\{0\}$.*

Proof. First, we recall that the initial value-problem $s(r_1)=s_1$, $s'(r_1)=s_1'$, for equation (1) (with φ treated as known) possesses exactly one solution. Second, we recall that whenever $S(s)$ is not empty for a minimizer, it is an interval $[0,r_0]$ with $r_0\geq 0$ (cf. Lemma 3.2 above). Thus, we assume that $r_0>0$ and we prove that this leads to a contradiction.

Let $\tau:[0,R]\to\mathbf{R}^+$ be any function of class C^1 such that

$$\tau(0)=\tau(R)=0\ . \tag{4.3}$$

For a given $\varepsilon\in\mathbf{R}$, let ρ_ε be the function defined by

$$\rho_\varepsilon(r):=r+\varepsilon\tau(r)\quad ,\quad r\in[0,R]\ . \tag{4.4}$$

For every function τ there is $\varepsilon_\tau>0$ such that ρ_ε is a C^1-diffeomorphism of $[0,R]$ onto $[0,R]$ for all $\varepsilon\in[-\varepsilon_\tau,\varepsilon_\tau]$. Once a function τ has been selected, if the pair (s,φ) belongs to $\mathcal{C}$, then the pair $(s_\varepsilon,\varphi_\varepsilon)$, whose members are defined by

$$s_\varepsilon(r):=s(\rho_\varepsilon(r))\quad ,\quad \varphi_\varepsilon(r):=\varphi(\rho_\varepsilon(r))\quad ,\ r\in[0,R]\ , \tag{4.5}$$

also belongs to $\mathcal{C}$ for all $\varepsilon\in[-\varepsilon_\tau,\ \varepsilon_\tau]$.

If (s,φ) is a minimizer of F, then the first variation

$$\delta F(s,\varphi)[\tau] := \frac{d}{d\varepsilon}\, F[s_\varepsilon,\varphi_\varepsilon]|_{\varepsilon=0} \tag{4.6}$$

must vanish for all τ of class C^1 that obey (3). When s vanishes on $[0,r_0]$ with $r_0>0$, a tedious but easy computation shows that

$$\delta F(s,\varphi)[\tau] = \int_{r_0}^{R} (r\tau' - \tau)\left\{ks'^2 + s^2\left(\varphi'^2 - \frac{\cos^2\varphi}{r^2}\right)\right\} dr \ . \tag{4.7}$$

Integrating by parts in (7), we arrive at

$$\delta F(s,\varphi)[\tau] = -\lim_{r\to r_0}(\tau(r) r w(r)) \quad - \int_{r_0}^{R} \tau(rw' + 2w)dr \ , \tag{4.8}$$

where we have set

$$w := ks'^2 + s^2\left(\varphi'^2 - \frac{\cos^2\varphi}{r^2}\right) \ . \tag{4.9}$$

Since $r_0>0$, the left-side of (8) vanishes for all functions τ if, and only if,

$$\lim_{r\to r_0^+} rw(r) = 0 \tag{4.10}$$

and

$$rw' + 2w = 0 \quad \text{in} \quad]r_0,R[\ . \tag{4.11}$$

By (11) w has the form

$$w(r) = \frac{c}{r^2} \quad , \quad r\in]r_0,R[\ , \tag{4.12}$$

whence (10) requires that $w\equiv 0$ on $]r_0,R[$. Since continuity of s yields $s(r_0)=0$, the boundedness of $\frac{\cos^2\varphi}{r}$ leads to $\lim_{r\to r_0^+} s'(r) = 0$. Since $s'\equiv 0$ on $]0,r_0[$ we are thus led to $s(r_0)=s'(r_0)=0$. Equation (1) subject to these conditions has only the solution $s=0$ in $[r_0,R]$, for each function φ of class $W^{1,2}$. Since s must satisfy $s(R)=s_0>0$, we get a contradiction that can be avoided only by setting $r_0=0$. □

REMARK. Notice that since $r_0 = 0$, (12) yields

$$w = 0 \qquad \text{on all of} \quad]0, R] \; . \tag{4.13}$$

It is easy to show that (13) is the du Bois–Reymond equation associated to (1) and (2).

5. The Hamilton–Jacobi Method.+ We consider the problem $(P_{1,1,0})$ of minimizing

$$\begin{cases} F_1[s,\varphi] := \displaystyle\int_0^1 f(r, s(r), \varphi(r), s'(r), \varphi'(r))dr \\ \text{over } \mathcal{A}(1;1,0) := \{(t,\psi) \in W^{1,1}_{\text{loc}} \times W^{1,1}_{\text{loc}} | t(1) = 1, \psi(1) = 0\} \; , \end{cases} \tag{5.1a}$$

where $W^{1,1}_{\text{loc}}$ denotes $W^{1,1}_{\text{loc}}]0,1]$ and where
(5.1b)

$$f(r,s,\varphi,p,q) = krp^2 + s^2rq^2 + s^2\frac{\cos^2\varphi}{r} \; , \; r \in]0,\infty[, (s,\varphi) \in [0,\infty[\times[0,\pi/2], (p,q) \in \mathbf{R}^2 \; .$$

[It will be seen later that the special choice $R = 1$ loses us nothing in the generality of our conclusions.] In order to facilitate the search for a minimizing pair $(s^*, \varphi^*) \in \mathcal{A}(1;1,0)$ we introduce the value function $V :]0,\infty[\times[0,\infty[\times[0,\pi/2] \to \mathbf{R}$ for the full class (P_{r_0,s_0,φ_0}) of variational problems defined by

$$V(r_0; s_0, \varphi_0) := \inf_{\mathcal{A}(r_0;s_0,\varphi_0)} F_{r_0} \quad r_0 \in]0,\infty[, (s_0,\varphi_0) \in [0,\infty[\times[0,\pi/2] \; , \tag{5.2}$$

where F_{r_0} denotes an integration of the integrand f over $[0, r_0]$ and $\mathcal{A}(r_0; s_0, \varphi_0)$ is defined analogously to $\mathcal{A}(1;1,0)$.

Under the assumption that the positive function V is smooth, the following *formal* scheme leads us to a Hamilton–Jacobi partial differential equation for V, and the latter will then be shown to serve as the basis for a rigorous verification theorem leading to the identification of (s^*, φ^*).

Now by (1) and the smoothness assumption, we have for each $(s,\varphi) \in \mathcal{A}(r_0; s_0, \varphi_0)$
(5.3)

$$\int_0^{r_0} f(r, s(r), \varphi(r), s(r), \varphi'(r))dr \geq V(r_0; s_0, \varphi_0) = \int_0^{r_0} (V_{,r} + s'V_{,s} + \varphi'V_{,\varphi})(r; s(r), \varphi(r))dr$$
$$+ \lim_{r_1 \to 0} V(r_1; s(r_1), \varphi(r_1)),$$

+In control theory this is usually referred to as the "dynamic programming" method.

where the validity of the last equation rests on the existence of the quantity $\lim_{r_1 \to 0} V(r_1; s(r_1), \varphi(r_1))$. Now if $F_{r_0}[s, \varphi] < \infty$, then the *inequality* in (3) when examined for all values $\overline{r}_0 \in]0, r_0[$ implies

$$\lim_{\overline{r}_0 \to 0} V(\overline{r}_0; s(\overline{r}_0), \varphi(\overline{r}_0)) = 0 ,$$

so that (3) leads to the integral inequality

(5.4)

$$\int_0^{r_0} [V_{,r} + s'(r)V_{,s} + \varphi'(r)V_{,\varphi} - f(r, s(r), \varphi(r), s'(r), \varphi'(r)]dr \leq 0 \quad , \quad \forall\, (s, \varphi) \in \mathcal{A}(r_0; s_0, \varphi_0) .$$

Notice that by the form (1b) of f it follows that

$$F_{r_0}[s, \varphi] < \infty \Rightarrow (s(r_1), \varphi(r_1)) \to [0, \infty[\times\{\pi/2\} \ \cup \ \{0\} \times [0, \pi/2] =: B_0 \ , \quad \text{as } r_1 \to 0.$$

Furthermore, since for any fixed $r_1 \in]0, r_0[$, $s'(r_1), \varphi'(r_1)$ can be substantially modified with only a small perturbation in (s, φ) near r_1, we are led to consider the following inequality for $V = V(r; s(r), \varphi(r))$

$$(5.4') \quad V_{,r} + p(r)V_{,s} + q(r)V_{,\varphi} - f(r, s(r), \varphi(r), p(r), q(r)) \leq 0 \ , \ r \in]0, r_0[, \ p, q \in L^1_{\text{loc}}]0, r_0[,$$

for all $(s, \varphi) \in \mathcal{A}(r_0; s_0, \varphi_0)$. We shall actually study the corresponding *Hamilton-Jacobi equation* for $V = V(r, s, \varphi)$,

$$(5.5) \qquad (\text{HJ}) \begin{cases} V_{,r} + \sup\limits_{p,q \in \mathbf{R}} \{pV_{,s} + qV_{,\varphi} - f(r, s, \varphi, p, q)\} = 0 \\ V(0^+; a, b) = 0 \quad \text{for all} \quad (a, b) \in B_0 \ . \end{cases}$$

REMARK 1. Steve Shreve has pointed out that with the substitution $r = e^{-t}$ the above argument leads to an *autonomous* partial differential equation in t, as opposed to (HJ) which is nonautonomous.

Now it is easily verified by using the explicit form (1b) of f that under the change of variables

$$\overline{r} = \alpha r \ , \ \overline{\varphi}(\overline{r}) = \varphi(\overline{r}/\alpha), \overline{s}(\overline{r}) = s(\overline{r}/\alpha), \overline{\varphi}'(\overline{r}) = \frac{1}{\alpha}\varphi'(\overline{r}/\alpha), \overline{s}'(\overline{r}) = \frac{1}{\alpha}s'(\overline{r}/\alpha), \ \alpha > 0,$$

one obtains

$$\begin{cases} (s, \varphi) \in \mathcal{A}(r_0; s_0, \varphi_0) \Rightarrow (\overline{s}, \overline{\varphi}) \in \mathcal{A}(\alpha r_0; s_0, \varphi_0) \\ F_{\alpha r_0}[\overline{s}, \overline{\varphi}] = \displaystyle\int_0^{\alpha r_0} f(\overline{r}, \overline{s}, \overline{\varphi}, \overline{s}', \overline{\varphi}')d\overline{r} = \int_0^{r_0} f(r, s, \varphi, s', \varphi')dr = F_{r_0}[s, \varphi] \ . \end{cases}$$

It follows from this that the value function V must be a solution of (4′) which is independent of r. Furthermore, since it is evident that

$$F_{r_0}[\beta s,\varphi] = \beta^2 F_{r_0}[s,\varphi] \ , \quad \forall\, \beta \in \mathbf{R} \ , \forall\, (s,\varphi) \in \mathcal{A}(r_0; s_0, \varphi_0),$$

we see that

$$V(r; s, \varphi) = s^2 B(\varphi) \qquad \text{for some smooth function } B \ .$$

[This provides the justification of the claim that the choice $R = 1$ in (1) came without loss of generality. We see that in general φ and s will depend on the ratio r/R.] By substituting the above expression into (5) we see that the above formula for V necessarily involves a solution B of the following ordinary differential equation:

$$\text{(5.6)} \qquad \sup_{p,q\in\mathbf{R}} \{2psB(\varphi) + qs^2B'(\varphi) - krp^2 - rs^2q^2\} = \frac{s^2\cos^2\varphi}{r} \qquad \text{(HJ}') \ .$$

On carrying out the indicated maximization in (6) we are led to three ordinary differential equations for determination of the value function $V = s^2B(\varphi)$ as well as of the optimal trajectories (s^*, φ^*) (at points where $s^*(r) \neq 0$):

$$\text{(5.7)} \qquad \begin{cases} \dfrac{(B'(\varphi))^2}{4} + \dfrac{B^2(\varphi)}{k} = \cos^2\varphi \ , \\ \varphi'(r) = \dfrac{B'(\varphi(r))}{2r} \ , \\ s'(r) = \dfrac{sB(\varphi(r))}{kr} \ . \end{cases}$$

REMARK 2. Substituting into (7a) from (7b) and (7c) leads to the du Bois–Reymond equation (4.13) (cf. also (4.9)).

Since it follows from the form of f that for $\varphi \equiv \pi/2$ and all constant functions $s \equiv s_0$ $F_{r_0}[s_0, \pi/2] = 0$, one also concludes that

$$V(r; s_0, \pi/2) = s_0^2 \ B(\pi/2) = 0 \qquad \text{for all} \quad s_0 \in]0, \infty[,$$

whence $B(\pi/2) = 0$. Furthermore, by utilizing the monotonicity properties of s and φ (cf. Lemma 3.1) we can write all differential equations in (7) in standard form. Thus we obtain the system of equations

$$\text{(5.8)} \qquad \begin{cases} B'(\varphi) = -2\sqrt{\cos^2\varphi - B^2(\varphi)/k} \quad , \quad \forall\varphi \in [\varphi_0, \pi/2] \ , \qquad B(\pi/2) = 0 \ ; \\ \varphi'(r) = \dfrac{B'(\varphi(r))}{2r} \quad , \quad \varphi(r_0) = \varphi_0 \ , \\ s'(r) = \dfrac{B(\varphi(r))}{kr}\, s(r) \quad , \quad s(r_0) = s_0 \ , \quad \forall r \in]0, r_0] \ \text{ such that } \ s^*(r) \neq 0 \ . \end{cases}$$

It remains of course to ascertain whether for a given $\varphi_0 \in [0, \pi/2[$ (8) possesses solutions $\overline{B}, \overline{\varphi}, \overline{s}$, with

$$\overline{B} \in C^2]\varphi_0, \pi/2[\ \cap \ C[\varphi_0, \pi/2] \quad , \quad s, \varphi \in C^1[0, r_0] \ .$$

We proceed to show that (8) leads to a rigorous *verification theorem* for determining optimal trajectories.

LEMMA 5.1. *Let $\overline{B}$ denote a nonnegative continuously differentiable solution to* (8a) *over the interval* $[0,\pi/2]$. *Then the function* W *defined by*

$$W(r;s,\varphi) := s^2\overline{B}(\varphi) \quad , \quad s \in [0,\infty[, \ \varphi \in [0,\pi/2[\ ,$$

provides a lower bound to the value function for each (P_{r_0,s_0,φ_0}):

(5.9)

$$W(r_0;s_0,\varphi_0) = s_0^2\overline{B}(\varphi_0) \le V(r_0;s_0,\varphi_0) = \inf_{\mathcal{A}(r_0;s_0,\varphi_0)} F_{r_0} \ , \quad \forall (r_0,s_0,\varphi_0) \in ([0,\infty[)^2 \times [0,\pi/2] \ .$$

Proof. Given any $(s,\varphi) \in \mathcal{A}(r_0;s_0,\varphi_0)$ and any $r_1 \in]0,r_0[$ we make use of the smoothness of W to write

(5.10)

$$W(r_0;s(r_0),\varphi(r_0)) - W(r_1;s(r_1),\varphi(r_1)) = \int_{r_1}^{r_0} (W_{,r} + s'(r)W_{,s} + \varphi'(r)W_{,\varphi})dr$$

$$= \int_{r_1}^{r_0} [2s(r)s'(r)\overline{B}(\varphi(r)) + s^2(r)\varphi'(r)\overline{B}'(\varphi(r))]dr \ .$$

Expressing this last integrand as an inner product of vectors in $\mathbf{R}^2$ and utilizing (7a) yields, via the Schwarz and arithmetic-geometric mean inequalities:

(5.11)

$$(2s'(r)\sqrt{kr}\ , 2\varphi'(r)s(r)\sqrt{r}) \cdot \left(\frac{s(r)\overline{B}(\varphi(r))}{\sqrt{kr}} \ , \ \frac{s(r)\overline{B}'(\varphi(r))}{2\sqrt{r}} \right) \le$$

$$\le 2\sqrt{\frac{s^2(r)\overline{B}^2(\varphi(r))}{kr} + \frac{s^2(r)(\overline{B}'(\varphi(r)))^2}{4r}} \sqrt{kr(s'(r))^2 + rs^2(r)(\varphi'(r))^2}$$

$$\le \frac{s^2(r)\cos^2\varphi(r)}{r} + kr(s'(r))^2 + rs^2(r)(\varphi'(r))^2 = f(r,s(r),\varphi(r),s'(r),\varphi'(r)) \ .$$

Inserting this into (10) now yields

(5.12)

$$W(r_0;s_0,\varphi_0) - W(r_1;s(r_1),\varphi(r_1)) \le \int_{r_1}^{r_0} f(r,s(r),\varphi(r),\varphi'(r))dr \qquad \forall\ (s,\varphi) \in \mathcal{A}(r_0;s_0,\varphi_0)$$

Since the inequality $W(r_0;s_0,\varphi_0) \le F_{r_0}[s,\varphi]$ is trivial when $F_{r_0}[s,\varphi] = +\infty$, we need only show that in (12) $F_{r_0}[s,\varphi] < \infty$ implies

(5.13)
$$\liminf_{r_1 \to 0} W(r_1;s(r_1),\varphi(r_1)) = \liminf_{r_1 \to 0} s^2(r_1)\overline{B}(\varphi(r_1)) = 0 \ .$$

By the form of f, finiteness of $F_{r_0}[s,\varphi]$ requires in particular that $r \mapsto \frac{s^2(r)\cos^2\varphi(r)}{r}$ is in $L^1(0,r_0)$, whence

$$\liminf_{r\to 0} s(r)\cos\varphi(r) = 0 \; .$$

For cases in which $\liminf\limits_{r\to 0}\; s(r) > 0$, this implies

$$\liminf_{r\to 0} \cos\varphi(r) = 0 \; ,$$

so that $\liminf |\pi/2 - \varphi(r)| = 0$. Thus the boundary condition $\overline{B}(\pi/2) = 0$ is clearly needed for (13) to hold in these circumstances.

To show sufficiency, note that $F_{r_0}[s,\varphi] < \infty$ implies

$$(5.14) \quad \int_0^{r_0} r(s'(r))^2 dr < \infty \quad \text{and} \quad \int_0^{r_0} \frac{s^2(r)\cos^2\varphi(r)}{r} dr = \int_0^{r_0} \frac{s^2(r)\cos^2\varphi(r)\ln\frac{1}{r}}{r\ln\frac{1}{r}}\, dr < \infty \; .$$

From the first relation we obtain

$$|s(r_0) - s(r_1)| = |\int_{r_1}^{r_0} s'(r)dr| \le \sqrt{\int_{r_1}^{r_0} r(s'(r))^2 dr}\;\sqrt{\int_{r_1}^{r_0} \frac{1}{r}\, dr} \; ,$$

whence

$$(5.15a) \qquad s(r) \le \text{const}\sqrt{\ln\frac{1}{r}} \quad , \quad r \in]0, r_0] \; .$$

Furthermore, since $r \mapsto \frac{1}{r\ln\frac{1}{r}}$ is not in $L^1(0,r_0)$, we deduce from the second relation that

$$(5.15b) \qquad \liminf_{r\to 0}\; s(r)\cos\varphi(r)\sqrt{\ln\frac{1}{r}} = 0 \; .$$

Now (7a) ensures that

$$(5.16) \qquad W(r_1; s(r_1), \varphi(r_1)) = s^2(r_1)\overline{B}(\varphi(r_1)) \le s(r_1)(\sqrt{k}s(r_1)\cos\varphi(r_1)) \; .$$

Estimating the first factor on the right by use of (15a) and applying (15b) to the result leads to

$$\liminf_{r_1\to 0} W(r_1; s(r_1), \varphi(r_1)) = 0 \; ,$$

so that (9) follows from (10). □

LEMMA 5.2. *For each $k > 0$ there is exactly one solution $\overline{B} = \overline{B}(k;\cdot) \in C^2]0,\pi/2[\cap C[0,\pi/2]$ to the problem*

$$(5.8') \qquad \overline{B}'(\varphi) = -2\sqrt{\cos^2\varphi - \frac{\overline{B}^2(\varphi)}{k}}\ , \ \overline{B}(\pi/2) = 0\ , \quad 0 \le \varphi \le \pi/2$$

Moreover,

$$(5.17) \qquad \begin{cases} \overline{B}(k;\varphi) < \sqrt{k}\ \cos\varphi\ , \ 0 < \varphi < \pi/2\ , \\ \overline{B}(k;0) = \sqrt{k} \quad , \ 0 < k \le 1 \\ \qquad\qquad < \sqrt{k} \quad , \ 1 < k < \infty\ . \end{cases}$$

This result will be proved in Section 6.

We can now state our main *verification theorem.*

THEOREM 5.3. *For each $k > 0$ the value function for the class of problems (P_{r_0,s_0,φ_0}) is given by the nonnegative C^1 function*

$$V(r_0;s_0,\varphi_0) = s_0^2\overline{B}(\varphi_0) \quad , \quad r_0, s_0 \in [0,\infty[, \quad \varphi_0 \in [0,\pi/2],$$

with $\overline{B} = \overline{B}(k;\cdot)$ as in Lemma 5.2. Furthermore the optimal trajectories (s^*,φ^*) for $(P_{1,1,0})$ are solutions on $[0,1]$ to

$$(5.18) \qquad \begin{cases} \varphi'(r) = \dfrac{\overline{B}'(\varphi(r))}{2r}\ , & \varphi(1) = 0 \\ s'(r) = \dfrac{s(r)\overline{B}(\varphi(r))}{kr}\ , & s(1) = 1\ , \end{cases}$$

possessing the cost $V(1;1,0) = \sqrt{k}$, for each $k \in]0,1]$. In particular for each $k \in]0,1]$ (but for no $k > 1$), the optimal trajectory is given by

$$\varphi^*(r) = 0\ , \qquad s^*(r) = r^{\frac{1}{\sqrt{k}}} \quad , \quad r \in [0,1]\ .$$

Proof. In view of equation (9) in Lemma 5.1, in order to prove that the value function is as claimed it suffices to produce for each (r_0,s_0,φ_0) a pair $(s^*,\varphi^*) \in \mathcal{A}(r_0;s_0,\varphi_0)$ satisfying

$$(5.19) \qquad F_{r_0}[s^*,\varphi^*] = s_0^2\overline{B}(\varphi_0)\ ,$$

with $\overline{B}$ as in Lemma 5.2. Now by reference to the inequalities in (11) it follows that equality will hold in (12) and in (19) *if and only if*

$$(s'(r)\sqrt{kr}\ , \ \varphi'(r)s(r)\sqrt{r}) = \left(s(r)\frac{\overline{B}(\varphi(r))}{\sqrt{kr}}\ , \ s(r)\frac{\overline{B}'(\varphi)r))}{2\sqrt{r}}\right) \quad , a.e.\ r \in]0,1[\ .$$

Equivalently, equality holds in (19) if and only if

$$\text{(5.20)}\qquad \begin{cases} s'(r) = \frac{\overline{B}(\varphi(r))}{kr}\, s(r) \\ s(r)\left[\varphi'(r) - \frac{\overline{B}'(\varphi(r))}{2r}\right] = 0 \end{cases} , \qquad a.e.\ r \in]0,1[\quad \begin{cases} s(r_0) = s_0 \\ \varphi(r_0) = \varphi_0 \ . \end{cases}$$

Since $\overline{B}$ is bounded it follows from (20a) that $s_0 \neq 0$ implies $s(r) \neq 0$ for all $r \in]0, r_0]$. Hence (20) simplifies to

$$\text{(5.20')}\qquad \begin{cases} s'(r) = \frac{\overline{B}(\varphi(r))}{kr}\, s(r) \\ \varphi'(r) = \frac{\overline{B}'(\varphi(r))}{2r} \end{cases} , \qquad a.e.\ r \in]0,1[\quad \begin{cases} s(r_0) = s_0 \\ \varphi(r_0) = \varphi_0 \ . \end{cases}$$

Now (20′b) clearly requires that $t_0 = \varphi(0^+)$ be a zero of $\overline{B}'$ in order for φ to satisfy $\varphi(r) \leq \pi/2$ on all of $[0, r_0]$; that is,

$$\overline{B}(k; t_0) = \sqrt{k}\cos t_0\ , \qquad \text{where} \quad t_0 = \varphi(0^+)\ .$$

Thus by (17a) existence of a $\varphi \in W^{1,1}_{\mathrm{loc}}]0, r_0]$ satisfying (20′b) requires

$$\text{(5.21)}\qquad \varphi(0^+) \in \{0, \pi/2\}\ ,\ 0 < k \leq 1 \quad , \varphi(0^+) = \pi/2\ ,\ k > 1\ .$$

Consider first the case $t_0 = \varphi(0^+) = 0$. Here the monotonicity properties of minimizers (cf. Lemma 3.1) imply

$$\text{(5.22a)}\qquad \varphi^*(r) = \varphi_0 = 0 \qquad \forall\, r \in [0,1]\ .$$

Inserting this into (20′a) we obtain

$$\text{(5.22b)}\qquad s^*(r) = s_0 \left(\frac{r}{r_0}\right)^{\frac{1}{\sqrt{k}}} \quad , \quad \forall\, r \in [0, r_0]\ .$$

Clearly this pair satisfies (20′), and we can verify that

$$F_{r_0}[s^*, \varphi^*] = \int_0^{r_0} \left[kr(s*\prime(r))^2 + \frac{s^{*2}(r)}{r} \right] dr = \int_0^{r_0} 2\frac{s_0^2}{r_0}\left(\frac{r}{r_0}\right)^{\frac{2}{\sqrt{k}}-1} dr = \sqrt{k}\ s_0^2 = s_0^2 \overline{B}(k;0)\ .$$

Next consider those cases with $t_0 = \varphi(0^+) = \pi/2$, so that by (8a) $\overline{B}(t_0) = \overline{B}'(t_0) = 0$. Since $\overline{B}'$ is smooth and bounded on $]0, \pi/2[$, the solution φ^* to (20′b) can be continued to all of $[0, r_0]$, so long as $\varphi^*(r) < \pi/2$, while if for some $r_1 > 0$ $\varphi^*(r_1) = \pi/2$ then φ^* can be (uniquely) continued to $[0, r_1[$ as the constant $\varphi^* = \pi/2$. Correspondingly the solution s^* to the linear equation (20′a) can be continued to all of $]0, r_0]$, as a C^∞ function in the former case or as a positive constant $s^* \equiv s^*(r_1)$ over $[0, r_1[$ in the latter case. Obviously $s^*, \varphi^* \in W^{1,1}_{\mathrm{loc}}$ in either of these situations. Moreover by the relation of equality in (12) for (s^*, φ^*) and the boundedness of $W = (s^*)^2\overline{B}(\varphi^*)$ it follows that $F_{r_0}[s^*, \varphi^*] < \infty$, so that (19) is a consequence of (13). This completes the proof that V is the value function as well as the proof that the designated trajectories $(s^*, \varphi^*) \in \mathcal{A}(r_0; s_0, \varphi_0)$ are indeed minimizers. Clearly (18) follows as a special case. We will complete the argument in Section 6 by proving that for $k \leq 1$ $\varphi(0^+) = 0$ (cf. Lemma 6.5). □

REMARK 3. Note that the issue of whether the minimizers s^*, φ^* happen to be constant on some interval near $r = 0$, which is a question of regularity, is not essential for the above verification result. It is not resolved by standard uniqueness results for differential equations in the real domain since in the present context $\overline{B}$ is not defined on a full neighborhood of $r = r_1, \varphi = \pi/2$. However an analysis utilizing the analytic nature of the differential equation does lead to a uniqueness result for each $r_1 > 0$, so that the case in which φ^* and s^* are constant on a proper subinterval of $]0, r_0[$ cannot arise. [cf. 12, Ch. 13].

6. Phase plane analysis. We have learned in Section 5 that all the solutions of (VP) solve also the following problem:

$$B'(\varphi) = -2\sqrt{\cos^2\varphi - \frac{B^2(\varphi)}{k}} \qquad B\left(\frac{\pi}{2}\right) = 0 \quad , \tag{6.1}$$

$$\varphi'(r) = \frac{B'(\varphi(r))}{2r} \qquad \varphi(R) = 0 \quad , \tag{6.2}$$

$$s'(r) = \frac{s(r)B(\varphi(r))}{kr} \qquad s(R) = s_0 \quad . \tag{6.3}$$

It is worth noting that since (5.7a), from which (1a) follows, is an analytic differential equation, one can refer to well known results concerning initial value problems for equations of this type. These will serve to justify our use of various formal expansions that occur below in the analysis of solutions of (1a) in the vicinity of its singular points. We refer the reader to INCE [12], Chapters 12 and 13 (especially §13.4) for this material.$^{\neq}$ In this section we complete the analysis of equations (1)–(3).

THEOREM 6.1. *For $k > 1$ the minimizer of F is such that $S(s^*) = \emptyset$ and ${\varphi^*}'(r) < 0$ for all $r \in [0, R]$.*

The proof of Theorem 6.1 rests upon a phase plane analysis of equation (1). We outline in a few Lemmata the main steps of this analysis, especially those involving qualitative features of the minimizers. The proof of Lemma 5.2 will also follow from the Lemmata below.

First we set the terminology we employ throughout this section. The ***integral trajectories*** are the curves that represent the solutions of (1a) in the (B, B') plane. They are confined within the region bounded by the co-ordinate axes and the quarter-ellipse described by

$$B' = -2\sqrt{1 - \frac{B^2}{k}} \quad , \quad B \geq 0 \quad . \tag{6.4}$$

$^{\neq}$We are indebted to David Kinderlehrer for supplying this reference.

This curve, which we call the *outer ellipse* for short, intersects the co-ordinate axes at $(\sqrt{k}, 0)$ and $(0, -2)$, respectively. The former of these intercepts, as we shall see later, plays a special rôle in our analysis. An integral trajectory hits the outer ellipse when $\varphi = 0$. For each $\varphi_0 \in \,]0, \frac{\pi}{2}[$ there is an ellipse inside the outer ellipse, described by

$$B' = -2\sqrt{\cos^2\varphi_0 - \frac{B^2}{k}} \quad , \quad B \geq 0 \quad ; \tag{6.5}$$

we call each of these curves an *inner ellipse*. For a given φ_0, the corresponding inner ellipse intersects the B-axis at $(\sqrt{k_0},\ 0)$, where

$$\sqrt{k_0} = \sqrt{k}\ \cos\varphi_0 \ . \tag{6.6}$$

We employ $k_0 \in [0, k[$ to label the inner ellipses. When $k_0 = 0$ the inner ellipse shrinks to the origin of the (B, B') plane. When $k_0 = k$ the inner ellipse reduces to the outer ellipse.

LEMMA 6.2. *There is exactly one solution to the initial value problem*

$$B(\varphi_0) = B_0 \in]0, \sqrt{k_0}] \quad , \quad \varphi_0 \in \left[0, \frac{\pi}{2}\right] \ , \tag{6.7}$$

for equation (1a), *except for the case* $\varphi_0 = 0$, $B_0 = \sqrt{k_0}$ *with* $k \neq 1$. *Moreover for* $B_0 = \sqrt{k_0}$, $\varphi_0 \in \,]0, \frac{\pi}{2}[$ *the domain of* B *is given by* $[0, \varphi_0]$.

Proof. Standard theorems ensure that the initial value problem (7) for (1a) possesses exactly one solution (which is analytic) except when $B(\varphi_0) = \sqrt{k_0}$ (cf. [12], Ch. 12). To complete the proof we need to analyze the behavior of the solutions of (1a) in the vicinity of the B-axis when $B(\varphi_0) = \sqrt{k_0}$.

Three cases arise: (a) $k_0 = 0$, (b) $0 < k_0 < k$, (c) $k_0 = k$. The corresponding asymptotic formulae (cf. [12], Ch. 13) for the solution to (1a) are given by

(6.8a)
$$B(\varphi) = \left(\frac{\pi}{2} - \varphi\right)^2 + o\left(\left(\frac{\pi}{2} - \varphi\right)^2\right) \qquad \varphi \leq \frac{\pi}{2} \ ,$$

(6.8b)
$$B(\varphi) = \sqrt{k_0} + \frac{4}{3}\sqrt{2}\left(\frac{k_0}{k}\left(1 - \frac{k_0}{k}\right)\right)^{1/4} (\varphi_0 - \varphi)^{3/2} + o((\varphi_0 - \varphi)^{3/2}) \quad \varphi \leq \varphi_0 \ ,$$

(6.8c)
$$B(\varphi) = \sqrt{k} - \alpha\varphi^2 + o(\varphi^2) \qquad \varphi \geq 0 \ ,$$

where α is a positive root of

$$\alpha^2 - \frac{2\alpha}{\sqrt{k}} + 1 = 0 \ . \tag{6.9}$$

Equation (9) has two positive solutions for $k < 1$, it has one for $k = 1$, and none for $k > 1$. Notice that when $B(\varphi_0) = \sqrt{k_0}, 0 < k_0 < k$, then by (8b) the solution to the initial value problem for (1a) has maximal domain $[0, \varphi_0]$ and it is only of class C^1 on this interval. □

LEMMA 6.3. *Let $\overline{B}(k;\varphi)$ be the solution of* (1). *Then*

$$\frac{\partial}{\partial k}\,\frac{\overline{B}(k;\varphi)}{\sqrt{k}} \le 0 \qquad k \in]0,\infty[\;,\; \varphi \in \left[0,\frac{\pi}{2}\right] \;. \tag{6.10}$$

Proof. For all $k \in]0,\infty[$ and all $\varphi \in \left[0,\frac{\pi}{2}\right]$ we define

$$b(k;\varphi) := \frac{\overline{B}(k;\varphi)}{\sqrt{k}} \;. \tag{6.11}$$

By (1), b satisfies the following equations

$$\frac{\partial b}{\partial \varphi} = -\frac{2}{\sqrt{k}}\,\sqrt{\cos^2\varphi - b^2}\;,\; b\left(k;\frac{\pi}{2}\right) = 0\;. \tag{6.12}$$

Differentiating in (12) with respect to k, we get

$$\frac{\partial}{\partial \varphi}\left(\frac{\partial b}{\partial k}\right) = \frac{1}{k^{3/2}}\,\sqrt{\cos^2\varphi - b^2} + \frac{1}{\sqrt{k}}\,\frac{2b}{\sqrt{\cos^2\varphi - b^2}}\,\frac{\partial b}{\partial k}\;,\; \frac{\partial b}{\partial k}\left(k;\frac{\pi}{2}\right) = 0\;. \tag{6.13}$$

Equation (1.3a) is known to be valid by Theorem 3.1 of [13], Ch. V. The solution of (13) satisfies

$$\frac{\partial b}{\partial k}(k;\varphi) = -\int_{\varphi}^{\pi/2} \frac{1}{k^{3/2}}\sqrt{\cos^2 x - b^2(x)}\,e^{-\int_{\varphi}^{x}\frac{1}{\sqrt{k}}\frac{2b(y)}{\sqrt{\cos^2\varphi - b^2(y)}}\,dy}\,dx\;. \tag{6.14}$$

This completes the proof of the Lemma. □

LEMMA 6.4. *The solution $\overline{B}$ of* (1) *satisfies*

$$\overline{B}(k;0)\begin{cases} = \sqrt{k} & \textit{for all} \quad k \in]0,1] \\ < \sqrt{k} & \textit{for all} \quad k \in]1,\infty[\;. \end{cases} \tag{6.15}$$

Furthermore,

$$\lim_{k\to\infty} \overline{B}(k;0) = 2\;. \tag{6.16}$$

Proof. It follows from Lemma 6.3 that if $k^* := \sup\{k \in]0,\infty[\,|\overline{B}(k;0) = \sqrt{k}\}$ then $\overline{B}(k;0) = \sqrt{k}$ for each $k \in]0,k^*]$. Moreover (15b) is an immediate consequence of the reasoning based on (8b) and (8c) since it ensures for $k > 1$ that $\overline{B}(k;0) \ne \sqrt{k}$. On the other hand (8c) is consistent with the possibility that k^* be any given number in $]0,1[$. Now it is easily checked that for $k = 1$ the function $B(\varphi) = \cos^2\varphi$ satisfies (1) as well as $B(0) = 1$. [It is worth mentioning that the likelihood of $k^* = 1$ was suggested by numerical computations (cf. Remark 2 below) prior to the discovery of the above explicit solution.]

Equation (16) follows from the asymptotic formula for (1) when $k \to \infty$:

$$B'_\infty = -2\cos\varphi \qquad , \quad B_\infty\left(\frac{\pi}{2}\right) = 0\;,$$

which yields $B_\infty(0) = 2$. □

REMARK 1. Note that Lemmata 6.2, 6.3 and 6.4 complete the proof of Lemma 5.2.

REMARK 2. Figure 1 shows the integral trajectory of (1) for $k = 1$ along with two other integral trajectories of (1a) originating from the inner ellipse with $k_0 = \frac{1}{2}$. (The dashed line is the outer ellipse.)

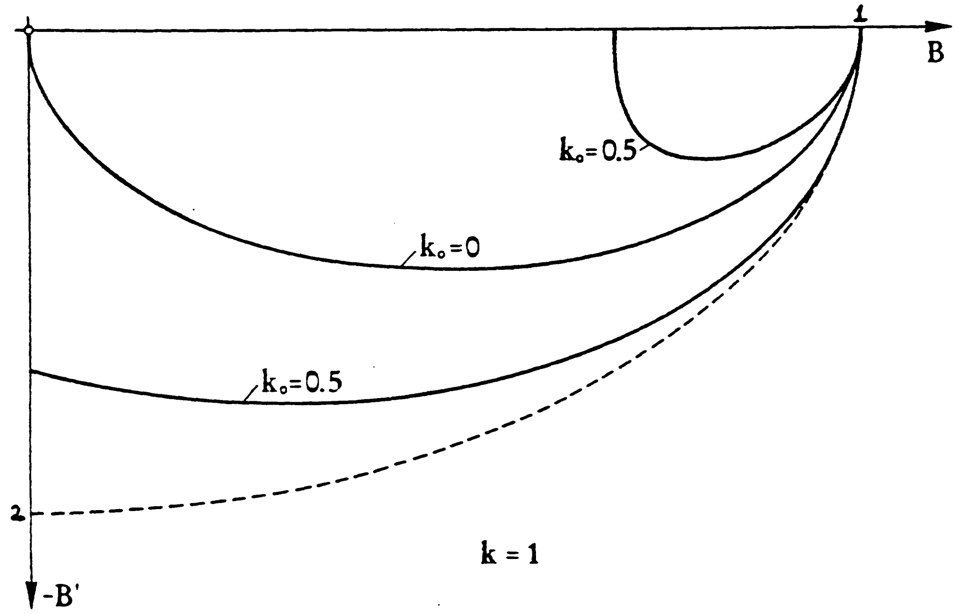

Figure 1

Figures 2 and 3 illustrate integral trajectories of (1a) for both $k < 1$ and $k > 1$.

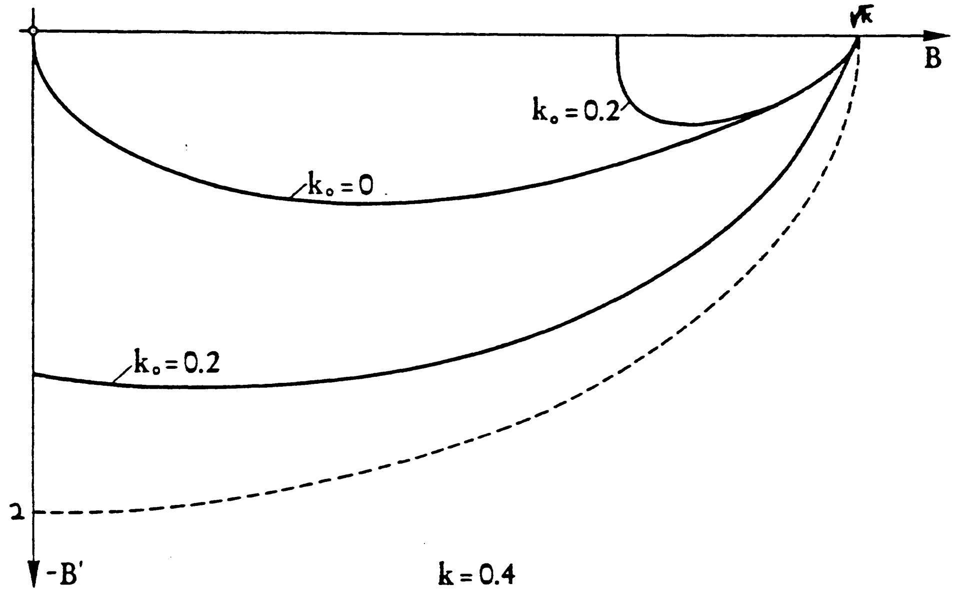

Figure 2

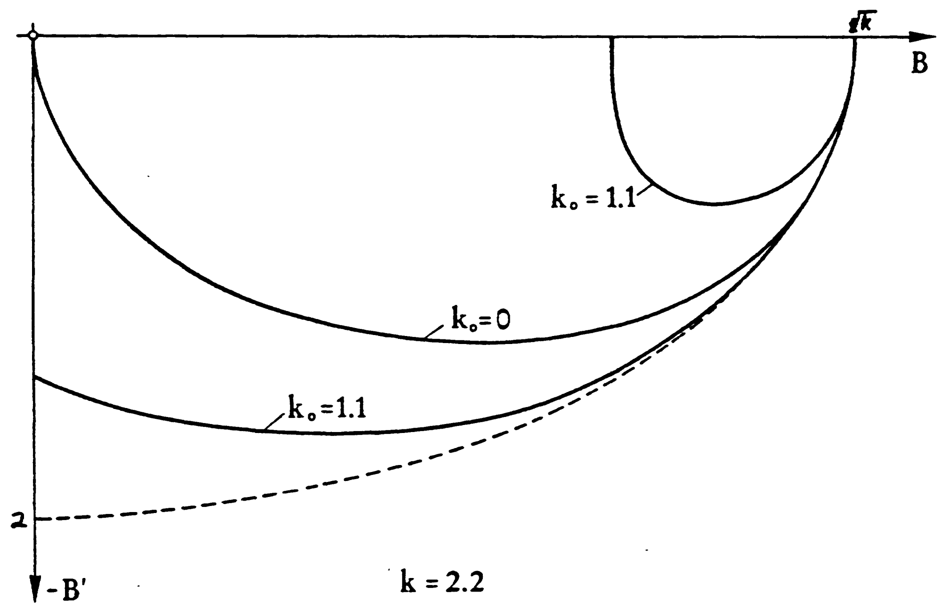

Figure 3

Figure 4 shows the graph of $\overline{B}(k;0)$ versus k; the dashed line is the graph of the function $k \mapsto \sqrt{k}$.

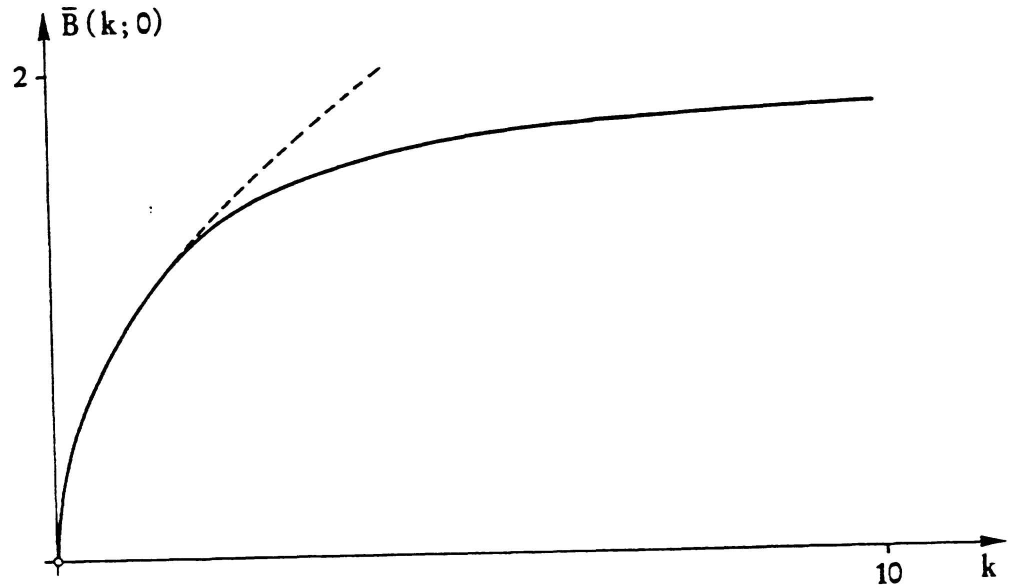

Figure 4

From Theorem 5.3 we know that

$$\min_{\mathfrak{C}} F = s_0^2 \overline{B}(k;0) . \tag{6.19}$$

Since $s_0 \leq 1$, comparing (19) with (1.10) and referring to (16) we learn that

$$\min_{\mathfrak{C}} F < F_{CK}[\varphi_{CK}] . \tag{6.20}$$

This inequality was already envisaged in [6], though in a special instance.

In the Lemmata below we take the last steps toward the proof of Theorem 6.1.

LEMMA 6.5. *For each $k \leq 1$ the solution of equation* (2) *satisfies* $\varphi(0^+) = 0$, *so that actually* $\varphi \equiv 0$ *and* $s(r) = s_0 \left(\frac{r}{R}\right)^{1/\sqrt{k}}$ *on* $[0, R]$.

Proof. Recall that (5.21a) states that $\varphi(0^+) \in \{0, \frac{\pi}{2}\}$ for $k \in]0,1]$. Now by the reasoning in Lemma 6.2 based on (8b), apart from the function $\varphi \equiv \frac{\pi}{2}$ which does not satisfy the boundary condition (2b), no solution φ of equation (2a) such that $\varphi(0^+) = \frac{\pi}{2}$ can satisfy $\varphi' = 0$ somewhere on $]0, R[$. Hence all such solutions satisfy $\varphi' < 0$ throughout $]0, R[$. In order for any such function to satisfy (2b) it would have to satisfy in the limit $r \to R$ the asymptotic approximation to (2a) near $\varphi = 0$, $B = \sqrt{k}$, namely (cf. (8c))

$$\varphi' = -\frac{\alpha \varphi}{r} .$$

However, the solutions of this equation with $\varphi' < 0$ have the form $\frac{\varphi(r)}{\varphi(r_0)} = \left(\frac{r_0}{r}\right)^\alpha$, $r \in]r_0, R[$ for some $r_0 \in]0, R[$, and hence do not vanish at R, contradicting the possibility $\varphi(0^+) = \frac{\pi}{2}$. Consequently $\varphi(0^+) = 0 = \varphi(R)$, whence $\varphi \equiv 0$ in $[0, R]$. □

LEMMA 6.6. *For $k > 1$ the solutions of* (2) *and* (3) *have the following asymptotic behavior as $r \to 0$:*

(6.21a) $$\varphi^*(r) = \frac{\pi}{2} - a^* r + o(r) ,$$

(6.21b) $$s^*(r) = s_0^* \left(1 + \frac{a^*}{2k} r^2\right) + o(r^2) ,$$

where both s_0^* and a^* are positive constants.

Proof. Recalling (5.21b) and inserting (8a) into both (2a) and (3a), we easily arrive at the expansions in (21). If a^* were to vanish then by use of (8a) the differential equation (2a) would ensure by uniqueness that $\varphi \equiv \pi/2$, contradicting (2b). Thus since $a^* \geq 0$ by Lemma 3.1, it follows that $a^* > 0$. Next consider what would occur if s_0^* were to vanish. In view of the form of (21b) and (8a) it would follow that s^* is a solution of a linear homogeneous equation whose coefficient is smooth at $r = 0$. Thus $s^*(0) = 0$ would imply $s^* \equiv 0$, contradicting (3b). This completes the argument. □

REMARK 3. Since $s^*(0) > 0$ for all $k > 1$, by Lemma 4.1 we see that $S(s^*) = \emptyset$. We now complete the proof of Theorem 6.1, recalling that $\varphi^{*'}(0) < 0$, by Lemma 6.6. By uniqueness for (2) it follows that $\varphi^{*'}(R) < 0$, as well.

We have computed both s^* and φ^* for different values of k. Their graphs are plotted in Figures 5 and 6.

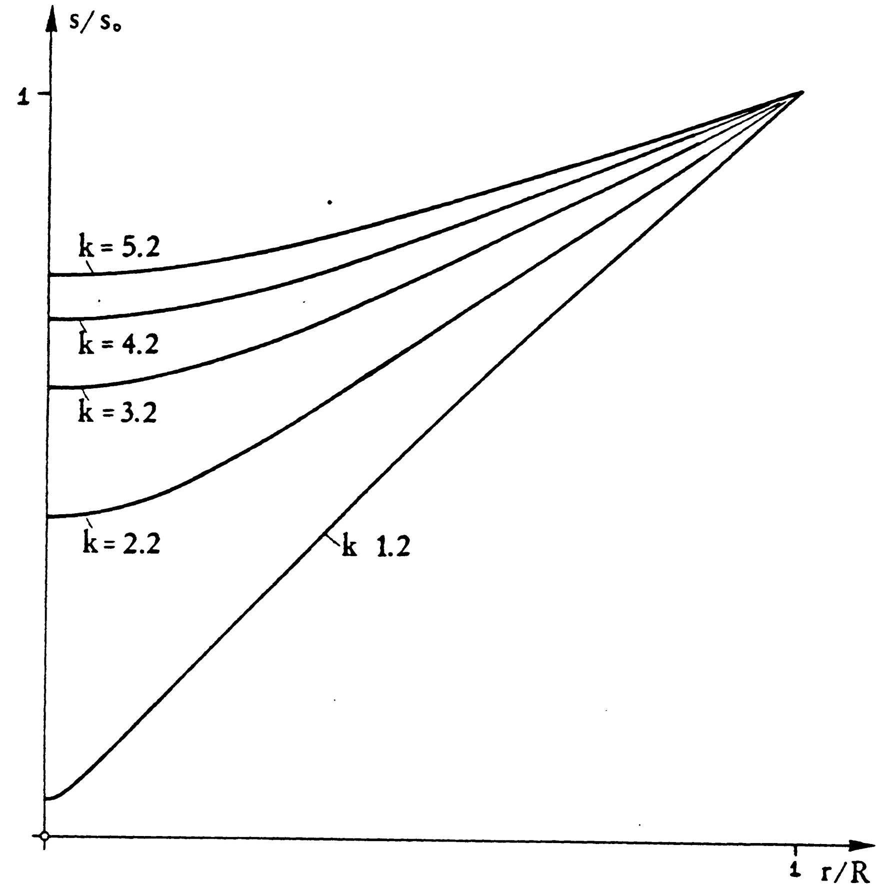

Figure 5

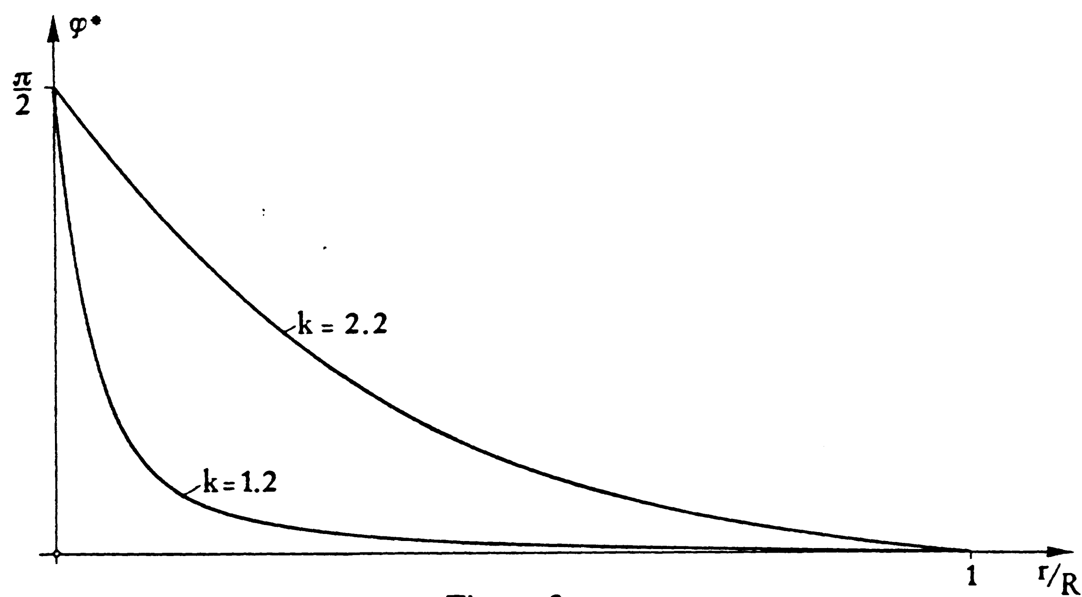

Figure 6

It is worth noting that while φ^* look much like φ_{CK} for all $k > 1$, s^* approaches 0 more rapidly near the axis of the cylinder as k gets closer to 1. Qualitatively, the size of the *core* where the liquid crystal is nearly isotropic becomes larger as k approaches 1 from above, while the orientation does not change dramatically.

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A version of Ericksen's order parameter theory of liquid crystals is studied in the case of a cylindrical container with anchoring on the curved surface only. The solutions are determined rather explicitly and the equilibrium orientation field is shown to vary between that of the FRANK solution (possessing an axial disclination) and that of the disclination-free CLADIS-KLEMAN solution as a scalar parameter in the free energy varies from 0 to ∞.

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