A Model for Disclinations in Nematic Liquid Crystal

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§1 Introduction

Nematic liquid crystals typically have many threadlike regions, called disclinations, along which the material displays singular behaviour. The standard Frank-Oseen model for nematic liquid crystals uses a field of unit-vectors to describe the equilibrium configurations, and line singularities in the vector field are interpreted as disclinations. The simplest possible line singularity has cylindrical symmetry, with a planar vector field that is everywhere radial and orthogonal to the cylinder axis. Such a disclination is a (formal) solution to the Frank-Oseen equilibrium equations, but the theory associates an infinite potential energy with this solution.

Physical arguments indicate that the difficulty of an infinite energy can be circumvented if the Frank-Oseen theory is modified by the addition of an extra variable called the order parameter. Ericksen (1976) describes this more general theory. The purpose of this note is to discuss some simple solutions of the extended model. In particular, it is shown that

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there is a solution described by a planar vector field with cylindrical symmetry that approximates a disclination, and which has finite energy.

It should be stated at the outset that the Frank-Oseen theory does admit a nonplanar singular solution with cylindrical symmetry and finite energy. The vector field corresponding to this configuration is parallel to the cylinder axis in the centre and then splays out to become a radial planar field. Moreover, there is considerable experimental evidence to suggest that amongst cylindrically symmetric singularities, the nonplanar configurations are the physically relevant ones (Williams et al, 1973). Nevertheless, there are more complicated singularities observed in experiment that cannot be fully described within the framework of the Frank-Oseen theory. Accordingly, an extended model is required, and this analysis can be regarded as a first simple investigation of one physically plausible modified theory.

§2 The Model

Ericksen (1976) assumes that any configuration of a nematic liquid crystal is described by a pair of functions $(n(x), S(x))$ defined over a region $\Omega \subset R^3$ containing the fluid, and that the equilibrium configurations are the extremals of a variational problem:

$$\min \int_{\Omega} W(n,S)\,dx\,, \qquad n\big|_{\partial\Omega} = n_0. \tag{2.1}$$

Here $n(x)$ is a unit vector called the director, and the scalar $S(x)$ is the order parameter or degree of orientation. The boundary condition that prescribes $n(x)$ on the surface $\partial\Omega$ is known as strong anchoring; other conditions are sometimes relevant.

Variational principle (2.1) reduces to the standard Frank-Oseen model if the variable S is assumed to be constant, that is $W(n,S) = W_1(n)$, and $W_1(n)$ is defined to be

$$2W_1(n) \equiv \kappa_1(\nabla\cdot n)^2+\kappa_2(n\cdot \mathrm{curl}\, n)^2 + \kappa_3\|n\times \mathrm{curl}\, n\|^2+(\kappa_2+\kappa_4)[\mathrm{tr}(\nabla n)^2+(\nabla\cdot n)^2] \qquad (2.2)$$

Here κ_1, κ_2, κ_3, and κ_4 are material constants.

The Frank-Oseen model gives excellent agreement with experiment, but it gives rise to the paradox concerning singularities that was described in §1. Several workers, for example Fan & Stephen (1970) and Fan (1971), argue that close to such singularities the scalar S cannot be accurately modelled as being constant. Accordingly, Ericksen (1985) proposed that W should take the form:

$$2W(n,S) = 2W_0(S) + S^2W_1(n) + \kappa_5\|\nabla S\|^2 + \kappa_6\|n\cdot\nabla S\|^2 . \qquad (2.3)$$

Here $W_0(S)\in C^2(-1/2,1)$ has the qualitative features of the function sketched in Figure 1, $W_1(n)$ is the Frank-Oseen energy defined in (2.2), and κ_5 and κ_6 are additional material constants. In the sequel the material constants κ_1, κ_5, and κ_6 will be assumed to satisfy the constitutive hypothesis

$$\kappa_5+\kappa_6>\kappa_1 . \qquad (2.4)$$

The role of this hypothesis is discussed in §8.

An <u>extremal</u> of (2.1) is a pair $(n(x), S(x))$ that satisfy the pertinent Euler-Lagrange equations and boundary conditions. With the further assumption that the "potential barrier" or "spinoidal" region of the function W_0 is sufficiently small (in a sense to be made precise), I shall show that when Ω is a circular cylinder, there is an extremal of (2.1) with W of the form (2.3), that has a line singularity in the vector field n(x), but has finite energy. Moreover, the singular vector field is everywhere radial and orthogonal to the cylinder axis.

§3 Cylindrical symmetry

The domain Ω is now taken to be a circular cylinder of radius R. The unit-vector n can be written in terms of the two scalar variables θ, and φ:

$$n(x) = \sin\theta\cos\varphi\, e_1 + \cos\theta\, e_2 + \sin\theta\sin\varphi\, e_3. \tag{3.1}$$

Here $\{e_1,e_2,e_3\}$ is the orthonormal basis for cylindrical coordinates (r,ψ,z) that is defined in terms of the usual Cartesian orthonormal basis $\{i,j,k\}$ by $e_1 = \cos\psi\, i + \sin\psi\, j$, $e_2 = -\sin\psi\, i + \cos\psi\, j$, and $e_3 = k$.

In principle, problem (2.1) can be stated in terms of the three scalar variables θ, φ, and S, which are each functions of the variables (r,ψ,z). We shall simplify our task by considering solutions that are both symmetric under rotations about the z-axis, and symmetric under translations along the z-axis; that is θ, φ, and S are assumed to be functions of r only. The following expressions can then be calculated:

$$\nabla\cdot n = r^{-1}\{r\sin\theta\cos\varphi\}', \tag{3.2}$$

$$n\cdot \operatorname{curl} n = -r\cos^2\theta\, \{r^{-1}\tan\theta\sin\varphi\}', \tag{3.3}$$

$$\operatorname{tr}(\nabla n)^2 = \{\sin\theta\cos\varphi\}'^2 - r^{-1}\{\cos^2\theta\}' + r^{-2}\sin^2\theta\cos^2\varphi\ , \tag{3.4}$$

$$\|n\times \mathrm{curl}\, n\|^2 = \sin^2\theta\cos^2\varphi\,\theta'^2 + \sin^4\theta\cos^2\varphi\,\varphi'^2$$
$$-2\sin^3\theta\cos\theta\sin\varphi\cos\varphi\,\theta'\varphi'$$
$$+\cos^2\theta\,\{r^{-1}\sin^2\theta\sin^2\varphi\}', \qquad (3.5)$$

$$\|\nabla S\|^2 = S'^2, \qquad \text{and} \qquad \|n\cdot\nabla S\|^2 = \sin^2\theta\cos^2\varphi\, S'^2. \qquad (3.6)$$

With the above expressions the energy density (2.3) can be expressed as a function $W(\theta(r),\varphi(r),S(r))$. Of course, this assumption of cylindrical symmetry, is only realistic if the imposed strong anchoring boundary conditions have the same symmetry.

The equilibrium equations are now a set of three coupled nonlinear ordinary differential equations that are the Euler-Lagrange equations of

$$\int_0^R r\, W(\theta(r),\varphi(r),S(r))\, dr. \qquad (3.7)$$

However the calculation of these equations is still a considerable task. Instead, symmetry is used to further simplify the problem.

§4 Solutions with No Twist

I define an equilibrium solution with no twist to be one for which $\theta(r)\equiv\pi/2$. On such solutions $n(r)$ has no azimuthal component. Consideration of (3.2) - (3.6) demonstrates that:

$$W(\pi/_2-\theta,\varphi,S) = W(\pi/_2+\theta,\varphi,S).$$

As a consequence, the Euler-Lagrange equation corresponding to θ must be satisfied for $\theta\equiv\pi/_2$, and the remaining two Euler-Lagrange equations can be determined after θ is set equal to $\pi/_2$. Of course, this procedure can only be adopted if such solutions are compatible with the boundary condition.

With $\theta \equiv \pi/_2$, the following expressions are obtained:

$$2W(\varphi,S) = 2W_0(S) + S^2 W_1(\varphi) + \{\kappa_5 + \kappa_6 \cos^2\varphi\} S'^2, \tag{4.1}$$

where

$$W_1(\varphi) = \{\kappa_1 \sin^2\varphi + \kappa_3 \cos^2\varphi\} \varphi'^2 + r^{-2} \kappa_1 \cos^2\varphi. \tag{4.2}$$

Accordingly the Euler-Lagrange equation with respect to φ is

$$\begin{aligned} -\{(\kappa_1 \sin^2\varphi + \kappa_3 \cos^2\varphi) S^2 r \varphi'\}' + \\ + \{(\kappa_1 - \kappa_3) \sin\varphi \cos\varphi\, \varphi'^2 r - \kappa_1 \cos\varphi \sin\varphi\, r^{-1}\} S^2 \\ - \kappa_6 \cos\varphi \sin\varphi\, S'^2 r = 0, \end{aligned} \tag{4.3}$$

and with respect to S is

$$-\{r(\kappa_5 + \kappa_6 \cos^2\varphi) S'\}' + rS\,W_1(\varphi) + rW_0'(S) = 0. \tag{4.4}$$

§5 A Planar Singular Solution of Finite Energy

When $\varphi(r) \equiv 0$, equation (4.3) is satisfied identically. The associated planar vector field has n everywhere purely radial, with no z-component, and the solution has a disclination on the z-axis. Equation (4.4) then becomes

$$-\{rS'\}' + \mu^2 r^{-1} S + r\,f(S) = 0, \tag{5.1}$$

where

$$\mu = \{\kappa_1/(\kappa_5 + \kappa_6)\}^{1/2}, \tag{5.2}$$

and

$$f(S) \equiv (\kappa_5 + \kappa_6)^{-1} W_0'(S). \tag{5.3}$$

The issue to be addressed is whether there is a nontrivial solution of (5.1) that satisfies the natural boundary condition

$$S'(R) = 0, \tag{5.4}$$

and which has finite energy.

Inspection of integral (3.7) and energy density (4.2) demonstrates that S must vanish at $r=0$ in order that the solution have finite energy. Moreover a series expansion about $r=0$ shows that the boundary condition

$$S(0) = 0 \tag{5.5}$$

is also sufficient to guarantee that the extremal in question has finite energy.

Existence of a nontrivial solution to boundary-value problem (5.1), (5.4) and (5.5) can be demonstrated by application of the theory of upper and lower solutions associated with monotone operators. One elementary, concise account of this technique is given by Hutson & Pym (1980, p211).

Equation (5.1) can be rewritten as

$$-\{rS'\}' + \{\mu^2/r + r\omega^2\}\, S \;=\; r\{\,\omega^2 S - f(S)\} \tag{5.6}$$

where ω^2 is a (large) constant chosen such that the right hand side is a monotone increasing function of S for $-1/2 < l \le S \le u < 1$, for given constants l and u. The assumed smoothness of $f(S)$ guarantees that such an ω^2 exists.

The left hand side of (5.6) is a modified Bessel operator which can be inverted with a positive Green's function $k(r,\rho)$, to obtain the integral equation

$$S = A[S], \tag{5.7}$$

where the nonlinear operator $A[.]$ is defined by

$$A[S](r) = \int_0^R \rho\; k(r,\rho)\;\{\omega^2 S(\rho) - f(S(\rho))\}\; d\rho. \tag{5.8}$$

If $\mu^2 < 1$ (cf. constitutive hypothesis (2.4) and definition (5.2)), the operator A is continuous from $L^2_r \to L^2_r$ (see, for example, Stakgold 1979 p.439) where the space L^2_r is the l^2-space on the interval [0,R] with weight function r. Moreover, by the choice of ω^2 and because the Green's function is positive, the operator A is monotone in the following sense:

if $v, w \in L^2_r$ satisfy $v(r) \leq w(r)$, a.e. , then $Av(r) \leq Aw(r)$, a.e. .

Upper and lower solutions of equation (5.7), say $l(r)$, $u(r) \in L^2_r$, are defined by the property $l(r) \leq Al(r)$, or $Au(r) \leq u(r)$, respectively. The abstract theory mentioned above exploits the monotonicity and continuity of the operator A to prove that if an upper and a lower solution satisfying $l(r) \leq u(r)$ can be found, then the sequences $A^n l$ and $A^n u$ both converge (in L^2_r) to solutions $\underline{S}(r)$, and $\overline{S}(r)$ of integral equation (5.7). Furthermore, the following bounds hold

$$l(r) \leq \underline{S}(r) \leq \overline{S}(r) \leq u(r). \qquad (5.9)$$

A standard argument can be used to demonstrate that the solutions of the integral equation are actually classical solutions of the pertinent boundary value problem.

In §6, I shall exhibit upper and lower solutions in C[0,R] that satisfy $-1/2 < l(r) \leq u(r) < 1$, and $l(r)$ is not less than the zero function. By the above development this is sufficient to guarantee the existence of a nontrivial solution to boundary value problem (5.1), (5.4) and (5.5).

Two remarks should be made. First, the above arguments provide a constructive iteration procedure by which solutions could be found. Second, there is often a uniqueness result associated with monotone iteration schemes (e.g. Stakgold, op.cit. p.612), but for the particular form of nonlinearity arising in this example the standard argument breaks down. Accordingly, it appears that the two solutions $\underline{S}(r)$ and $\overline{S}(r)$ could be distinct.

§6 Upper and lower solutions

Upper solutions of (5.7) are easily obtained. The one that will be used here is:

$$u(r) \equiv K_1 , \tag{6.1}$$

where the constant K_1 is the largest root of $f(S) = 0$ (cf. Figure 2).

Construction of lower solutions is more intricate, and several preliminary steps are necessary. Consider the nonhomogeneous Bessel equation:

$$-\{rv'\}' + \{\mu^2/r - r\} v = -r, \qquad v(0) = v'(0) = 0, \tag{6.2}$$

and define S^* and r^* to be the ordinate and abscissa of the first local maximum of the function $v(r)$ defined by (6.2). In the case $\mu = 1$, the function $v(r)$ is a Struve function, which functions are tabulated. In the more general case, simple contradiction arguments demonstrate that S^* and r^* satisfy the estimates

$$S^* > 1 + \{\mu/r^*\}^2, \tag{6.3}$$

and

$$\rho_1 < r^* \leq \rho_2 , \tag{6.4}$$

where ρ_1 is the abscissa of the first local maximum of $J_\mu(r)$ (i.e. the Bessel function of order $\mu>0$), and ρ_2 is the first nontrivial zero of $J_\mu(r)$.

The smallness condition on the nonlinear term can now be introduced. The assumption that will be made is that there exists a constant K with the property

$$f(x) \le \gamma^2(K/S^* - x), \quad -1/2 < x \le K. \tag{6.5}$$

Here γ^2 is defined to be

$$\gamma^2 = \{-f(K)/K\}\{S^*/(S^* - 1)\}. \tag{6.6}$$

Thus, condition (6.5) is the requirement that the straight line through the points $(0, K/S^*)$ and $(K, f(K))$ lies above the graph of f for $x \le K$ (cf. Figure 2).

If smallness requirement (6.5), and the further condition

$$\gamma R \ge r^*, \tag{6.7}$$

are satisfied, then the following function is a lower solution of integral equation (5.7) (cf. Figure 3):

$$l(r) = \begin{cases} (K/S^*)\, v(\gamma r), & 0 \le r \le r^*/\gamma, \\ K, & r^*/\gamma \le r \le R. \end{cases} \tag{6.8}$$

Recall that the function $v(r)$ was defined by (6.2). It is straightforward to verify that (6.8) represents a lower solution once it has been observed that, by (6.5) and (6.8), the function $l(r)$ satisfies (in a piecewise sense) the differential inequality:

$$-(rl')' + (\mu^2/r - \gamma^2 r)l + \gamma^2 K/S^*\, r \le -r\{f(l) + \gamma^2(l - K/S^*)\}. \tag{6.9}$$

Inequality (6.9) can be rewritten in the form

$$-(rl')' + (\mu^2/r + \omega^2 r)l \le r(\omega^2 l - f(l)), \tag{6.10}$$

and provided that (6.7) is valid, multiplication of (6.10) by the Green's function followed by integrations by parts over the intervals $[0, r^*/\gamma]$ and $[r^*/\gamma, R]$ yield the desired result, namely

$$l(r) \le Al(r). \tag{6.11}$$

It should be remarked that if condition (6.7) does not hold then boundary terms of the wrong sign appear in the integrations by parts, and (6.11) no longer follows from (6.10).

The lower solution $l(r)$ is sketched in Figure 3. In particular the following estimates hold

$$0 \le l(r) \le K \le K_1 = u(r). \tag{6.12}$$

Consequently, all the requirements of the previous section are satisfied, and the existence of a solution is guaranteed. Moreover $l(r)$ vanishes only at $r=0$, which, with the left hand inequality of (6.12), implies that the solution is nontrivial.

§7 Estimates on the solution

A major benefit of the existence result described in §§5 and 6 is that the solutions $\overline{S}$ and $\underline{S}$ satisfy bounds (5.9). Of course, when different upper and lower solutions are used in the existence proof, different estimates are obtained. In this section the parameters arising during the construction of the lower solution are varied, and improved estimates are obtained. Throughout, the upper solution is taken to be that given by (6.1). Consequently, because the sequence $A^n u(r)$ is independent of the choice of lower bound, the solution $\overline{S}$ is actually bounded below by the upper envelope of all lower solutions that are found. It should be reiterated that there is no guarantee that the solutions $\overline{S}$ and $\underline{S}$ coincide, and, as $\underline{S}$ depends upon the choice of lower bound, there is no estimate on $\underline{S}$ in terms of the envelope of lower solutions. Nevertheless, estimates can be obtained on one solution, namely $\overline{S}$.

A function of the general form (6.8) must satisfy inequalities (6.5) and (6.7) in order that it be a lower solution, and the existence result was predicated on there being one value of K that satisfies the inequalities. But typically one expects there to be either no such values of K, or a range of admissible values. In the latter case K can be regarded as a parameter in the problem.

If K is chosen to be as large as is permissible, the lower solution obtained eventually reaches a relatively high value, namely K, but has slow growth near $r=0$. This last conclusion arises because the assumed form of f (cf. Figure 2) associates a large value of K with a small value of γ. Contrariwise, when K is chosen to maximize $-f(K)/K$ amongst admissible K, the lower solution grows relatively quickly close to the origin, but is eventually smaller than lower solutions corresponding to larger values of K. The best of both worlds is obtained when the envelope of lower solutions is constructed.

A few remarks concerning the range of values of K are in order. First, it is pointless to consider values of K below that which maximizes $-f(K)/K$; the corresponding lower solutions lie entirely below some other lower solution. Thus maximization of $-f(K)/K$ provides an effective lower bound. Inequality (6.5) implies another lower-bound, and one of these two bounds determines the best growth estimate for small r.

Upper bounds on the range of admissible K are determined by (6.5) and (6.7). The domain size R appears only in (6.7), and this condition can be expected to be the active one in small domains. Notice that (6.5) is in some sense a measure of the "hump" region of f, and if this region is high (6.5) will determine the optimal bound. However there are cases of interest in which the energy density $W_0(S)$ has only an inflexion point at

$S=0$, with the associated function $f(S)$ being non-positive for $x \leq K_1$. In this circumstance (6.5) is irrelevant, and the upper bound is provided by (6.7). Notice that inequalities (6.3) and (6.7) imply that admissible K satisfy

$$-f(K)/K > \mu^2/R^2. \tag{7.1}$$

Consequently, the lower solution on any finite domain is strictly less than K_1.

More refined estimates can be obtained if S^* is also treated as a parameter. This strategy can be adopted if the inner-part of lower solution (6.8) is redefined in terms of the function $w(r) = \alpha J_\mu(r) + v(r)$, which is a solution of

$$-\{rw'\}' + \{\mu^2/r - r\}\, w = -r, \qquad w(0) = 0. \tag{7.2}$$

Here the constant α can be chosen such that the first local maximum of w is achieved at any r^* satisfying (6.4). Moreover, the corresponding value of S^* is given by the formula

$$S^*(r^*) = -\{r^* J_\mu'(r^*)\}^{-1} \int_0^{r^*} r J_\mu(r)\, dr. \tag{7.3}$$

The function $S^*(r^*)$ so defined is monotone decreasing in the interval $(\rho_1, \rho_2]$ with a local minimum at ρ_2. More importantly, inequality (6.3) remains valid when the left hand side is regarded as a function of r^*. All of the above arguments and estimates hold when S^* and r^* are interpreted in the sense of (7.3). The one added complication is that account must be taken of the requirement

$$l(r) > -{}^1/_2\,, \tag{7.4}$$

that was used in §5 to guarantee the monotonicity of the operator A.

Inequality (7.4) did not arise explicitly in §6 because it was satisfied trivially, the lower solution under consideration being positive. It appears that the values of α that arise are either positive, or negative and of small magnitude, so that (7.4) is not an active constraint, but I have not been able to prove this.

The more general interpretation of S^* strengthens the existence result described previously; the hypothesis that there exist a pair S^* and K satisfying the pertinent inequalities is a less stringent requirement than the hypothesis that there exist some K for a fixed value of S^*. However, when μ is close to one little benefit is gained. This is apparent from the tabulated values of the Struve function, which show that the simple definition of S^* given in §6 happens to be close to optimal. A numerical study for the case of small μ would be of some interest.

The main benefit of allowing S^* (or, equivalently, α) to vary, lies in the estimates that can be obtained. When α is positive the associated lower solutions have a positive derivative at $r = 0$. Consequently, although these lower solutions provide no better estimate at large values of r, the envelope of lower solutions obtained by varying both S^* and K is a significantly improved bound for small values of r.

The following less general version of the existence and estimate results is perhaps the most practical result described here. When μ is set equal to 1 in either the definition (6.2) of v(r), or (7.3) of w(r), it can be verified that the function l(r) that is constructed as before, is still a lower solution. Consequently, if inequalities (6.3), (6.5), and (7.4) hold for some S^* (defined with $\mu = 1$) and K, then there is a nontrivial extremal of finite energy for all values of $\mu < 1$. This result has associated estimates that are not as sharp as those described previously, but its main significance is that it encompasses the physically realistic case in which there is uncertainty in the value of μ.

§6 Discussion

The objective of this work was to model disclinations in nematic liquid crystals by a solution of Ericksen's model that has a planar vector field and finite energy. That goal has been attained under various simplifying assumptions and restrictions. The most restrictive condition is that of cylindrical symmetry, which reduces the governing equations to ordinary differential equations. This simplification has two justifications, it is required to make the problem tractable, and there is a reasonable expectation that singular solutions for more general domains and boundary conditions are a smooth perturbation of a radially symmetric singular solution.

The mathematical development is based on three hypotheses that are encapsulated in inequalities (2.4), (6.5) and (6.7). If any of these conditions fail, the method employed to prove existence breaks down. It has not been proven that the problem has no solution when the inequalities are invalid. However, each of the conditions has a plausible physical interpretation, so there is some possibility that the inequalities are not entirely technical artifices.

Inequality (2.4) is a constitutive hypothesis on various material constants. The condition is used to guarantee that the nonlinear operator A is continuous. To my knowledge there is no direct experimental evidence either to support or to refute the assumption. Indirect support for the validity of the condition is lent by the following argument. The Frank-Oseen model assumes the variable S to be constant, and the theory provides good agreement with experiment away from singularities. Accordingly, any modification of the Frank-Oseen theory should heavily penalize the appearance of gradients in S. Inequality (2.4) is a requirement of this type.

Inequalities (6.5) and (6.7) are coupled conditions of a somewhat complicated geometrical type, that are used in the construction of the lower solutions. Inequality (6.5) is primarily a restriction on the shape of the potential function $W_0(S)$, and (6.7) is primarily a restriction on the domain size (cf. Figures 1 & 2). Inequality (6.5) will be satisfied unless the barrier region of W_0 is too large in comparison to the depth of the wells, and this seems to be a physically reasonable requirement. Inequality (6.7) will be satisfied unless the domain size is too small. This is also a reasonable condition because the imposed boundary conditions are radial strong anchoring, and as the domain size approaches zero it is to be expected that the only solution is $S \equiv 0$, in which the molecules of the liquid crystal have no coherence.

Two issues have so far been ignored, namely: is the solution of the Euler-Lagrange equations that has been found either a global or local minimum of the potential? Neither of these questions has an obvious answer. As was mentioned in the Introduction, the Frank-Oseen model has a nonplanar singular extremal with finite energy that satisfies the radial boundary conditions described in §3. This solution has no twist ($\theta \equiv \pi/2$), and $\varphi(r)$ is defined implicitly by

$$r^2\varphi'^2 = \cos^2\varphi / \{\kappa_1 \sin^2\varphi + \kappa_3 \cos^2\varphi\}.$$

The function $\varphi(r)$ corresponds to a segment of the separatrix in the phase-plane diagram that arises after the change of variable $r = Re^t$. Presumably Ericksen's model has an analogous nonplanar singular solution, and, a priori, either of the two singular solutions could have the lesser energy. Verification of the conditions for a local minimum are also nontrivial. In particular, it appears that the second variation of (4.1) with respect to perturbations in S need not be positive definite. An analysis based on bifurcation theory might be profitably pursued here.

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References

J.L.Ericksen, 1976, Equilibrium theory of liquid crystals, in Advances in Liquid Crystals, Academic Press, New York.

J.L.Ericksen, 1985, Private communication.

C.Fan & M.J.Stephen, 1970, Isotropic nematic phase transitions in liquid crystals, Phys. Review Letters V.25 pp.500-503.

C.Fan, 1971 Disclination lines in liquid crystals, Phys. Letters V.34A pp.335-336.

V.Hutson & J.S.Pym, 1980, Applications of Functional Analysis and Operator Theory, Academic Press, New York.

I.Stakgold, 1979, Green's Functions and Boundary Value Problems, Wiley-Interscience, New York.

C.E.Williams, P.E.Cladis & M.Kleman, (1973), Screw disclinations in nematic samples with cylindrical symmetry, Mol. Cryst. & Liquid Cryst. V.21 pp.355-373.

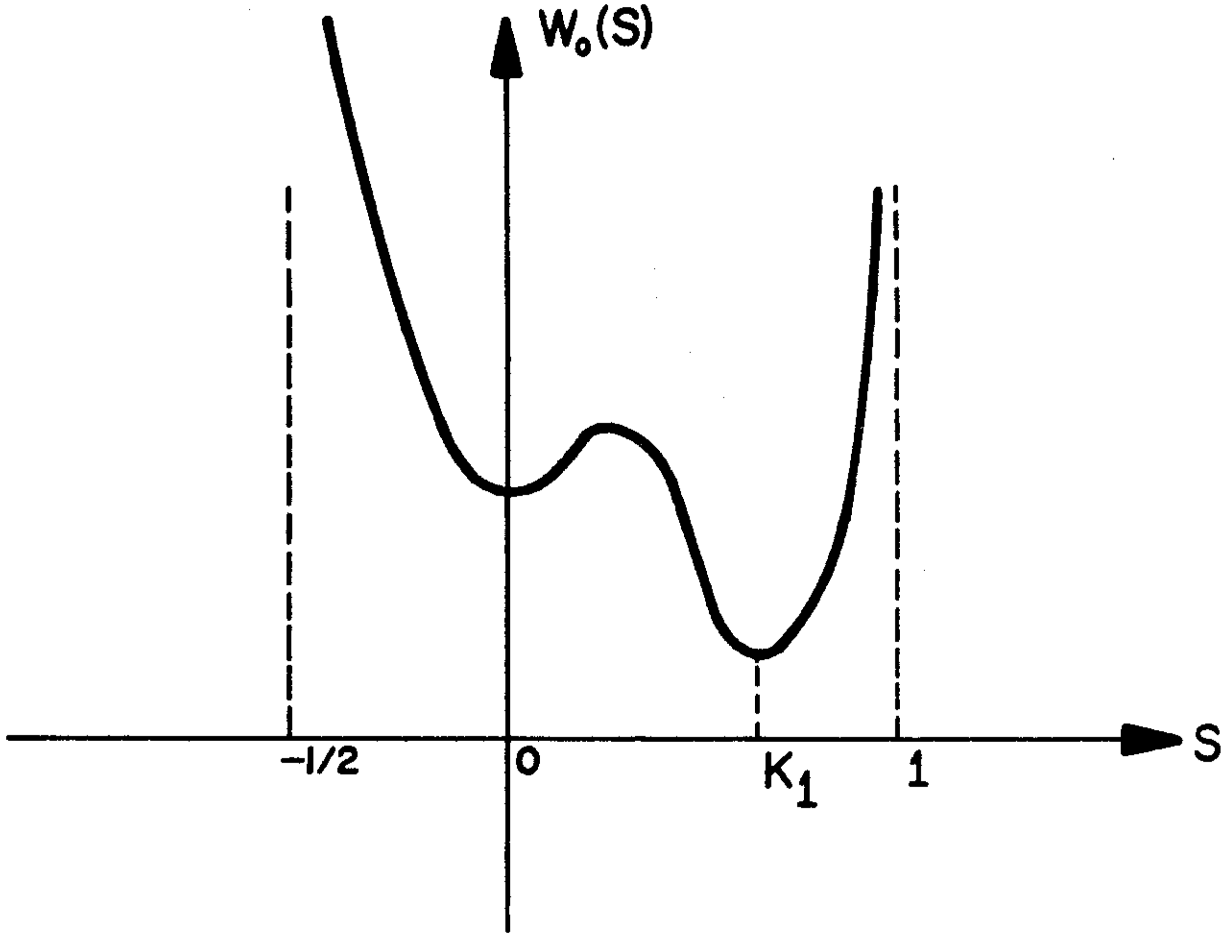

Figure 1: The qualitative form of potential $W_0(S)$. There is a global minimum at $S = K_1$, $0 < K_1 < 1$, and either a local minimum or inflexion point at $S = 0$.

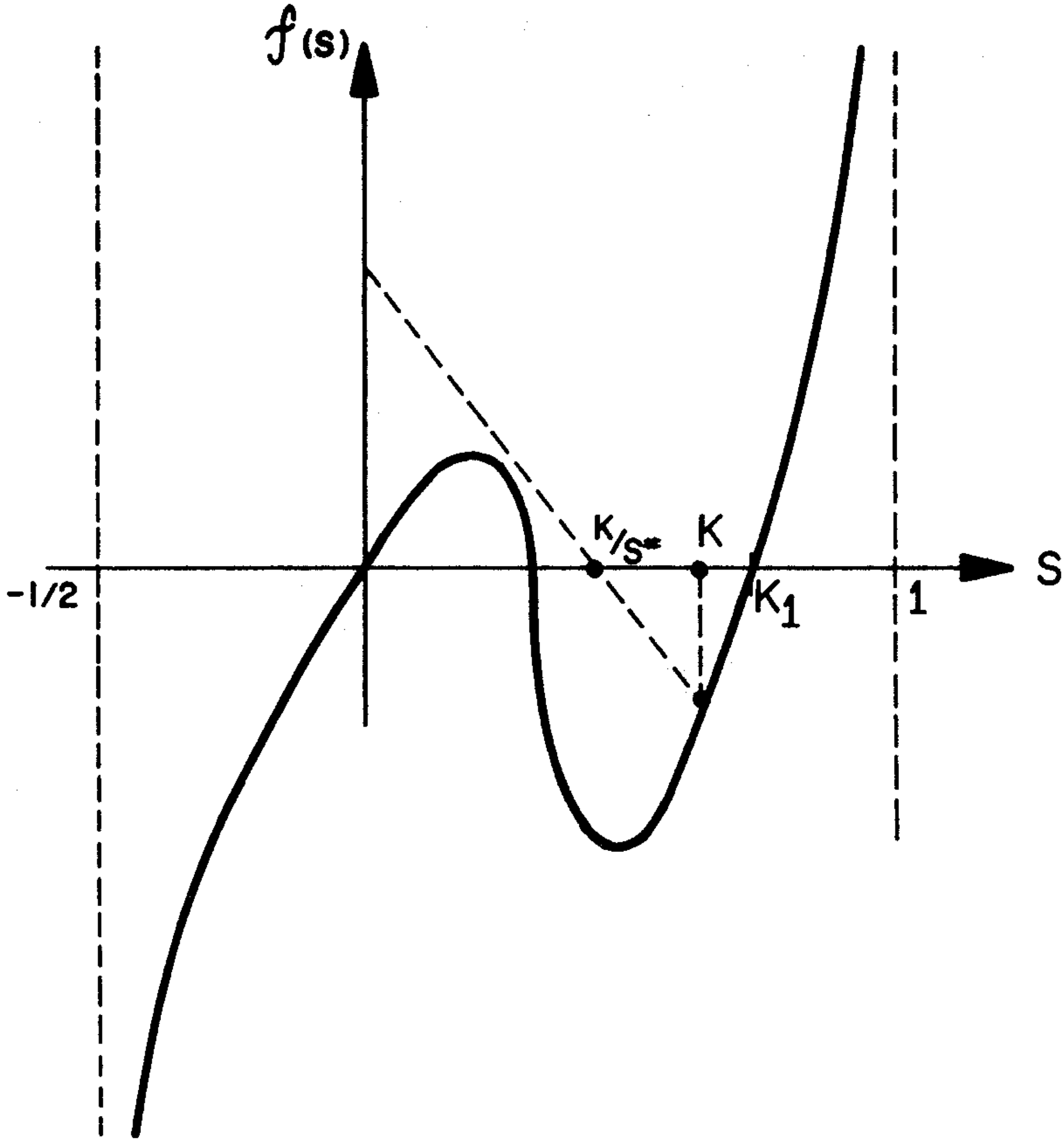

Figure 2: The qualitative form of the function f(s). H is assumed that for a given $S^* > 1$, there exists a constant K such that the line through the points $(K/S^*,0)$ and $(K,f(K))$ lies above the graph of f for $S < K$.

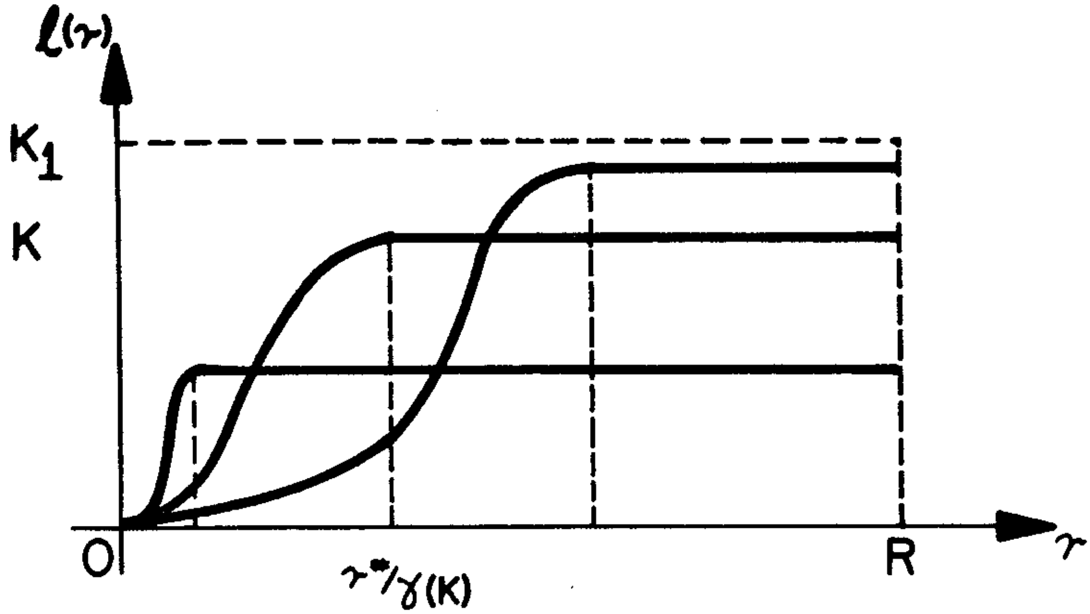

Figure 3: The qualitative form of the lower solution $\ell(r)$ defined in (6.8). K may assume a range of values, and three lower solutions are illustrated. The upper envelope of the lower solutions is a lower bound for a solution of integral equation (5.7).