NAMS
91-23

VARIATIONAL PROBLEMS FOR LIQUID CRYSTALS WITH VARIABLE DEGREE OF ORIENTATION

by

V. J. Mizel
Department of Mathematics
Carnegie Mellon University
Pittsburgh, PA 15213

WORKSHOP ON CALCULUS OF VARIATIONS AND NONLINEAR MATERIAL BEHAVIOR
November 1-4, 1990

Research Report No. 91-122-NAMS-23

July 1991

Variational Problems for Liquid Crystals with Variable Degree of Orientation

Victor J. Mizel, Department of Mathematics, CMU

This represents joint work with E. Virga and D. Roccato in the analysis of a model associated with J. Ericksen's recently proposed theory of nematic liquid crystals [Er]. In that theory an order parameter s is employed to describe the extent to which the local arrangement of molecules at a point lines up molecular axes sufficiently strongly to justify the nematic description via a unit vector which represents the optical axis of the material at the point in question. The parameter s varies between -1/2 and +1, with -1/2 corresponding to the case where all molecular axes are aligned parallel to a plane and +1 corresponding to the other extreme in which all the molecular axes are aligned along a fixed direction; the value s=0 indicates isotropy of the liquid crystal, in which the molecules are randomly distributed and the optical axis of the macroscopic site is undefined.

One goal of the analysis is to determine how well the model describes *defects,* namely regions or curves where the optical axis vector is a discontinuous function of position. Such defects are commonly observed in experiments on liquid crystals and the prediction of their occurrence provides a major test for the theorist.

In the present work we consider a finite cylinder of liquid crystal possessing a free energy density which is a (somewhat degenerate) case of the Ericksen scheme. The challenge is to analyze the analytic consequences of cylindrical symmetry for the equilibrium (i.e.,minimal energy) states and in particular to describe any cylindrically symmetric equilibrium states which possess defects.

The three dimensional bulk free energy involves both the order parameter s and the gradient of the optical axis field $\mathbf{n}$. The formula to which our simplification of Ericksen's energy density leads is:

$$\mathcal{F}[s,\mathbf{n}] = \kappa\int[k(\text{grad } s)^2 + s^2(\text{grad } \mathbf{n})^2]\, dV$$
$$= 2\pi H\kappa\; F[s, \varphi],$$

for a cylindrically symmetric configuration, where φ denotes the angle from the horizontal plane made by the unit vector $\mathbf{n}$ at any point, H denotes the height of the cylinder and κ is a material constant.

Here the reduced bulk energy F takes the form:

(1) $$F[s,\varphi] = \int_0^R [k(s')^2 + s^2((\varphi')^2 + (\cos^2\varphi)/r^2)]\ r dr,$$

where R is the radius of the cylinder and k is a material parameter. The corresponding reduced bulk energy for the classical Oseen-Frank theory [Fr] [Ch], which does not involve an order parameter, is given by:

$$\mathbb{F}[\varphi] = \int_0^R [(\varphi')^2 + (\cos^2\varphi)/r^2]\ r dr.$$

The problem which we analyze is that in which the optical axis is specified to be horizontal and pointed away from the axis of the cylinder at all points of the lateral boundary, but is unspecified at the circular faces of the cylinder. This reduces to the end condition

(2) $$\varphi(R) = 0.$$

It is worth noting that Frank observed that one choice of optical axis field **n** consistent with this condition is that in which $\mathbf{n} \equiv \mathbf{e_r}$ so that it is horizontal and points away from the axis of the cylinder at all points off the cylinder axis. This solution was consistent with certain experimental observations in which the cylindrical axis seemed to yield a defect curve or *disclination* for **n**. Nevertheless it was inconsistent with the requirement of being an energy minimizing field, since a simple computation reveals that $\mathbb{F}[\mathbf{e_r}] = \infty$. The clarification of this difficulty was provided by Cladis and Kle'man in [CK]. There they showed that the field **n** minimizing $\mathbb{F}$ is one in which

$$\mathbf{n} = (\cos\varphi)\ \mathbf{e_r} + (\sin\varphi)\ \mathbf{e_z},$$

where φ is a C^1 radial function which is 0 only for r= R, namely

$$\varphi(r) = \pi/2 - 2\arctan(r/R), \qquad r \in [0, R].$$

This particular field was described as *escaping into the third dimension*; although it is fluted at the cylindrical axis it does not possess a defect anywhere.

In order to examine the same situation for the order parameter model which leads to (1) we take, in addition to the *anchoring condition* (2) for **n,** a cylindrically symmetric lateral boundary condition for s:

(3) $$s(R) = s_0, \qquad \text{where } s_0 \in (0, 1].$$

The purpose of the present research was to analyze the variational problem (1) - (3). In particular it is of interest to ascertain whether the Cladis and Kle'man fluted solution or the Frank defect solution is more closely mirrored by the equilibrium **n** field which arises in the present model [note that with an appropriate field for the order parameter s the Frank solution does **not** require that $F[s,\varphi] = \infty$].

We proceed to describe the results obtained for the variational problem (1) - (3), hereafter denoted by (VP), where the admissible class is taken to be

$\mathcal{C} = \{(s,\varphi) \mid s \in AC[0,R], \varphi \in AC_{loc}((0,R)\backslash S(s)), s(R) = s_0 \in (0, 1], \varphi(R)=0\}$,

with $S(s) = \{r \in [0,R) \mid s(r) = 0\}$ the *singular set* on which the optical axis is undefined.

Direct comparisons demonstrate the validity of the following lemmas, where we resolve the fact that $\pm\varphi$ have the same effect on F by restricting attention to functions φ which are everywhere nonnegative.

Lemma 1 *If the pair* (s,φ) *minimizes* (VP) *then*

(a) $s(r) \geq 0, \quad \varphi(r) \leq \pi/2 \qquad$ for $r \in [0, R]$

(b) $s'(r) \geq 0, \quad \varphi'(r) \leq 0 \qquad$ a.e. $r \in [0, R]$

Lemma 2 *If the pair* (s,φ) *minimizes* (VP) *then either* $S(s) = \{0\}$ *or* $S(s) = \varnothing$.

Theorem A *If* $V(r_0;s_0,\varphi_0)$ *denotes the infimum for the variational problem analogous to* (VP) *in which the cylinder radius is taken to be* $r_0 \in \mathbb{R}$ and the boundary values for s,φ *are*

$$s_0 \in (0,1], \qquad \varphi_0 \in [0,\pi/2],$$

then the value function V *has the form*

$$V(r_0; s_0, \varphi_0) = s_0^2 B(\varphi_0).$$

Moreover the value of V at r_0, s_0, φ_0 *and the (unique) optimizing pair* (s^*, φ^*) *are determined (at points where* $s^*(r) \neq 0$*) as solutions of the following* <u>optimality system</u>:

$$B'(\varphi) = -2\sqrt{[\cos^2\varphi - (B(\varphi))^2/k]}, \qquad \varphi \in [\varphi_0, \pi/2],$$

$$B(\pi/2) = 0$$

$$(\#) \qquad \varphi'(r) = B'(\varphi(r))/2r, \qquad s'(r) = sB(\varphi(r))/kr, \quad \text{a.e. } r \in [0, r_0]\backslash S(s^*).$$

$$\varphi(r_0) = \varphi_0 \qquad\qquad s(r_0) = s_0$$

Theorem B *For each* $k > 0$ *the solution to the original problem*(VP) *is a solution to the optimality system* (#). *Moreover for* $s(R) = s_0$, $\varphi(R) = 0$, $k \in (0, 1]$ *the total energy is* $F[s^*, \varphi^*] = s_0^2 \sqrt{k}$. *In particular when* $s_0 = 1$, *for each* $k \in (0, 1]$ (*but for no* $k > 1$) *the optimal trajectories are given by*

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

so that $S(s^*) = \{0\}$ *and the axis* $r = 0$ *corresponds to a disclination defect.*

On the other hand, for each $k > 1$ *the optimal trajectories satisfy*

$$\varphi^{*\prime}(r) < 0, \qquad s^*(r) > 0, \quad r \in [0, R],$$

so that $S(s^*) = \varnothing$ *and there are no defects.*

We may summarize the results of the analysis by pointing out that when $k > 1$ then the solution does not possess defects and the optical axis field is similar to that of Cladis and Kle'man in the sense that it too escapes into the third dimension. By contrast, when $k \leq 1$ then the optical axis field is identical to the Frank solution and, in particular, possesses a defect along the cylindrical axis consistent with some of the experimental observations.

The full analysis, which makes use of Hamilton-Jacobi theory (i.e., *dynamic programming*), will appear in the Archive for Rational Mechanics and Analysis [MRV].

References

[Ch] S. Chandrasekhar, *Liquid Crystals*, Cambridge U. Press, Cambridge, 1977.

[CK] P.E. Cladis&M. Kle'man, Non-singular disclinations of strength $S = +1$ in nematics, J. Phys. (Paris) **33**(1972), 591-598.

[Er] J.L. Ericksen, Liquid crystals with variable degree of orientation, Archive for Rat. Mech. Anal. **113**(1991), 97-120.

[Fr] F.C. Frank, On the theory of liquid crystals, Discuss. Faraday Soc. **25**(1958), 19-28.

[MRV] V.J.Mizel, D.Roccato&E.G.Virga, A variational problem with variable degree of orientation, Res.Report 90-91-NAMS-6 (1990) Carnegie Mellon U. (to appear in Arch. Rat. Mech. Anal.)

MASTER COPY KEEP THIS COPY FOR REPRODUCTION PURPOSES

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE

3. REPORT TYPE AND DATES COVERED

4. TITLE AND SUBTITLE

Variational Problems for Liquid Crystals with Variable Degree of Orientation

5. FUNDING NUMBERS

6. AUTHOR(S)

Victor J. Mizel

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Carnegie Mellon University
Department of Mathematics
Pittsburgh, PA 15213

8. PERFORMING ORGANIZATION REPORT NUMBER

NAMS-23

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The analysis of a nematic liquid crystal, filling a bounded cylindrical container, whose free energy is a (simplified) version of Ericksen's model with variable degree of orientation, leads to a variational problem of the form

$$F[s,\phi] = \int_0^1 [k(s')^2 + s^2((\phi')^2 + \frac{\cos^2\phi}{r^2})]rdr$$

subject to $s(1) = s_0, \phi(1) = 0$, with k a positive constant.

It will be shown that a surprisingly explicit solution is obtainable. Moreover an interesting bifurcation takes place at $k = 1$.

14. SUBJECT TERMS

15. NUMBER OF PAGES 5

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

NSN 7540-01-280-5500

Standard Form 298 (Rev 2-89)
Prescribed by ANSI Std Z39-18
298-102