REMARKS ABOUT THE MATHEMATICAL THEORY OF LIQUID CRYSTALS

BY

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- 165 D. Arnold and R.S. Falk, Continuous Dependence on the Elastic Coefficients for a Class of Anisotropic Materials
- 166 I.J. Bakelman, The Boundary Value Problems for Non-linear Elliptic Equation and the Maximum Principle for Euler-Lagrange Equations
- 167 Ingo Müller, Gases and Rubbers
- 168 Ingo Müller, Pseudoplasticity in Shape Memory Alloys - an Extreme Case of Thermoelasticity
- 169 Luis Magalhães, Persistence and Smoothness of Hyperbolic Invariant Manifolds for Functional Differential Equations
- 170 A. Damiani and M. Vogelius, Homogenization limits of the Equations of Elasticity in Thin Domains
- 171 H.C. Simpson and S.J. Spector, On Hadamard Stability in Finite Elasticity
- 172 J.L. Vazquez and C. Yaurur, Isolated Singularities of the Solutions of the Schrödinger Equation with a Radial Potential
- 173 G. Dal Maso and U. Mosco, Wiener's Criterion and Γ -Convergence
- 174 John H. Maddocks, Stability and Folds
- 175 R. Hardt and D. Kinderlehrer, Existence and Partial Regularity of Static Liquid Crystal Configurations
- 176 M. Nerukar, Construction of Smooth Ergodic Cycles for Systems with Fast Periodic Approximations
- 177 J.L. Ericksen, Stable Equilibrium Configurations of Elastic Crystals
- 178 Patricio Aviles, Local Behavior of Solutions of Some Elliptic Equations
- 179 S.-N. Chow and R. Lauterbach, A Bifurcation Theorem for Critical Points of Variational Problems
- 180 R. Pego, Phase Transitions: Stability and Admissibility in One Dimensional Nonlinear Viscoelasticity
- 181 Mariano Giaquinta, Quadratic Functions and Partial Regularity
- 182 J. Bona, Fully Discrete Galerkin Methods for the Korteweg De Vries Equation
- 183 J. Maddocks and J. Keller, Mechanics of Robes
- 184 F. Bernis, Qualitative Properties for some nonlinear higher order Nonlinear Higher Order Parabolic Equations with Asymptotic Rates for some Bernis, Finite Speed of Propagation and Asymptotic Rates for some
- 185 F. Bernis, Game Forms with Minimal Strategy Spaces
- 186 S. Reichelstein and S. Reiter, Problem on Boundedness
- 187 An Answer to Littlewood's Problem on Periodic Media
- 188 J. Rubinstein and P.E. Sogami, Dispersion and Convection in Periodic Media
- 189 W.H. Fleming and P.E. Sogami, Asymptotic Series and the Method of Vanishing Viscosity
- 190 H. Beltracchi, Existence and Asymptotic Behavior for Strong Solutions of Navier-Stokes Equations in the Whole Space
- 191 L.A. Caffarelli, J.L. Vazquez, and N.I. Wolanski, Lipschitz Continuity of Solutions and Interfaces of the N-Dimensional Porous Medium Equation
- 192 R. Johnson, m-Functions and Floquet Exponents for Linear Differential Systems
- 193 F.V. Atkinson and L.A. Peletier, Ground States and Dirichlet Problems for $-\Delta = F(u)$ in $\mathbb{R}^n$
- 194 G. Dal Maso, U. Mosco, The Wiener Modulus of a Radial Measure
- 195 H. A. Levine and H.F. Weinberger, Inequalities between Dirichlet and Neumann Eigenvalues
- 196 J. Rubinstein, On the Macroscopic Description of Slow Viscous Flow Past a
- 197 G. Dal Maso and U. Mosco, Wiener Criteria and Energy Decay for Relaxed Dirichlet Problems
- 198 V. Ofler and P. Walfman, On the Monge-Ampere Equation Arising in the Reflect Mapping Problem
- 199 M. Chipot, D. Kinderlehrer and L. Caffarelli, Some Smoothness Properties of Linear Laminates
- 200 Y. Giga and R. Kohn, Characterizing Blow-up Using Similarity Variables
- 201 P. Cannarsa and H. M. Sonner, On the Singularities of the Viscosity Solutions to Hamilton-Jacobi-Bellman Equations
- 202 Andrew Majda, Nonlinear Geometric Optics for Hyperbolic Systems of Conservation Laws
- 203 G. Buttazzo, G. Dal Maso and U. Mosco, A Derivation Theorem for Capacities with Respect to a Radon Measure
- 204 S. Cowlin, M. Mehrabadi, On the Identification of Material Symmetry for Anisotropic Elastic Materials
- 205 R.W.R. Darling, Constructing Nonhomeomorphic Stochastic Flows.
- 206 M. Chipot, On the Reynolds Lubrication Equation
- 207 R.V. Kohn and G.W. Milnor, On Bounding the Effective Conductivity of Anisotropic Composites
- 208 I.J. Bakelman, Notes Concerning the Torsion of Hardening Rods and its N-Dimensional Generalizations
- 209 I.J. Bakelman, The Boundary Value Problems for Non-linear Elliptic Equations
- 210 Guanglu Gong and Mingping Qian, On the Large Deviation Functions of Markov Chains
- 211 Arle Leizarowitz, Control Problems with Random and Progressively Known Targets
- 212 R.W.R. Darling, Ergodicity of a Measure-Valued Markov Chain Induced by Random Transformations
- 213 G. Gong, M. Qian and Zhongxin Zhao, Killed Diffusions and its Conditioning
- 214 Arle Leizarowitz, Controlling Diffusion Processes on Infinite Horizon with the Overfaking Criterion
- 215 Milard Beatty, The Poisson Function of Finite Elasticity
- 216 David Terman, Traveling Wave Solutions Arising From a Combustion Model
- 217 Yuh-Jia Lee, Sharp Inequalities and Regularity of Heat Semi-Group on Infinite Dimensional Spaces
- 218 D. Stroock, Lecture Notes
- 219 Claudio Canuto, Spectral Methods and Maximum Principle
- 220 Thomas O'Brien, A Two Parameter Family of Pension Contribution Functions and Stochastic Optimization
- 221 Takeyuki Hida, Analysis of Brownian Functionals
- 222 Leonid Hurwicz, On Information Decentralization and Efficiency of Resource Allocation Mechanisms
- 223 E.B. Fabes and D.W. Stroock, A New Proof of Moser's Parabolic Harnack Inequality via the Old Ideas of Nash
- 224 Minoru Murata, Structure of Positive Solution to $(-\Delta + V)u = 0$ in $\mathbb{R}^n$
- 225 Paul Dupuis, Large Deviations Analysis of Reflected Diffusion
- 226 F. Bernis, Constrained Stochastic Approximation Algorithms in Convex Sets
- 227 S. Orey and S. Pelikan, Existence Results for Doubly Nonlinear Higher Order Parabolic Equations on Unbounded Domains.
- 228 R. Gulliver and S. Hildebrandt, Boundary Configurations Spanning Continua of Minimal Surfaces.
- 229 J. Baxter, G. Dal Maso, U. Mosco, Stopping Times and T-Convergence.
- 230 Juffo Bouillet, Self-Similar Solutions, Having Jumps and Intervals of Constancy of a Diffusion-heat Conduction Equation
- 231 R. Hardt, D. Kinderlehrer & F.-H. Lin, A Remark About the Stability of Smooth Equilibrium Configurations of Static Liquid Crystal
- 232 M. Chipot and M. Luskin, The Compressible Reynolds Lubrication Equation
- 233 J.H. Maddocks, A Model for Disclinations in Nematic Liquid Crystal
- 234 C. Folas, G.R. Sell and R. Temam, Inertial Manifolds for Nonlinear Evolutionary Equations
- 235 P.L. Chow, Expectation Functionals Associated with Some Stochastic Evolution
- 236 Giuseppe Buttazzo, Reinforcement by a Thin Layer with Oscillating Thickness
- 237 W.H. Fleming, S.J. Sheu and H.M. Sonner, On Existence of the Dominant Eigenfunction and its Application to the Large Deviation Properties of an Ergodic Markov Process
- 238 R. Jensen and P.E. Sogami, A Regularity Result for Viscosity Solutions of Hamilton-Jacobi Equations in one Space Dimension
- 239 B. Boczar-Karakl, J.-L. Bona and D.L. Cohen, Interaction of Shallow-Water Waves and Bottom Topography
- 240 F. Colonius and W. Klemann, Infinite Time Optimal Control and Periodicity Dirichlet Problems

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5 JOB NUMBER[illegible]

Remarks about the mathematical theory of liquid crystals

Robert Hardt, David Kinderlehrer, and Mitchell Luskin

dedicated to Hans Lewy

1. Liquid crystals and liquid crystal theory

A liquid crystal is a mesomorphic phase of a material which occurs between its liquid and solid phases. Frequently the material is composed of rod like molecules which display orientational order, unlike a liquid, but lacking the lattice structure of a solid. It may flow easily and so may also be thought of as an anisotropic fluid. This anisotropy is evident in the way it transmits light; for example, a nematic liquid crystal is optically uniaxial. We take this opportunity to discuss a few of the analytical and computational issues which arise in the attempt to study static equilibrium configurations. One attractive feature of this subject is that it has a well developed continuum description in the Ericksen-Leslie theory [9].

Some of the questions have significance in the context of harmonic mappings into the sphere and we shall attempt to clarify these connections. Indeed, at this point in time, we are able to answer questions about harmonic mappings which we had not conceived of asking several years ago. This is especially true of the study of singularities, cf. sect. 4 and the recent work of Brezis, Coron, and Lieb [2], [3] and the authors [18].

A general exposition of the static theory is given in Ericksen [9]. The flow theory is developed in Leslie [22], cf. also [23]. Accessible books about this subject have been written by de Gennes [8] and Chandross [6]. What we describe here is primarily work with F.-H. Lin [15],[16]. The numerical aspects have been studied with R. Cohen and S. Y. Lin [7]. A more complete exposition of the topics discussed here may be found in [14]. The volume [11] is a source of contemporary issues in liquid crystal research. A particular experiment which has served as a focus for us and to which we have returned frequently to test our ideas and our results is related by Williams, Pieranski, and Cladis [27]. This is also described in the expository article of Brinkman and Cladis [4]. A retrospective view of the issues posed by this experiment is given in sect. 6.

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The kinematic variable in the nematic and cholesteric phases, which are our concern, may be taken to be the optic axis, which is a unit vector field n defined in the region Ω occupied by the material. The bulk energy at fixed temperature is given by the Oseen-Frank density

$$W(\nabla n, n) = \frac{1}{2} \kappa_1 (\text{div} n)^2 + \frac{1}{2} \kappa_2 (n \cdot \text{curl} n + q)^2 + \frac{1}{2} \kappa_3 (n \wedge \text{curl} n)^2 + \frac{1}{2} \alpha (\text{tr}(\nabla n)^2 - (\text{div} n)^2), \quad (1.1)$$

where the constants $\kappa_i > 0$, $i = 1, 2, 3$, q and α are real. A static equilibrium configuration corresponds to an extremal of the functional defined by W , namely,

$$\delta \int_{\Omega} W(\nabla n, n) dx = 0. \quad (1.2)$$

(figure)

Another means of understanding the differences between ordinary liquids and liquid crystals may be achieved by examining the stress of the material as a function of temperature, (figure). In the high temperature isotropic phase,

$$T = -p1$$

where p is a constant, whereas in the liquid crystal phases T has a molecular component,

$$T = -p1 + T_M$$

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$$T_M = wI - (\partial w / \partial \nabla n) \nabla n^T ,$$

cf. [9]. For a solid, the stress is rather complicated.

With (1.2) in mind, it is reasonable to seek equilibrium configurations by a variational principle. A typical situation, called strong anchoring in the literature, is to prescribe the optic axis on the boundary $\partial\Omega$ of the region $\Omega \subset \mathbb{R}^3$ occupied by the fluid. So let n_0 be defined on $\partial\Omega$ with $|n_0| = 1$ and

$$Q(n_0) = \{ u \in H^1(\Omega; \mathbb{R}^3) : |u| = 1 \text{ in } \Omega \text{ and } u = n_0 \text{ on } \partial\Omega \}. \quad (1.3)$$

Problem Find

$$n \in Q(n_0) : \int_{\Omega} W(\nabla n, n) \, dx = \inf_{Q(n_0)} \int_{\Omega} W(\nabla u, u) \, dx . \quad (1.4)$$

We have been rather glib in our choice of admissible functions. It is not obvious that $Q(n_0)$ is not empty nor that W is coercive in a suitable sense. We return to this in section 2. In as much as the variational problem (1.4) is constrained, some observations may be in order.

1. In the special case

$$\kappa_1 = \kappa_2 = \kappa_3 = \alpha = 1 \text{ and } q = 0,$$

$$W = \frac{1}{2} |\nabla n|^2 , \quad (1.5)$$

which is the integrand for a harmonic mapping of Ω into S^2 . The equilibrium equation here is the system

$$\Delta n + |\nabla n|^2 n = 0 \text{ in } \Omega, \quad (1.6)$$

which exhibits quadratic growth in $|\nabla n|$. This is a known peril in the study of elliptic systems, [5],[13].

2. The constraint on n seems to be very mild considering those imposed on the determinant of a deformation gradient in finite

$$T_m = W - \int_{\partial\Omega} \nabla u^6 \cdot \nu^T.$$

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Problem Find

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elasticity, but it leads to an equilibrium equation which, unlike (1.6), is not always elliptic. This is because the Lagrange multiplier generally involves second derivatives. The implications of this are not well understood. However, it seems evident that continuity methods will be of little use to find and analyze solutions.

3. When the degree of $n_0: \partial\Omega \rightarrow S^2$ differs from zero, it does not admit any smooth extensions to Ω . Thus any element of $\Omega(n_0)$ must have singularities. Singularities are called defects in the liquid crystal literature. They give insight into the behavior of the material.

4. There can be many solutions for given boundary data. Circumstances which ensure uniqueness are known only in special cases.

5. Other fields may be imposed, especially magnetic or electric ones, cf. Ericksen [9], de Gennes [8], or [14],[16] for a mathematical treatment.

2. Existence

To begin our discussion we state

Proposition 2.1 If $\partial\Omega$ is Lipschitz and n_0 is Lipschitz, then $\Omega(n_0) \neq \emptyset$.

The proof of this is given in [16], Lemma 1.1. A more complete, if more technical discussion, of this point will be given later.

In order to have a reasonable theory, we would prefer that a solution $n \in H^1(\Omega; S^2)$. Are there any conditions for which

$$W(\nabla u, u) \geq \text{const.} |\nabla u|^2 \quad ? \quad (2.1)$$

If such a constant exists in a class of functions, the boundary conditions of this class must play a role. The unconstrained functional is not coercive on $H^1(\Omega; S^2)$. Brief consideration of the cases $\alpha = 0$ and α very large serve to convince one of this. To resolve this issue, observe that

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3. When the degree of u_0 is $2s + 2$, it does not admit any smooth extensions to Ω . Thus any element of $D(u_0)$ must have singularities. Singularities are called defects in the fluid crystal literature. They give insight into the behavior of the material.

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In order to have a reasonable theory, we would prefer that a solution $u \in H^1(\Omega; \mathbb{R}^2)$. Are there any conditions for which

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if such a constant exists in a class of functions, the boundary conditions of this class must play a role. The unconstrained functional is not coercive on $H^1(\Omega; \mathbb{R}^2)$. Brief consideration of the cases $\alpha = 0$ and α very large serve to convince one of this. To resolve this issue, observe that

$$\begin{aligned}
 S(\nabla u) &= \frac{1}{2}(\text{tr}(\nabla u)^2 - (\text{div} u)^2) \\
 &= \frac{1}{2}\text{div}(\nabla u u - \text{div} u u)
 \end{aligned}
 \tag{2.2}$$

is a divergence. Indeed, as observed by Ericksen [10] and Oseen, it is a surface energy in the sense that

$$\int_{\Omega} S(\nabla u) \, dx = \int_{\partial\Omega} f(\nabla_{\text{tan}} u, u) \, dx = \int_{\partial\Omega} f(\nabla_{\text{tan}} n_0, n_0) \, dx$$

depends only on n_0 for $u \in Q(n_0)$. Obviously,

$$-\text{div} S_p(\nabla u) = 0 \quad \text{in } \Omega \text{ for any } u,$$

so this term offers no contribution to the equilibrium equations. For this reason it is often dropped and, in fact, there are no known ways to measure the constant α experimentally. For the same motive, it may be added to W . Choosing

$$\alpha = \min\{\kappa_1, \kappa_2, \kappa_3\} > 0,$$

it is elementary to calculate ([16], Lemma 1.4) that

$$W(\nabla n, n) \geq \frac{1}{2} \alpha |\nabla n|^2.$$

Thus by addition of a constant to W , it becomes coercive on $Q(n_0)$. We assume this to be done, which leads to the

Theorem 2.2 *There is at least one $n_0 \in Q(n_0)$ satisfying (1.4).*

3. Examples

If Ω is diffeomorphic to a ball and the degree of the data $n_0: \partial\Omega \rightarrow S^2$ is not zero, then any solution must have singularities. Moreover, Hardt and Lin [20] give an example of an n_0 with degree zero for which any minimizing n must have singularities.

Solutions of the equilibrium equations (1.6), the equal constant or

$$(2.2) \quad 2(\nabla u) = \kappa(\operatorname{div} u) - \kappa(\nabla u) \cdot \nabla u$$

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$$\int_{\Omega} 2(\nabla u) \, dx = \int_{\partial\Omega} \kappa(u, u) \, d\mathcal{H}^n = \int_{\partial\Omega} \kappa(u, u) \, d\mathcal{H}^n$$

depends only on u for $u \in Q(u)$. Obviously,

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so this term offers no contribution to the equilibrium equations. For this reason it is often dropped and, in fact, there are no known ways to measure the constant κ experimentally. For the same motive, it may be added to W choosing

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It is elementary to calculate ([16], Lemma 1.4) that

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Solutions of the equilibrium equations (1.6), the dual constant or

harmonic mapping case, may be constructed by homogeneous extension of conformal mappings of S^2 onto itself. Such mappings are essentially rational functions of z or $\bar{z}$. More precisely, let Π denote stereographic projection of S^2 from the north pole onto an equatorial plane and f a rational function of z so that

$$\Pi^{-1} f(\Pi \xi) \quad \text{and} \quad \Pi^{-1} f(\overline{\Pi \xi}), \quad \xi \in S^2,$$

are conformal and anticonformal maps of S^2 onto itself. Then for any $\Omega \subset S^2$,

$$\begin{aligned} \text{and} \quad n(x) &= \Pi^{-1} f(\Pi(x/|x|)) \\ n(x) &= \Pi^{-1} f(\overline{\Pi(x/|x|)}) \end{aligned} \quad x \in \Omega \quad (3.1)$$

are solutions of (1.6).

Write $f = p/q$ with p and q relatively prime polynomials and set

$$\deg f = \max\{\deg p, \deg q\}.$$

The solutions (3.1) have the special property that

$$\rho^{-1} \int_{B_\rho} |\nabla n|^2 dx = 8\pi \deg f \quad (3.2)$$

for any $\rho > 0$.

Another family of solutions easy to construct is what serves as the analogue of viscometric flows in fluids or St.-Venant solutions in elasticity. These are the solutions which lie in a plane. They illustrate the instability and the non-uniqueness of solutions as well. We found this with M. Luskin. For example,

$$n(x) = (\cos qx_3, \sin qx_3, 0) \quad (3.3)$$

is a solution of (1.2) for any choice of constants. Generalizing this but confining our attention to the equal constant case, suppose that

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harmonic mapping case, may be constructed by homogeneous extension of conformal mappings of S^2 onto itself. Such mappings are essentially rational functions of z or $\bar{z}$. More precisely, let π denote stereographic projection of S^2 from the north pole onto an equatorial plane and f a rational function of z so that

$$S^2 \ni z \mapsto \pi^{-1}(f(z)) \text{ and } \pi^{-1}(f(\bar{z}))$$

are conformal and anticonformal maps of S^2 onto itself. Then for any $\Omega \subset S^2$,

$$(1.2) \quad \Omega \ni x \quad \begin{aligned} \pi^{-1}(f(x)) &= (x) \text{ and} \\ \pi^{-1}(f(\bar{x})) &= (x) \end{aligned}$$

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Write $f = p/q$ with p and q relatively prime polynomials and set

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The solutions (3.1) have the special property that

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Another family of solutions easy to construct is what serves as the analogue of viscous flows in fluids or St.-Venant solutions in elasticity. These are the solutions which lie in a plane. They illustrate the instability and the non-uniqueness of solutions as well. We found this with M. Lukin. For example,

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is a solution of (1.2) with finite Dirichlet integral. One may infer from this, [1] for example, the existence of an angle

$$\theta \in H^1(\Omega): -\Delta \theta = 0 \quad \text{in } \Omega \quad (3.5)$$

such that

$$\begin{aligned} n &= (\cos \theta, \sin \theta, 0), \\ |\nabla n|^2 &= |\nabla \theta|^2. \end{aligned} \quad (3.6)$$

In particular, all planar solutions are smooth. However, they are not always stable. Suppose that $\Omega = B_{2r}$ and let

$$u(x) = \cos \eta(x) n(x) + \sin \eta(x) e, \quad x \in B_{2r}, \quad (3.7)$$

where $e = e_3$ and η is a suitable cut-off function,

$$\begin{aligned} \eta &= 0 \quad \text{on } \partial B_{2r}, \quad |\nabla \eta| \leq \pi/2r, \\ &\quad \pi/2 \quad \text{in } B_r. \end{aligned}$$

Thus $u = n$ on ∂B_r and, by (3.6),

$$|\nabla u|^2 = \cos^2 \eta |\nabla \theta|^2 + |\nabla \eta|^2 \quad (3.8)$$

Hence for some constant $C > 0$,

$$\int_{B_{2r}} |\nabla u|^2 dx \leq \int_{B_{2r} - B_r} |\nabla \theta|^2 dx + Cr.$$

Now n fails to minimize whenever

$$\int_{B_{2r} - B_r} |\nabla \theta|^2 dx + Cr < \int_{B_{2r}} |\nabla \theta|^2 dx,$$

or whenever

$$C < r^{-1} \int_{B_r} |\nabla \theta|^2 dx. \quad (3.9)$$

is a solution of (1.2) with finite Dirichlet integral. One may infer from this, [1] for example, the existence of an angle

$$(3.2) \quad \theta \in H^1(\Omega); \quad -\Delta \theta = 0 \quad \text{in } \Omega$$

such that

$$(3.3) \quad \begin{aligned} n &= (\cos \theta, \sin \theta), \\ |\nabla n|_2 &= |\nabla \theta|_2. \end{aligned}$$

In particular, all planar solutions are smooth. However, they are not always stable. Suppose that $\Omega = B^2$ and let

$$(3.4) \quad u(x) = \cos \pi(x)u(x) + \sin \pi(x)v(x), \quad x \in B^2.$$

where $e = e_3$ and π is a suitable cut-off function,

$$\pi = 0 \quad \text{on } \partial B^2, \quad |\nabla \pi|_2 \geq \pi/2 \quad \text{in } B^2.$$

Then $u = u$ on ∂B^2 and, by (3.3),

$$(3.5) \quad |\nabla u|_2 = \cos \pi |\nabla \theta|_2 + |\nabla \pi|_2$$

Hence for some constant $C > 0$,

$$\int_{B^2} |\nabla u|_2^2 dx \geq \int_{B^2} |\nabla \theta|_2^2 dx + C.$$

Now u fails to minimize whenever

$$\int_{B^2} |\nabla \theta|_2^2 dx + C < \int_{B^2} |\nabla \theta|_2^2 dx,$$

or whenever

$$(3.6) \quad C < \int_{B^2} |\nabla \theta|_2^2 dx.$$

Let θ be harmonic in all of $\mathbb{R}^3$. Then (3.9) holds for r sufficiently large unless $\theta = \text{const.}$ First, it is easily shown that for any harmonic θ ,

$$M(r) = r^{-1} \int_{B_r} |\nabla \theta|^2 dx$$

is an increasing function of r . If it remains bounded, then so does

$$M(a,r) = r^{-1} \int_{B_r(a)} |\nabla \theta|^2 dx$$

for any $a \in \mathbb{R}^3$. On the other hand, by the subharmonic character of $|\nabla \theta|^2$,

$$\begin{aligned} |\nabla \theta(a)|^2 &\leq |B_r|^{-1} \int_{B_r(a)} |\nabla \theta|^2 dx \\ &\leq (4/3)\pi r^{-2} M(a,r) \rightarrow 0, \quad \text{as } r \rightarrow \infty, \end{aligned}$$

whenever $M(a,r)$ remains bounded. Thus $\theta = \text{const.}$

We have shown that

a harmonic mapping of $\mathbb{R}^3$ into S^2 whose image lies in a plane and which minimizes energy with respect to its boundary values on arbitrarily large balls is constant.

Consider now a smooth harmonic function $\theta(x)$ for which $n(x)$ defined by (3.6) does not minimize energy on a ball B . By the existence theorem, there is some minimizing $n^* \in Q(n)$ and if it is also planar, there is a harmonic function $\theta^* \in H^1(B)$ for which $\cos \theta = \cos \theta^*$ and $\sin \theta = \sin \theta^*$ on ∂B . Hence

$$\theta - \theta^* \in H^1(B) \quad \text{and} \quad \theta - \theta^* \text{ has discrete values on } \partial B.$$

But this can only happen if $\theta - \theta^*$ is constant, whence $n = n^*$. So the minimum n^* is not planar, and has a nonzero component n^{*3} . Since the energies of n^* and $(n^{*1}, n^{*2}, -n^{*3})$ are the same, the minimum is not unique and there are at least three solutions of the equilibrium equation (1.6) in B with the same boundary values on ∂B , [19].

Let θ be harmonic in all of $\mathbb{R}^3$. Then (3.2) holds for r sufficiently large unless $\theta = \text{const}$. First, it is easily shown that for any harmonic θ ,

$$M(r) = r^{-1} \int_{\mathbb{R}^3} |\nabla \theta|^2 dx$$

is an increasing function of r . If it remains bounded, then so does

$$M(s, r) = r^{-1} \int_{\mathbb{R}^3(s)} |\nabla \theta|^2 dx$$

for any $s \in \mathbb{R}^3$. On the other hand, by the subharmonic character of $|\nabla \theta|^2$,

$$|\nabla \theta(s)|^2 \geq |\nabla \theta|^{-1} \int_{\mathbb{R}^3(s)} |\nabla \theta|^2 dx$$

$$2 \leq (4\pi)^{-1} M(s, r) \rightarrow 0 \text{ as } r \rightarrow \infty.$$

whenever $M(s, r)$ remains bounded. Thus $\theta = \text{const}$.

We have shown that

a harmonic mapping of $\mathbb{R}^3$ into $\mathbb{S}^2$ whose image lies in a plane and which minimizes energy with respect to its boundary values on arbitrarily large balls is constant.

Consider now a smooth harmonic function $\theta(x)$ for which $n(x)$ defined by (3.6) does not minimize energy on a ball B . By the existence theorem, there is some minimizing $n^* \in Q(n)$ and it is also planar, there is a harmonic function $\theta^* \in H^1(B)$ for which $\cos \theta^* = \cos \theta$ and $\sin \theta^* = \sin \theta$ on ∂B . Hence

$$\theta^* - \theta \in H^1(B) \text{ and } \theta^* - \theta \text{ has discrete values on } \partial B.$$

But this can only happen if $\theta^* - \theta$ is constant, whence $n^* = n$. So the minimum n^* is not planar, and has a nonzero component n^*_3 . Since the energies of n^* and $(n^*_1, n^*_2, -n^*_3)$ are the same, the minimum is not unique and there are at least three solutions of the equilibrium equation (1.6) in B with the same boundary values on ∂B , [12].

Planar solutions have also been studied by E. MacMillan [24]. The instability of the solution (3.3) has been checked numerically.

4. Regularity theory

We begin our brief discussion of the regularity theory for liquid crystals by stating our principal result.

Theorem 4.1 *Let n be a minimum of W , that is, a solution of (1.4). Then*

(1) *There exist constants σ and C (depending on κ_1) such that if*

$$r^{-1} \int_{B_r(a)} W(\nabla n, n) \, dx < \sigma,$$

then

(i) $\rho^{-1} \int_{B_\rho(a)} W(\nabla n, n) \, dx \leq C\rho, \quad \rho \leq r/2, \text{ and}$

(ii) n is Hölder continuous in a neighborhood of a .

(2) *There is a relatively compact subset $Z \subset \Omega$ such that*

$$n|_{\Omega-Z} \text{ is analytic and } \mathcal{H}^1(Z) = 0.$$

In the statement above, $\mathcal{H}^1(X)$ denotes the 1-dimensional Hausdorff measure of X . The proofs of these statements are in Corollary 2.5 and Theorem 2.6, [16]. Part (2) may be extended to the boundary of Ω , Theorem 5.6 [16]. Analogous theorems hold when the effects of magnetic or electric fields are included.

The main idea in the proofs is to use the blow-up method, which has a long history dating at least to Almgren, DeGiorgi, and Guisti-Miranda. The method is also closely related to the Schoen-Uhlenbeck [26] argument for harmonic mappings, but it differs significantly from this even though the equal constant case concerns harmonic mappings. There are three elements to the argument which we found unusual:

1. The blow-up sequence is normalized by energy instead of radius.

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4. Regularity theory

We begin our brief discussion of the regularity theory for liquid crystals by stating our principal result.

Theorem 4.1. Let n be a minimum of W , that is, a solution of (1.1). Then there exist constants α and C (depending on n) such that if

$$\int_{B_r(a)} |\nabla n|^2 dx < \alpha, \quad (4.1)$$

then

$$|\nabla n| \leq C \quad \text{in } B_{r/2}(a), \quad (4.2)$$

$$n \text{ is Hölder continuous in a neighborhood of } a. \quad (4.3)$$

$$\text{There is a relatively compact subset } \Sigma \subset \Omega \text{ such that} \quad (4.4)$$

$$n|_{\Sigma} \text{ is analytic and } H^1(\Sigma) = 0.$$

In the statement above, $H^1(X)$ denotes the 1-dimensional Hausdorff

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1. The blow-up sequence is normalized by energy instead of radius.

2. The blow up limit is the solution of a linear system with two dependent variables.
3. An estimate due to Hardt and Lin,[21], cf also Lemma 2.3 [16].

Rather than give technical details of proofs, let us describe the Hardt-Lin estimate and illustrate some of its additional consequences. Let n be a minimizer of W in Ω and suppose that $B_{2\rho} \subset \Omega$. Then there is a constant $C_0 = C_0(\kappa_1, \kappa_2, \kappa_3)$ such that

$$\int_{B_\rho} |\nabla n|^2 dx \leq C_0 \left(\int_{\partial B_\rho} |\nabla n|^2 dS \int_{\partial B_\rho} |n - \bar{n}|^2 dS \right)^{1/2} \quad (4.1)$$

for any $\bar{n} \in \mathbb{R}^3$.

This estimate reads precisely as the Schoen-Uhlenbeck estimate of [26], but there it is required that the right hand side of (4.1) be very small before the inequality be valid. Here are some applications:

1. Upper density bound *There is a number $M = M(\kappa_1, \kappa_2, \kappa_3)$ such that*

$$\limsup_{\rho \rightarrow 0} \rho^{-1} \int_{B_\rho(a)} W(\nabla n, n) dx \leq M, \quad a \in \Omega, \quad (4.2)$$

for any minimizer n of W in Ω .

It is to be emphasized that the number M does not depend on the boundary values of n nor on the domain Ω , but only on the material constants $\kappa_1, \kappa_2, \kappa_3$. As a special case, consider the solutions of the equilibrium equation (1.6) which are given by homogeneous extension of conformal maps of S^2 into itself, cf. (3.1), for which (3.2) holds. They are smooth mappings except at $x = 0$, where they have singularities of degree equal to $\deg f$. If the $\deg f$ is large enough that

$$8\pi \deg f > M,$$

then the associated n is not a minimizer. *There is a maximum possible degree of a stable singularity of a harmonic mapping.*

2. The blow up limit is the solution of a linear system with two dependent variables.
3. An estimate due to Hardy and Lin [21], cf also Lemma 2.3 [16].

Rather than give technical details of proofs, let us describe the Hardy-Lin estimate and illustrate some of its additional consequences. Let n be a minimizer of W in Ω and suppose that $\Omega \subset \mathbb{R}^n$. Then there is a constant $C = C(n, k_1, k_2)$ such that

$$(4.1) \quad \int_{\Omega} |\nabla n|^2 dx \leq C \int_{\Omega} |\nabla n|^2 dx \quad \text{for any } n \in \mathbb{R}^n.$$

This estimate reads precisely as the Schoen-Uhlenbeck estimate of [26], but there it is required that the right hand side of (4.1) be very small before the inequality be valid. Here are some applications:

1. Upper density bound. There is a number $M = M(n, k_1, k_2)$ such that

$$(4.2) \quad \limsup_{r \rightarrow 0} \frac{1}{r^n} \int_{B_r} |\nabla n|^2 dx \leq M, \quad \text{if } \Omega \subset \mathbb{R}^n.$$

for any minimizer n of W in Ω .

It is to be emphasized that the number M does not depend on the boundary values of n nor on the domain Ω , but only on the material constants k_1, k_2, k_3 . As a special case, consider the solutions of the equilibrium equation (1.6) which are given by homogeneous extension of conformal maps of $\mathbb{R}^2$ into itself, cf. (3.1), for which (3.2) holds. They are smooth mappings except at $x = 0$, where they have singularities of degree equal to $\deg$. If the $\deg$ is large enough that

$$\deg > M,$$

then the associated n is not a minimizer. There is a maximum possible degree of a stable singularity of a harmonic mapping.

We prove this statement, which follows in an elementary way from the estimate (4.1). Restricting our attention to the equal constant case, set $\bar{n} = 0$. Note that

$$\int_{\partial B_\rho} |n|^2 dS = |\partial B_\rho| = 4\pi\rho^2$$

implies that

$$\int_{B_\rho} |\nabla n|^2 dx \leq C\rho \left(\int_{\partial B_\rho} |\nabla n|^2 dS \right)^{1/2}.$$

We square this and integrate it from r to $2r$, using the most elementary estimates for the various terms.

$$\begin{aligned} \left(\int_{B_\rho} |\nabla n|^2 dx \right)^2 &\leq C^2 \rho^2 \int_{\partial B_\rho} |\nabla n|^2 dS, \\ r \left(\int_{B_r} |\nabla n|^2 dx \right)^2 &\leq 4C^2 r^2 \int_{B_{2r}} |\nabla n|^2 dx, \\ (r^{-2} \int_{B_r} |\nabla n|^2 dx)^2 &\leq 4C^2 r^{-1} \int_{B_{2r}} |\nabla n|^2 dx. \end{aligned} \tag{4.3}$$

Set

$$E(\rho) = \rho^{-1} \int_{B_\rho(a)} |\nabla n|^2 dx,$$

which allows us to rewrite (4.3) as

$$E(r)^2 \leq ME(2r) \quad \text{or} \quad E(\tfrac{1}{2}r)^2 \leq ME(r) \quad \text{whenever } B_{2r} \subset \Omega.$$

This may be iterated in the following way:

$$E(2^{-k}r)^{2^k} \leq M^{2^k} E(r) \quad \text{or}$$

$$E(2^{-k}r) \leq ME(r)^{-2^k}.$$

Letting $k \rightarrow \infty$, we obtain that $E(0) \leq M$.

We prove this statement, which follows in an elementary way from the estimate (4.1). Restricting our attention to the equal constant case, set $\bar{n} = 0$. Note that

$$\int_{\partial B} |\nabla u|^2 dx = |\partial B| = 4\pi b^2$$

implies that

$$\int_{\partial B} |\nabla u|^2 dx \geq C(b) \int_{\partial B} |\nabla u|^2 dx^2.$$

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261

$$E(b) = \int_{\partial B} |\nabla u|^2 dx^2.$$

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Letting $k \rightarrow \infty$, we obtain that $E(0) \geq M$.

Now the M established by our estimate is very general in that it holds for any liquid crystal integrand, even when contributions are given by other energies. In the harmonic mapping case, it ought to be possible to give a precise statement, as was suggested when the conference on which this note is based was presented. In the meantime, our numerical results had shown that the minimizer associated to the boundary values determined by $f(z) = z^2$ had two singularities of degree one and markedly less energy than its homogeneous extension, Cohen et al [7].

This was taken up by Brezis, Coron, and Lieb [2],[3] who proved the remarkable result that in the harmonic mapping case $M/8\pi = 1$, so that only singularities of degree one are present in minima, and moreover such singularities are, asymptotically, homogeneous extensions of rotations.

2. Higher integrability *There is a $q > 2$ such that*

$$n \in H^{1,q}_{loc}(\Omega; S^2) \quad (4.4)$$

for any minimizer n of W in Ω .

The estimate (4.1) permits us to show (4.4) by a reverse Holder inequality, cf. [12],[13],[25]. As a consequence, $\mathcal{H}^{1-\delta}(Z) = 0$ for some $\delta > 0$, slightly improving (2) of Theorem 4.1. There remains the question of whether the singular set Z consists in fact of only isolated points as in the harmonic mapping case [26].

3. Convergence of minimizers *If $\{n_i\}$ is a sequence of minimizers of W in Ω which converges weakly in $H^1(\Omega; S^2)$ to n , then a subsequence $\{n_{i_j}\}$ converges strongly in $H^1(\Omega; S^2)$ to n and n is also a minimizer of W .*

For the proofs of these statements, we refer to [18].

A major step in the proof of (4.1) is to show that for any $v \in H^1(B)$, with $|v| = 1$ on ∂B , or equivalently, for any $v \in H^{1/2}(\partial B)$ with $|v| = 1$, there is a $\zeta \in H^1(B)$ satisfying

$$|\zeta| = 1 \quad \text{in } B \quad \text{and}$$

Now the M established by our estimate is very general in that it holds for any kind of integral, even when contributions are given by other energies. In the harmonic mapping case, it ought to be possible to give a precise statement, as was suggested when the conference on which this note is based was presented. In the meantime, our numerical results had shown that the minimizer associated to the boundary values determined by $f(z) = z^2$ had two singularities of degree one and markedly less energy than its homogeneous extension, Cohen et al [7].

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2. Higher integrability There is a $p > 2$ such that

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for any minimizer u of W in Ω .

The estimate (4.1) permits us to show (4.4) by a reverse Hölder inequality, cf. [12], [13], [25]. As a consequence, $M^{1/2}(z) = 0$ for some z slightly improving (2) of Theorem 4.1. There remains the question of whether the singular set S consists in fact of only isolated points as in the harmonic mapping case [26].

3. Convergence of minimizers If (u_n) is a sequence of minimizers of W in Ω which converges weakly in $H^1(\Omega; \mathbb{R}^2)$ to u , then a subsequence $(u_{n'})$ converges strongly in $H^1(\Omega; \mathbb{R}^2)$ to u and u is also a minimizer of W .

For the proofs of these statements, we refer to [18].

A major step in the proof of (4.1) is to show that for any $v \in H^1(B)$ with $|v| = 1$ on ∂B , or equivalently, for any $v \in H^1(B)$ with $|v| = 1$, there is a $\zeta \in H^1(B)$ satisfying

$$|\zeta| = 1 \quad \text{in } B \quad \text{and}$$

$$\int_B |\nabla \zeta|^2 dx \leq 32 \left(\int_{\partial B} |\nabla_{\tan} v|^2 dS \int_{\partial B} |v - c|^2 dS \right)^{1/2}, \quad (4.5)$$

for any $c \in \mathbb{R}^3$. In this way we may place the issue of admissibility in its proper functional setting:

4. Admissibility *If Ω is diffeomorphic to a ball and $n_0 \in H^{1/2}(\partial\Omega)$, then $\Omega(n_0) \neq \emptyset$.*

5. Computational results

Two numerical algorithms have been employed to compute minimum energy configurations. The results of these experiments illustrate that the functions $n_f(x)$ defined by (3.1) with $f(z) = z$ minimizes the energy and $f(z) = z^2$, $f(z) = \bar{z}^2$, $f(z) = z^3$, and $f(z) = \frac{1}{2}z$ do not minimize energy, all in the equal constant case, (1.5). The unusual features of these algorithms are that they must accommodate the nonconvex constraint $|n| = 1$ and the possible singularities of the configuration. Details appear in [7].

The first method consists in applying the relaxation method to a discretized version of the functional

$$\frac{1}{2} \int_{\Omega} |\nabla n|^2 dx,$$

or more generally,

$$\int_{\Omega} w(\nabla n, n) dx$$

subject to the constraint that

$$|n| = 1 \quad \text{in } \Omega$$

and the boundary condition

$$n = n_0 \quad \text{on } \partial\Omega.$$

For the Gauss-Seidel relaxation, this method has the desirable stability

$$(2.2) \quad \int_{\Omega} |\nabla u|^2 dx = 2 \int_{\Omega} (u - c)^2 dx.$$

for any $c \in \mathbb{R}$. In this way we may place the issue of admissibility in its proper functional setting:

4. Admissibility. If Ω is diffeomorphic to a ball and $u \in H^1_0(\Omega)$, then $Q(u) = 0$.

2. Computational results

Two numerical algorithms have been employed to compute minimum energy configurations. The results of these experiments illustrate that the function $u(x)$ defined by (3.1) with $f(z) = z$ minimizes the energy and $f(z) = z_j$, $f(z) = \bar{z}_j$, and $f(z) = z_j$ do not minimize energy. All in the equal constant case, (1.2). The unusual features of these algorithms are that they must accommodate the nonconvex constraint $|u| = 1$ and the possible singularities of the configuration. Details appear in [7].

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and the boundary condition

$$u = 0 \quad \text{on } \partial\Omega.$$

For the Gauss-Seidel relaxation, this method has the desirable stability

property that it is energy decreasing in the usual sense. That is, if $\hat{W}(n^k)$ denotes the energy of the k^{th} iterate n^k , then

$$\hat{W}(n^{k+1}) \leq \hat{W}(n^k). \quad (5.1)$$

Also, $|n^k| = 1$ at all mesh points. Improved rates of convergence have been obtained with a version of the over-relaxation method modified to enforce the pointwise constraint. Unfortunately, the energy decreasing property (5.1) is lost with over-relaxation.

The second algorithm is a fractional step method which is motivated by penalty methods for achieving constraints. One might think of approximating minima of

$$\int_{\Omega} W(\nabla n, n) \, dx$$

by penalization of the constraint. For example, if $f(t)$, $t \geq 0$, is a smooth function of t satisfying

$$f(t) > 0, \quad t \geq 0, \quad t \neq 1, \quad \text{and} \quad f(1) = 0,$$

a penalization is given by minimizing the functional

$$E_{\lambda}(n) = \int_{\Omega} W(\nabla n, n) \, dx + \lambda \int_{\Omega} f(|n|) \, dx \quad (5.2)$$

in $H^1(\Omega; \mathbb{R}^3)$. It is not difficult to show that the minima n_{λ} of E_{λ} converge suitably to a minimum of (1.4) as $\lambda \rightarrow \infty$.

A computational technique to construct a minimum of the functional (5.2) is to solve to steady state the time dependent problem

$$\partial n / \partial t = \operatorname{div} \partial W / \partial p - \partial W / \partial n - \lambda \partial f / \partial n. \quad (5.3)$$

The algorithm that we found most efficient for computation approximated the penalty term in (5.2) and (5.3) by an "indicator" function and used a fractional step algorithm for the energy and the penalty to advance in time [7].

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The second algorithm is a fractional step method which is motivated by penalty methods for achieving constraints. One might think of approximating minima of

$$\int_0^1 w(\nabla u) dx$$

by penalization of the constraint. For example, if $f(t)$ is a smooth function of t satisfying

$$f(t) > 0, \quad t \leq 0, \quad f(t) \approx 1, \quad \text{and } f(t) = 0, \quad t \geq 1,$$

a penalization is given by minimizing the functional

$$(2.2) \quad E_\lambda(u) = \int_0^1 w(\nabla u) dx + \lambda \int_0^1 f(t) |u|^2 dx$$

in $H^1(\Omega; \mathbb{R}^2)$. It is not difficult to show that the minima u_λ of E_λ converge suitably to a minimum of (1.1) as $\lambda \rightarrow \infty$.

A computational technique to construct a minimum of the functional (2.2) is to solve to steady state the time dependent problem

$$(2.3) \quad \partial_t^2 u - \nabla \cdot (\nabla u) - \partial_t^2 u = 0 \quad \text{in } \Omega.$$

The algorithm that we found most efficient for computation approximated the density term in (2.2) and (2.3) by an indicator function and used a fractional step algorithm for the energy and the penalty to advance in time [7].

Figures 1 and 2 are indicative of our results in the equal constant case. The calculations were performed on the unit cube $Q = (0,1) \times (0,1) \times (0,1)$ with $(21)^3$ grid points. Figure 1 is a picture of

$$n(x) = n_T(x) = \Pi^{-1} f \Pi(x-a/|x-a|) \quad (5.4)$$

where $f(z) = z^2$ and $a = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ in the plane $x_3 = \frac{1}{2}$. Clearly visible is a singularity of degree 2 at the center. Figure 2 is a picture of our 'solution' with given boundary data (5.4) in the plane $x_3 = \frac{1}{2}$, after 152 time steps of the fractional step method. At this number of iterations,

$$\hat{W}(n^{k+1} - n^k) < \delta \quad \text{for } \delta = 10^{-7}.$$

The graphical output indicates that the solution has two singularities of degree 1. Moreover,

$$\hat{W}(n^k) = 24.651 < 27.978 = \hat{W}(n_T), \quad k = 152.$$

The computations were executed on the Cray-2 at the University of Minnesota.

6. Further remarks: the Williams, Pieranski, and Cladis experiment

When nematic material is introduced into a capillary tube which has been prepared to render the director perpendicular to the tube walls, two point singularities, of degree +1 and -1, may appear along the axis of the tube. Taking account of the faces of the tube, and assuming its axis to be the x_3 -axis, the boundary orientation of $n(x)$ is roughly

$$n_0(x) = (x_1/r, x_2/r, 0), \quad r^2 = x_1^2 + x_2^2,$$

which has degree zero. The two defects gradually move closer together, then coalesce, resulting in a configuration free of singularities. This experiment is described in [27]. This was our first exposure to singularities and was related to us by J. L. Ericksen.

One is led to surmise the existence of a family of solutions of (1.4)

Figures 1 and 2 are indicative of our results in the equal constant case. The calculations were performed on the unit cube $Q = (0,1) \times (0,1) \times (0,1)$ with $(2,1)^2$ grid points. Figure 1 is a picture of

$$(2.4) \quad n(x) = n^*(x) = \pi^{-1} \pi(x - x_0) \sqrt{x - x_0}$$

where $(z) = z_2$ and $a = (x, x, x)$ in the plane $x_3 = x$. Clearly visible is a singularity of degree 2 at the center. Figure 2 is a picture of our solution with given boundary data (2.4) in the plane $x_3 = x$, after 125 time steps of the fractional step method. At this number of iterations,

$$\hat{w}(n^{k+1} - n^k) > \delta \quad \text{for } \delta = 10^{-7}.$$

The graphical output indicates that the solution has two singularities of degree 1. Moreover,

$$\hat{w}(n^k) = 24.621 > 27.978 = \hat{w}(n^k), \quad k = 125.$$

The computations were executed on the Cray-2 at the University of Minnesota.

6. Further remarks: the Williams, Pieranski, and Cladis experiment

When nematic material is introduced into a capillary tube which has been prepared to render the director perpendicular to the tube walls, two point singularities, of degree +1 and -1, may appear along the axis of the tube. Taking account of the faces of the tube, and assuming its axis to be the x_3 -axis, the boundary orientation of $n(x)$ is roughly

$$n_0(x) = (x_1 \sqrt{x_2}, x_2 \sqrt{x_1}, 0), \quad x_1^2 + x_2^2 = r^2.$$

The two defects gradually move closer together, then coalesce, resulting in a configuration free of singularities. This experiment is described in [27]. This was our first exposure to singularities and was related to us by J. L. Erickson.

One is led to surmise the existence of a family of solutions of (1.1)

whose limit is a smooth configuration when the defects coalesce. Two points of view have been adopted to investigate this.

In [3], as described by Brezis in this volume and to which we refer for a complete explanation, the location and degree of each singularity in a configuration are assumed known and the minimum of energy with respect to this constraint is studied. It is not achieved.

In [17] it is shown that if a minimizing configuration is sufficiently close to one which is free of defects, then it too is free of defects. This result employs the regularity theory we have described as well as section 4.3, the Convergence of minimizers.

Both results suggest that static theory alone does not suffice to explain this phenomenon. It remains a challenging problem to analyse the dynamical equations, cf. [22],[23], pertinent to this situation.

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Figure 1

$$n_f \text{ for } f = z^2$$

Figure 2

n^K for $K = 152$ and with boundary data n_f