

**RECENT DEVELOPMENTS IN LIQUID CRYSTAL THEORY**

By

**David Kinderlehrer**

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## Recent developments in liquid crystal theory

David Kinderlehrer

School of Mathematics  
University of Minnesota

*Dedicated to J.-L. Lions*

Liquid crystals are interesting systems to study because they are mesomorphic phases between solid and isotropic liquid phases. Generally composed of rigid rod-like molecules with large aspect ratios, they possess long range orientational order, unlike a liquid, but lack the configurational order characteristic of a solid. They flow easily and thus may be thought of as anisotropic liquids. Their optical properties are highly sensitive to electromagnetic fields and sometimes temperature, which is the basis of their application in display devices and calorimetry<sup>1</sup>.

The nematic and cholesteric phases, which are our topic here, enjoy a well developed continuum theory due to J. L. Ericksen and F. Leslie [20,38] which is based on the Oseen - Frank bulk energy density. Recent years have witnessed developments in the analysis and numerical analysis of the Ericksen - Leslie equations and comparison of the results with experimental evidence. This has led to interesting questions, many with unexpected answers<sup>2</sup>.

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<sup>2</sup> In addition to the books by Chandross [12] and de Gennes [17], we refer the reader to Ericksen [20] and Leslie [38,39] for reviews of the static and flow theories, respectively, of nematics and cholesterics. The article by Brinkman and Cladis [10] provides a short introduction to defects. The collection [21] contains papers about a variety of topics, including some of those discussed here. The lucid early paper by G. Friedel is available in [23]. A preliminary exposition of some of the work discussed here was given in [35].

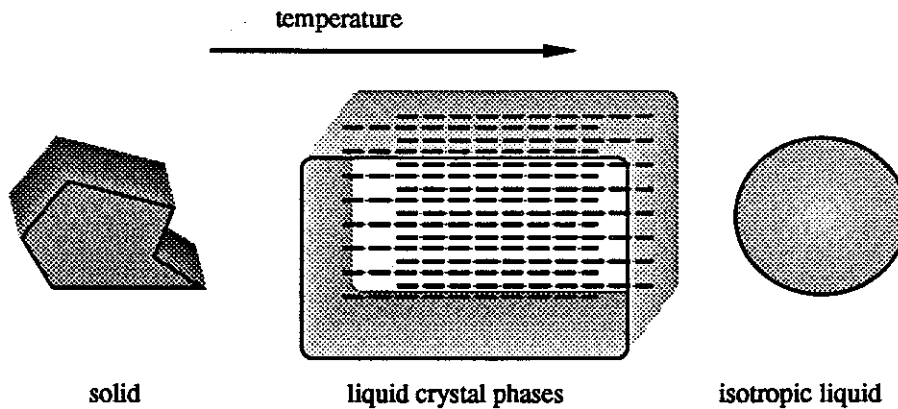


Fig. 1

In this brief review we wish to report on some of these developments, primarily as we have investigated them, [14,15,30-35,43], and with particular attention to the collateral work of Brezis, Coron, and Lieb, [8,9], and successive results. To organize this article we present the ideas leading to the notion of a stable defect in a liquid crystal configuration and the issues it suggested. Here is an outline.

- A brief resumé of liquid crystals and the continuum theory
- The variational formulation for static configurations
- The phenomenon of stable defects: theory and computation
- The determination of stable defects for harmonic mappings
- The general liquid crystal: implications for uniqueness and further development of the computational program

Additional discussion of some other directions in the investigation of liquid crystals may be found in the papers of R. Hardt [26] and F.-H. Lin [41].

## 1 Liquid crystals

Since the nematic and cholesteric phases are optically uniaxial, the order parameter describing the long range orientational order is commonly identified with the material optic axis. In

this way, the kinematic variable is a unit vector  $n(x)$  for  $x$  in the region occupied by the fluid. The Oseen - Frank bulk energy is

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

where  $\kappa_i > 0$ ,  $i = 1, 2, 3$ , and  $q$  and  $\alpha$  depend on temperature.

This formula was derived originally by Oseen, in the 1930's, on the basis of molecular theory, [46]. It was later shown to be a consequence of Galilean invariance by Frank [22], cf. also [19]. This simply places in evidence that the material is composed of rod-like molecules whose heads and tails are indistinguishable; hence,

$$W(\nabla n, n) = W(-\nabla n, -n) \quad \text{and} \quad (1.2)$$

$$W(\nabla n, n) = W(Q \nabla n Q^T, Qn) \quad \text{for any rotation } Q \text{ with } \det Q = 1.$$

Expanding such a  $W$  to quadratic terms in  $\nabla n$  gives rise to (1.1).

When  $q = 0$ , the liquid crystal is nematic and

$$n = \text{const.} \quad (1.3)$$

represents a rest state. Here  $W$  enjoys the additional symmetry that

$$W(\nabla n, n) = W(\nabla n, -n).$$

When  $q \neq 0$ , the liquid crystal is cholesteric<sup>1</sup> and displays chirality. The vector field

$$n(x) = (\cos qx_3, \sin qx_3, 0) \quad (1.4)$$

represents a rest state.

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<sup>1</sup> After cholesterol benzoate, which was the first liquid crystal discovered, by Reinitzer and Lehmann, about 1880. See [53] for interesting comments about this.

The special case  $\kappa_1 = \kappa_2 = \kappa_3 = \alpha = 1$ ,  $q = 0$  gives

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

the energy density of a harmonic mapping from a domain  $\Omega \subset \mathbb{R}^3$  into  $S^2$ . Of course, much is known about this special case, of particular relevance here are [49,50], sufficiently so that in our early investigations we did not anticipate anything more than recovering the analogous information about (1.1).

In equilibrium, the optic axis is stationary for the functional defined by (1.1), namely,

$$\delta \int_{\Omega} W(\nabla n, n) dx = 0. \quad (1.6)$$

Additional fields may be imposed. For example when a constant magnetic field  $H \in \mathbb{R}^3$  is present, its contribution is given by

$$W_M = \frac{1}{2} (\chi_o 1 + \chi_a n \otimes n) H \cdot H, \quad H \in \mathbb{R}^3,$$

where  $\chi_o$  and  $\chi_a$  are the diamagnetic susceptibilities. The condition for equilibrium is

$$\delta \int_{\Omega} (W(\nabla n, n) - W_M(n, H)) dx = 0, \quad |n| = 1. \quad (1.7)$$

That the system can maintain equilibrium when a magnetic or electric field is imposed means that the static fluid is capable of supporting couple stresses; thus, the stress tensor is not a pressure. This tensor has been derived by Ericksen and Leslie [20,38] by means of a suitable principle of virtual work and is given by

$$T = -p 1 + T_M,$$

where  $T_M$ , the molecular stress, is the expression

$$T_M = -\nabla n^T \frac{\partial W}{\partial \nabla n} + W 1. \quad (1.8)$$

This is the connection between the Oseen - Frank bulk energy density and the mechanical properties of the liquid crystal.

## 2 Variational formulation

With (1.6) in mind, it is reasonable to seek equilibrium configurations by direct methods. A typical situation, called *strong anchoring* in the literature, is to prescribe the optic axis on the boundary of the vessel occupied by the fluid.

To formulate such a question, let  $n_0$ ,  $|n_0| = 1$ , be defined on the boundary  $\partial\Omega$  of the region  $\Omega \subset \mathbb{R}^3$  and let

$$A = A_{\Omega}(n_0) = \{v \in H^1(\Omega; \mathbb{R}^3) : |v| = 1 \text{ a.e. in } \Omega \text{ and } v = n_0 \text{ on } \partial\Omega\}. \quad (2.1)$$

Our problem is to

$$\text{Find } n \in A : \int_{\Omega} W(\nabla n, n) \, dx = \inf_A \int_{\Omega} W(\nabla v, v) \, dx. \quad (2.2)$$

or, more generally,

$$\begin{aligned} \text{Given } H \in \mathbb{R}^3, \text{ find } n \in A : \int_{\Omega} (W(\nabla n, n) - W_M(n, H)) \, dx = \\ \inf_A \int_{\Omega} (W(\nabla v, v) - W_M(v, H)) \, dx. \end{aligned} \quad (2.3)$$

We shall return to the question of whether or not  $A_{\Omega}(n_0)$  is empty later.

This result, although neither the most precise nor the most general, serves as the starting point of our analysis, cf. [30,32] where this is discussed in detail.

**THEOREM 1.1 (A)** *Given  $n_0 \in H^1(\Omega; \mathbb{R}^3)$  with  $|n_0| = 1$  on  $\partial\Omega$ , there is an  $n \in A$  which minimizes, that is, which satisfies (2.2) (when  $H = 0$ ) or (2.3).*

(B) Any minimizer is analytic except on a relatively closed set  $Z$  of vanishing one dimensional Hausdorff measure. The points  $a \in Z$  are precisely the points  $a \in \Omega$  for which

$$\Theta(a) = \limsup_{\rho \rightarrow 0} \frac{1}{8\pi\rho} \int_{B_\rho(a)} |\nabla n|^2 dx > 0. \quad (2.4)$$

A few remarks may serve to illustrate some of our difficulties.

#### EXISTENCE

Perhaps it is not obvious that a minimizing sequence for (2.2) or (2.3) is bounded in  $H^1(\Omega)$ . To check this, observe that the term involving  $\alpha$  is a null-lagrangian and depends only on the data  $n_0$ , [19,32]. Formally, this may be seen by calculating that

$$\begin{aligned} \int_{\Omega} (\text{tr}(\nabla n)^2 - (\text{div } n)^2) dx &= \int_{\partial\Omega} [(\nabla n)n - \text{div } n n] \cdot \nu dx \\ &= \int_{\partial\Omega} [(\nabla_{\text{tan}} n)n - (\text{tr } \nabla_{\text{tan}} n)n] \cdot \nu dx \\ &= \int_{\partial\Omega} [(\nabla_{\text{tan}} n_0)n_0 - (\text{tr } \nabla_{\text{tan}} n_0)n_0] \cdot \nu dx \quad \text{for } n \in A_{\Omega}(n_0) \\ &= S(n_0). \end{aligned} \quad (2.5)$$

Hence, changing the parameter  $\alpha$  alters only the minimum value of the functional without altering a minimizer, so we may choose it at will. Choosing

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

leads to the expression

$$W(\nabla n, n) = \frac{1}{2} \alpha |\nabla n|^2 + V(\nabla n, n), \quad (2.6)$$

where

$$V(\nabla n, n) \geq 0 \quad \text{for all } n \in H^1(\Omega; \mathbb{S}^2). \quad (2.7)$$

We always assume  $\alpha$  to be chosen so that (2.6) and (2.7) hold. This also will be useful in understanding how estimates may be achieved for minima.

- EQUILIBRIUM EQUATIONS

The equilibrium equations of the system (2.2) are

$$\left\{ \begin{array}{ll} -\operatorname{div} \frac{\partial W}{\partial \nabla n} + \frac{\partial W}{\partial n} + \lambda n = 0 & \text{in } \Omega \\ |n| = 1 & \\ n = n_0 & \text{on } \partial\Omega \end{array} \right. \quad (2.8)$$

where  $\lambda$  is the Lagrange multiplier arising from the constraint. In the harmonic mapping case, this system reduces to

$$\Delta n + |\nabla n|^2 n = 0 \quad \text{in } \Omega, \quad (2.9)$$

namely,  $\lambda = -|\nabla n|^2$ . Quadratic growth of lower order terms in elliptic systems is a known peril, eg. [24,27]. The general case (2.4) here is further complicated because in general

$$\lambda = \lambda(\nabla^2 n, \nabla n)$$

is also dependent on second derivatives of  $n$ . This may compromise the ellipticity of the system, [27]

- DEFECTS

If  $\Omega$  is topologically a ball and

$$n_0: \partial\Omega \rightarrow S^2$$

has nonzero topological degree, then every element of  $A(n_0)$  has singularities. These singularities are the defects.



Now it may appear that defects are a mathematical artifact since we have, in some sense, chosen a unit vector instead of some other parameter as our kinematic variable. However, point defects are present in actual configurations and they correspond to singularities of the function  $n(x)$  which minimizes in (2.2), [12,17,20].

Hardt and Lin [28] have given an example where high oscillation of the boundary data alone gives rise to defects in the solution.

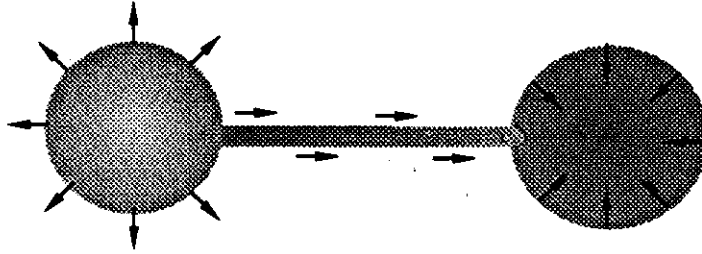


Fig. 2 Any minimizing harmonic map from the "dumbbell" above into  $S^2$  with the indicated data must have at least two defects.

Brezis gives an example [7] of data of degree zero on  $\partial\Omega$  which illustrates clearly how

$$\inf_A \int_{\Omega} W(\nabla v, v) \, dx < \inf_{A \cap C^1(\Omega)} \int_{\Omega} W(\nabla v, v) \, dx .$$

Indeed,  $C^1(\Omega; S^2)$  is not dense in  $H^1(\Omega; S^2)$ . This question was taken up by Bethuel and Zheng, as we briefly indicate in §5.

- UNIQUENESS

Uniqueness of configurations is generally unknown and frequently not available. For example, with boundary data

$$n_0(x) = (\cos kx_3, \sin kx_3, 0) ,$$

$n_0(x)$  is a solution of the Euler equation (2.8) for any nematic ( $q = 0$  in (1.1).) It is a planar solution. When  $k$  is too large, minimum energy for this boundary data is achieved by at least two nonplanar solutions of the form

$$n(x) = (n^1(x), n^2(x), m(x)) \quad \text{and} \quad \bar{n}(x) = (n^1(x), n^2(x), -m(x)).$$

This was discovered by S.-Y. Lin [42] by computation and verified in [35], cf. [13] for additional details. More dramatic examples of the multiplicity of solutions will be discussed in the sequel. Planar solutions were previously investigated by MacMillan, [44].

#### • HARMONIC MAPPINGS

The variety of solutions available may be seen by considering the homogeneous extension of conformal mappings of  $S^2$  onto itself. To be explicit, let

$$g: S^2 \rightarrow S^2$$

be conformal or anticonformal. Then

$$n(x) = g\left(\frac{x}{|x|}\right), \quad |x| < 1,$$

is a solution of (2.9). For later use, let

$$\Pi: S^2 \rightarrow \mathbb{R}^2$$

denote stereographic projection of  $S^2$  onto  $\mathbb{R}^2$  from the south pole to the meridian hyperplane. Set

$$n_f(x) = \Pi^{-1} f\left(\Pi\left(\frac{x}{|x|}\right)\right), \quad |x| < 1, \quad (2.10)$$

for  $f$  rational in  $z$  or  $\bar{z}$ . Then  $n_f$  is a solution of (2.9) with a single defect, generally rather complicated, at  $x = 0$ .

One may readily calculate that, writing  $f = p/q$ ,  $p$  and  $q$  relatively prime, that

$$\begin{aligned} \deg f &= \max(\deg p, \deg q) = \Theta(0) \\ &= \frac{1}{8\pi\rho} \int_{B_\rho(0)} |\nabla n|^2 dx, \quad \text{for any } \rho > 0. \end{aligned} \quad (2.11)$$

• SPECIAL SOLUTION

Finally, we point out that

$$n(x) = \frac{x}{|x|} \quad (2.12)$$

is a solution of (2.4) for any nematic, that is (1.1) for any choice of constants  $\kappa_i$ ,  $\alpha$  with  $q = 0$ .

### 3 The phenomenon of stable defects

In the proof of partial regularity, THEOREM 1.1 part B, an estimate originally due to Hardt and Lin was used whose implications were not fully appreciated at the time. This estimate states that if  $n \in A_\Omega(n_0)$  is a minimizer of (2.2) (or (2.3)) and  $B_{2r}(a) \subset\subset \Omega$ , then

$$\int_{B_r(a)} |\nabla n|^2 dx \leq C_0 \left( \int_{\partial B_r(a)} |\nabla_{\tan n}|^2 dS + \int_{\partial B_r(a)} |n - \xi|^2 dS \right)^{\frac{1}{2}}, \quad (3.1)$$

for any  $\xi \in \mathbb{R}^3$ , where  $C_0 = C_0(\kappa_1, \kappa_2, \kappa_3)$ , [32], cf. also [33]. This estimate is distinguished from the well known one of Schoen and Uhlenbeck [49] in that no *a priori* smallness is assumed about the right hand side of (3.1).

This led us to the notion of a stable defect, which we describe for stationary points of the functional. Suppose that  $n$  has the property that

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

and that

$$\Theta(a) = \limsup_{\rho \rightarrow 0} \frac{1}{8\pi\rho} \int_{B_\rho(a)} |\nabla n|^2 dx > 0 \text{ at } a \in \Omega.$$

Let us say that  $a$  is a *stable defect* provided that for all  $r > 0$  sufficiently small,  $n$  minimizes the functional (2.2) in  $B_r(a)$  subject to its own boundary values. Namely,

$$\int_{B_r(a)} W(\nabla n, n) dx = \inf_A \int_{B_r(a)} W(\nabla v, v) dx$$

for all  $r > 0$  sufficiently small where

$$A = A_{B_r(a)}(n).$$

**THEOREM 3.1** *If  $a \in \Omega$  is a stable defect of  $n$ , then*

$$\Theta(a) \leq M,$$

where the constant  $M = M(\kappa_1, \kappa_2, \kappa_3)$ .

So what this result asserts is that the density  $\Theta(a)$  of a stable defect depends only on the material constants of the liquid crystal and in particular is independent of the boundary data  $n_0$ . In fact,  $M = 6\sqrt{\pi}C_0$ . For a harmonic mapping, the immediate consequence is

**COROLLARY 3.2** *A defect suffered by a minimizing configuration of a harmonic mapping has a limited degree.*

Comparing with the formula (2.11) shows that if the degree of the rational function determining  $n_f$  is too large, then the defect at the origin is unstable and thus  $n_f$  does not minimize the functional (2.2).

The proof of THEOREM 3.1 follows almost immediately from (3.1). Set  $a = 0$ . Squaring both sides of (3.1), setting  $\xi = 0$ , and integrating, between  $r$  and  $2r$ , say, we obtain

$$\left(\frac{1}{r} \int_{B_r} |\nabla n|^2 dx\right)^2 \leq \frac{C}{2r} \int_{B_{2r}} |\nabla n|^2 dx.$$

Setting

$$E(r) = \frac{1}{r} \int_{B_r} |\nabla n|^2 dx$$

and iterating yields that

$$E(2^{-k}r) \leq C^{1+2^{-1}+\dots+2^{-k}} E(2r)^{2^{-k-1}}.$$

Passing to the limit as  $k \rightarrow \infty$  gives the result.

What are the stable defects? They are bounded in degree, but may be limited in other ways as well. For a given rational function of degree  $m$  and for  $\varepsilon > 0$ , consider the harmonic mapping of the unit ball  $B$  into  $S^2$  defined by  $n_{\varepsilon f}$ , cf. (2.10). Let  $u_\varepsilon$  denote a minimizer of the Dirichlet integral with boundary data  $n_{\varepsilon f}$ , that is a solution of (2.2) in  $A_B(n_{\varepsilon f})$ . So  $n_{\varepsilon f}$  is a solution of the equilibrium equations and

$$\int_B |\nabla n_{\varepsilon f}|^2 dx = 8\pi \deg f.$$

On the other hand, since  $\varepsilon f(z) \rightarrow 0$  as  $\varepsilon \rightarrow 0$  in the complex plane, it is immediate that

$$n_{\varepsilon f} \rightarrow -e_3 \text{ (the south pole) in } L^2(S^2).$$

Moreover,  $\nabla_{\tan} u_\varepsilon = \nabla_{\tan} n_{\varepsilon f}$  on  $S^2$ . Now we apply (3.1) with  $\xi = -e_3$  to see that

$$\begin{aligned} \int_B |\nabla u_\varepsilon|^2 dx &\leq C_0 \left( \int_{\partial B} |\nabla_{\tan} n_{\varepsilon f}|^2 dS \int_{\partial B} |n_{\varepsilon f} + e_3|^2 dS \right)^{\frac{1}{2}} \\ &\leq C_0 (8\pi \deg f \int_{\partial B} |n_{\varepsilon f} + e_3|^2 dS)^{\frac{1}{2}} \\ &\rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0. \end{aligned}$$

Thus it is immediate that  $n_{\epsilon f}$  is not a minimizer for  $\epsilon$  sufficiently small, even when  $m = 1$ .

Other consequences of these ideas include the compactness of minimizing configurations, for example, [33].

**THEOREM 3.3**      *The set  $N$  of minimizers of the functional*

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

*is locally bounded in  $H^1(\Omega)$  and any weakly convergent sequence  $(n_j) \subset N$  converges strongly in  $H^1_{loc}(\Omega)$  and its limit  $n \in N$ , that is,  $n$  is a minimizer as well.*

This result has been used to discuss an experiment of Williams, Pieranski, and Cladis [54]. We refer to [33] for details.

#### 4      The computation of stable defects

The computational program in liquid crystals, under the direction of M. Luskin, has been developed with the objective of finding three dimensional configurations, perhaps containing defects. Several features of the variational principle (1.5) or the equilibrium equations (2.8) immediately reveal their presence. One is the clearly three dimensional nature of the problem. Another is the combination of a pointwise nonconvex constraint, which is infinite dimensional in  $H^1$ , with the possible failure of ellipticity of the system. For this reason, the methods devised were closely linked to seeking minima of the functional. A relaxation method and a finite element fractional step/conjugate gradient method were employed. For information about these methods and their origins we refer to [14]. The results of both methods were identical on all problems considered. As we have already mentioned, a first conclusion was that the high frequency nematic simple twist solution is unstable, S.-Y. Lin [42].

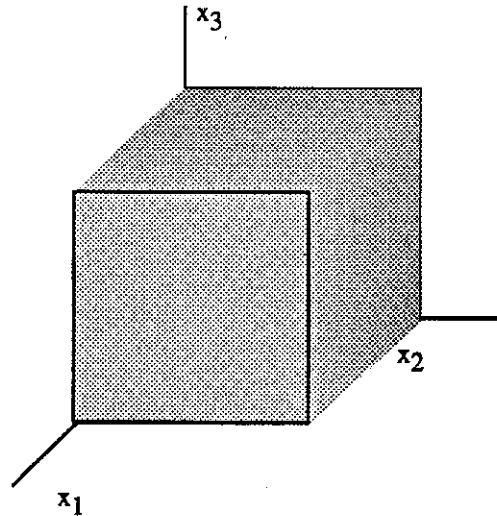


Fig. 3 The computational cube

To investigate the stability of defects, we first considered the functional

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

in the domain  $\Omega = (0,1) \times (0,1) \times (0,1)$ . Let

$$n_0(x) = n_f(x-a), \quad \text{where } a = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \text{ and } f(z) = z^2.$$

Thus

$$n_0(x) = \Pi^{-1} \left[ \left( \Pi \left( \frac{x-a}{|x-a|} \right) \right)^2 \right] \quad (4.1)$$

and has a dipole like singularity of degree 2 at  $x = a$ . Consider the

*Problem:* Find  $I = \inf_A \int_{\Omega} |\nabla v|^2 dx$  where

$$A = A_{\Omega}(n_0).$$

The computed answer is that

$$I = .88 \int_{\Omega} |\nabla n_o|^2 dx$$

and thus  $n_o$  is not a minimizer. The graphical displays illustrate very clearly the results of the computation. The minimizing configuration has two defects, each of degree one and approximately asymptotic to

$$Q\left(\frac{x - x_o}{|x - x_o|}\right), \text{ where } Q \text{ is a rotation by } \frac{\pi}{2} \text{ about } e_3 \text{ and } x_o \text{ is the singular point.}$$

Similar results were found for the boundary conditions  $n_f$  for  $f(z) = z^3, \bar{z}^2, \bar{z}^3,$  and  $\frac{1}{2}z$ . None were found to minimize and all stable defects were of degree one. On the other hand,  $\sqrt{F(x - a, |x - a|)}$ , which is  $n_f$  for  $f(z) = z$ , was found to minimize. Qualitatively equivalent results were found for other values of the Frank constants  $\kappa_i$ .

Convergence of the relaxation method has been proven by Lin and Luskin [43]. The properties of the finite element fractional step and conjugate gradient methods have been investigated by R. Cohen [13]. We refer to [15] for a more complete discussion.

We shall have more to say about computation of configurations later.



## 5 The identification of stable defects for harmonic mappings

Using the computational evidence as a guide, Brezis, Coron, and Lieb [8] were able to identify the stable defects of harmonic mappings of a domain  $\Omega \subset \mathbb{R}^3$  into  $S^2$ . Let us begin by noting that Schoen and Uhlenbeck [50] had already determined that a minimizing harmonic mapping with smooth data is analytic with the exception of a finite number of defects. The ability to prove such facts about harmonic mappings owes to the close connection of the integrand of (2.2) to the geometry of the sphere in this case. This permits the derivation of certain monotonicity properties which are unavailable in the general situation.

The result of Brezis, Coron, and Lieb is

**THEOREM 5.1** *A stable defect of a harmonic mapping from  $\Omega \subset \mathbb{R}^3$  into  $S^2$  of the form*

$$n(x) = g\left(\frac{x}{|x|}\right)$$

*is of the form*

$$n(x) = Q \frac{x}{|x|} \quad \text{where } Q \text{ is a rotation.} \quad (5.1)$$

A description of this work is given in Brezis [7]. The proof in [8] is notable. It employs results from the Monge-Kantorovich mass transfer problem, [47], and Birkhoff's theorem about doubly stochastic matrices. They also use these ideas to study a different variational problem which is motivated by the Williams, Pieranski, and Cladis experiment to which we have alluded previously.

Using L. Simon's result [52] and a theorem of Gulliver and White [25], it follows that any stable defect is asymptotically of this form.

Some of the more recent investigations have focussed on the actual number of singular points exhibited by a configuration. For example, in the Hardt and Lin example already mentioned, the topological degree of the data is zero, but the number of singular points may be arbitrarily

large. In a subsequent work [29], they are able to demonstrate a stability result about the possible coalescence of defects as the data is varied. They show

**THEOREM 5.2** *The number of defects in a minimizing configuration of a harmonic mapping from  $\Omega \subset \mathbb{R}^2$  into  $S^2$  with boundary data  $n_0$  is bounded by a constant which depends on  $\Omega$  and*

$$\|n_0\|_{H^1, \infty(\partial\Omega)}.$$

A similar theorem was proved by Almgren and Lieb [1], but with a rather different proof. They show that

$$\# \text{ of defects} \leq C_\Omega \int_{\partial\Omega} |\nabla_{\tan} n_0|^2 dS.$$

Both of the analyses have the compactness result THEOREM 3.3 and the Brezis, Coron, and Lieb result THEOREM 5.1 as their point of departure.

A different proof of (5.1) was given by Coron and Gulliver [16] on the basis of the co-area formula. Their proof also applies to the case where the functional to be minimized is, where  $p$  has an appropriate range,

$$\int_{\Omega} |\nabla v|^p dx \quad \text{subject to} \quad |v| = 1.$$

Another line of investigation suggested by these considerations concerns the density of smooth functions in Sobolev spaces. For example,  $C^\infty(\Omega, S^2)$  is not dense in  $H^1(\Omega, S^2)$  when  $\Omega \subset \mathbb{R}^3$ , as the example of

$$\frac{x - a}{|x - a|}, \quad \text{where } a \text{ is any fixed point of } \Omega,$$

illustrates. In several papers, Bethuel and Zheng [5,6] and Bethuel [4] have given fairly complete answers to the question of when  $C^\infty(M, N)$  is dense in  $H^1(M, N)$  in terms of the homotopy group  $\pi_{[p]}(N)$  when  $p < \dim M$ .

## 6 The general liquid crystal

One may suspect that the qualitative behavior of an arbitrary nematic liquid crystal is much like that of a harmonic mapping, and indeed, this is a common simplification in some analyses, cf. Chandrasekhar [12]. On the other hand, critical points of

$$\int_{\Omega} W(\nabla n, n) \, dx \quad (6.1)$$

for

$$\begin{aligned} W(\nabla n, n) = & \frac{1}{2} \kappa_1 (\operatorname{div} n)^2 + \frac{1}{2} \kappa_2 (n \cdot \operatorname{curl} n)^2 + \frac{1}{2} \kappa_3 |n \wedge \operatorname{curl} n|^2 \\ & + \frac{1}{2} \alpha (\operatorname{tr} (\nabla n)^2 - (\operatorname{div} n)^2) \end{aligned} \quad (6.2)$$

are rather different. For example,

$$n(x) = Q \frac{x}{|x|}, \quad Q \text{ a rotation, } Q \neq 1,$$

is not a minimizer of (6.1); in fact, it is not even a stationary point of (6.1) unless all the  $\kappa_i$ 's are equal.

In the table below, the Frank constants for a few nematics are reported. PBT and PBG are liquid crystal polymers. Also, for example, the measured constants may vary widely within the nematic phase, as the graph indicates.

material	$\kappa_1$	$\kappa_2$	$\kappa_3$
PAA 120° (†)	1.3	1	2.67
125°	1.55	1	3.27
129°	1.6	1	3.2
MBBA 22° (†)	1.75	1	3.5
PBT (‡)	15.8	1	7.3
PBG (‡)	11.3	1	13.1

$\kappa_2$  has been normalized to 1.

Fig. 4 Frank constants for some nematic liquid crystals. (†) from [12] and (‡) from [3].

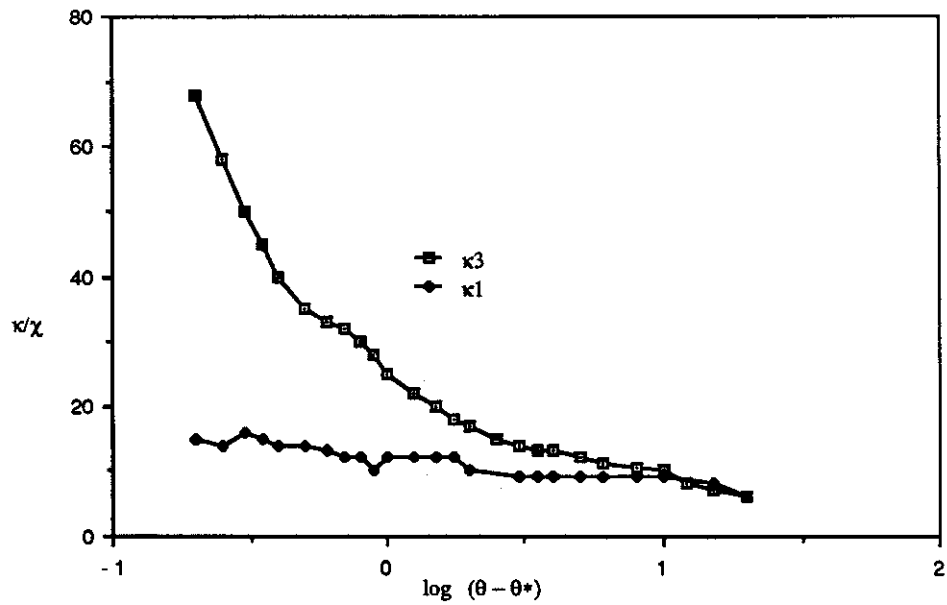


Fig. 5 Temperature dependence in  $C^\circ$  of the splay and bend elastic constants in the nematic CBOOA prior to nematic/smectic A transition. CBOOA prior to nematic/smectic A transition.  $\chi$  is the diamagnetic anisotropy. The critical temperature is  $\theta^*$ . The clearing point is about  $\theta - \theta^* = 18$  (from [12], p.308)

In summary, it is unlikely that a given liquid crystal corresponds to a harmonic mapping. A few of the issues which arise in the study of general liquid crystals, both from the study of experiments and in the analysis of the functional (6.1) are

- the uniqueness of configurations,
- the stability of configurations, and
- the role of  $n(x) = x/|x|$  as a minimizer.

Our discussion may be unified, in a somewhat artificial manner, by consideration of the situation where  $\kappa_1$  is large, since all of the aberrant behavior is manifested in this case.

## 7 The role of $n^*(x) = \frac{x}{|x|}$

F.-H. Lin recently found a very simple proof based on (2.5) that (2.12) is a minimizing harmonic mapping which is valid in any dimension larger than 2, [40]. It extends to a case of (6.2), so we report it here.

**THEOREM 7.1** *If  $\kappa_1 \leq \min\{\kappa_2, \kappa_3\}$ , then  $n^*(x) = \frac{x}{|x|}$  is a minimizer of (6.1) in  $A_B(n^*)$ , where  $B$  is a ball with center 0.*

To prove this, Lin observes that if  $u: \mathbb{R}^3 \rightarrow S^2$ , then

$$|\nabla u|^2 \geq (\operatorname{div} u)^2 - \operatorname{tr}(\nabla u)^2.$$

Now if  $\kappa_1 = \min\{\kappa_1, \kappa_2, \kappa_3\}$ , then (cf. (2.6), (2.7)),

$$\begin{aligned} W(\nabla u, u) &= \frac{1}{2} \kappa_1 (\operatorname{div} u)^2 + \frac{1}{2} \kappa_2 (u \cdot \operatorname{curl} u)^2 + \frac{1}{2} \kappa_3 |u \wedge \operatorname{curl} u|^2 \\ &\quad + \frac{1}{2} \alpha (\operatorname{tr}(\nabla u)^2 - (\operatorname{div} u)^2) \\ &= \frac{1}{2} \alpha |\nabla u|^2 + \frac{1}{2} (\kappa_2 - \alpha) (u \cdot \operatorname{curl} u)^2 + \frac{1}{2} (\kappa_3 - \alpha) |u \wedge \operatorname{curl} u|^2 \end{aligned}$$

$$\begin{aligned} &\geq \frac{1}{2} \alpha |\nabla u|^2 \\ &\geq \frac{1}{2} \alpha \{(\operatorname{div} u)^2 - \operatorname{tr}(\nabla u)^2\}. \end{aligned}$$

Hence

$$\begin{aligned} \int_B W(\nabla u, u) \, dx &\geq \frac{1}{2} \alpha \int_B \{(\operatorname{div} u)^2 - \operatorname{tr}(\nabla u)^2\} \, dx \\ &= -\frac{1}{2} \alpha \int_{\partial B} [(\nabla_{\tan} u)u - (\operatorname{tr} \nabla_{\tan} u)u] \cdot \nu \, dx \\ &= -\frac{1}{2} \alpha \int_{\partial B} [(\nabla_{\tan} n^*)n^* - (\operatorname{tr} \nabla_{\tan} n^*)n^*] \cdot \nu \, dx \\ &= \left(\frac{1}{2} \alpha\right) (8\pi) \\ &= \int_B W(\nabla n^*, n^*) \, dx, \end{aligned}$$

since  $\operatorname{curl} n^* = 0$ .

The table shows that  $\kappa_1$  is not always the smallest Frank constant. S.-Y. Lin [42] and F. Helein [36] have shown that if  $\kappa_1$  is too large, then  $n^*$  is unstable. The essence of Helein's argument, for example, is that for the vector field

$$u(x) = x + \frac{1}{r} \sqrt{1 - \rho^2} (x_2, -x_1, 0), \quad r^2 = (x_1)^2 + (x_2)^2, \quad \rho = |x|,$$

one has

$$\int_B (\operatorname{div} u)^2 = 12\pi$$

whereas

$$\int_B (\operatorname{div} n^*)^2 = 16\pi.$$

Thus, in the limit as  $\kappa_2$  and  $\kappa_3$  tend to 0,  $u$  has less energy than  $n^*$ . By perturbing  $u$  one finds a trial vector field  $n \in H^1(B; S^2)$  with energy less than that of  $n^*$  when  $\kappa_2$  and  $\kappa_3$  are small compared with  $\kappa_1$ . To summarize we state

**THEOREM 7.2** *If  $\kappa_1$  is sufficiently large with respect to  $\kappa_2$  and  $\kappa_3$ , then  $n^*(x) = x/|x|$  is an unstable stationary point of the functional (6.1).*

We now give an argument of Ericksen's which illustrates how many minimizers may occur. Let us assume that  $n^*(x)$  is not a minimizer in  $B$ . It has, of course, the special property that  $Qn^*(x) = n^*(Qx)$  for any rotation  $Q$ . Consider any unit vector field  $u(x)$  such that

$$Qu(x) = u(Qx), \quad x \in \Omega, \quad \text{for all rotations } Q \quad (7.1)$$

which is continuously differentiable in a neighborhood  $\Omega$ . Differentiating with respect to the rotation gives that

$$\Lambda u(x) = \nabla u(x) \Lambda x \quad \text{for all } \Lambda, \Lambda + \Lambda^T = 0,$$

or

$$\xi \wedge u(x) = \nabla u(x) (\xi \wedge x) \quad \text{for all } \xi \in \mathbb{R}^3.$$

Choosing  $\xi = x$  shows that  $u(x)$  is parallel to  $x$  so  $u(x) = \pm n^*(x)$  in  $\Omega$ .

Let  $u(x) \in A_B(n^*)$  be a minimizer which satisfies (7.1). Were it to have a defect  $a \neq 0$ , it would have an entire sphere of defects in contradiction to the regularity result, Theorem 1.1, part B. So it must be smooth except at  $a = 0$ . We may apply the conclusion of the paragraph above, with the  $+$  sign since this holds on  $\partial B$ .

Thus if  $u(x) \in A_B(n^*)$  is a minimizer of (6.1), then the group  $G$  of rotations  $Q$  satisfying (7.1) is not all of  $O(3)$ . For any rotation  $P$  not in the group  $G$ ,

$$v(x) = P^T u(Px)$$

is a different minimizer by virtue of the frame indifference condition (1.2). Since  $G$  is not all of  $O(3)$ , there is at least a smooth one parameter family of rotations  $P \notin G$ , as may be verified by inspecting the Lie algebra of  $G$ , for example. In summary,

**THEOREM 7.3** *If  $n^*$  is not a stable minimizer of the liquid crystal functional (6.1), then there is a continuum of minimizers of (6.1) with boundary data  $n^*$ .*

This sort of qualitative behavior is not restricted to high anisotropy. The discussion which follows was motivated by a conversation with E. Lieb. Consider, for example, the harmonic mapping of the unit ball  $B$  into  $S^2$

$$n^{**}(x) = n_f(x) \quad \text{for } f(z) = z^2,$$

that is,

$$n^{**}(x) = \Pi^{-1}\left[\left(\Pi\left(\frac{x}{|x|}\right)\right)^2\right], \quad x \in B,$$

as in (4.1). This vector field enjoys the symmetry property that

$$Q^2 n^{**}(Q^T x) = n^{**}(x) \quad \text{for any rotation } Q \text{ about the } x_3\text{-axis, (7.2)}$$

since  $e^{2i\theta}(e^{-i\theta} z)^2 = z^2$ . The minimizer of (6.1) in  $B$  with boundary data  $n^{**}$  for the harmonic mapping case is not  $n^{**}$ . If it has a defect off the  $x_3$ -axis, then it cannot satisfy the symmetry property (7.2) owing to the regularity theorem, as we have seen. Hence, there would be an infinite family of minimizers.



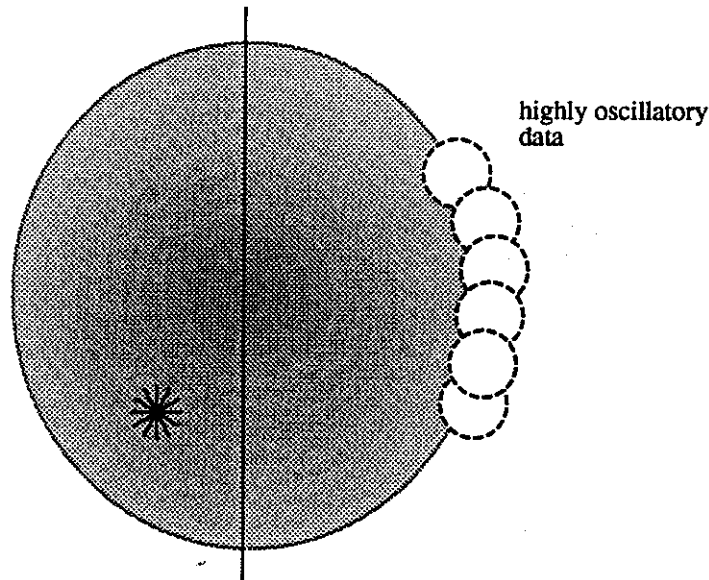


Fig 6 At least one defect is not on the  $x_3$ -axis

Suppose, however, that the data  $n_0$  satisfies

$$Q^N n_0(Q^T x) = n_0(x), \quad x \in \partial B, \quad (7.3)$$

for any rotation  $Q$  about the  $x_3$ -axis and some integer  $N$ . If some minimizer has at least one defect not on the  $x_3$ -axis, it follows that for this data there is an infinite family of minimizers. If  $a \in B$  is a defect on the  $x_3$ -axis, by the Brezis, Coron, and Lieb result [8], the solution has the local expansion

$$n(x) = R \frac{x - a}{|x - a|} + \dots \quad \text{near } x = a,$$

for some rotation  $R$ , and thus cannot admit the symmetry (7.3) for *all* rotations  $Q$  about the  $x_3$ -axis. Hence, whenever the data satisfies (7.3), there is a continuum of minimizers.

The experimental evidence confirms both situations. In particular, the work of Candau *et al.* [11,45] describes the behavior of droplets of a variety of liquid crystals, some of which are also subjected to external fields. In these experiments, the director orientation at the boundary of the droplet is known. Easily accessible, a photograph in [17] figure 4.17 illustrates that  $n_0(x)$  is not a

minimizer. Our understanding from P. Cladis is that the Frank constants for this particular material have not been measured.

## 8 Development of the computational program: an example

Another situation where there are some interesting connections among the experimental evidence, theory, and simulation has been the study of a classical Freederickz transition, cf. [12,17,20]. Here, too, large values of  $\kappa_1$  play a role.

Freederickz transitions are the consequence of competition between the boundary condition and an imposed magnetic field. The concept is that the exchange of stability resulting in the dominance of the magnetic field permits evaluation of the Frank constants  $\kappa_1, \kappa_2, \kappa_3$ . For example, in the experiment used to evaluate  $\kappa_1$ , the liquid crystal is confined between two narrowly separated parallel plates and anchored in the same direction on each, say in the direction of the  $x_1$ -axis. A magnetic field parallel to the vertical, say  $x_3$ -axis, is imposed. Assuming the optic axis to be a function of  $x_3$  only and to lie in the  $(x_1, x_3)$  plane, one obtains an ordinary differential equation nearly identical to the classical Euler bar for the angle of deflection. Bifurcation occurs at the first eigenvalue, explaining the exchange of stability and determining  $\kappa_1$ .

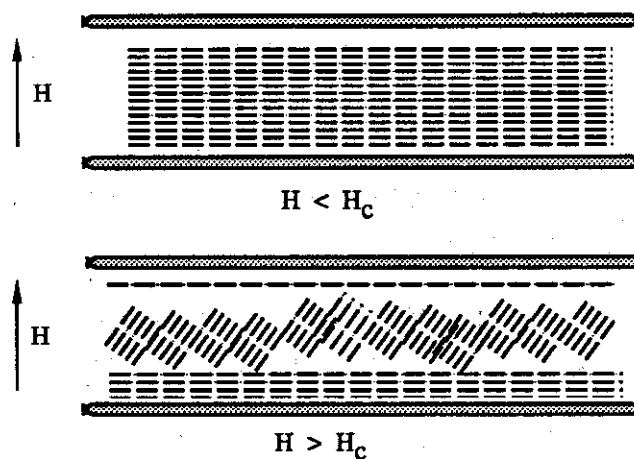


Fig. 7 Schematic view of a Freederickz transition

Berry et al. [2,3,51] observed, in the course of their investigations, unstable behavior in the liquid crystal polymer PBT where  $\kappa_1 = 15.8$ ,  $\kappa_2 = 1$ , and  $\kappa_3 = 7.3$ , cf. the table. Of course, many effects are present in long flexible chain polymers which are absent in small molecule liquid crystals, for which the Oseen - Frank bulk energy density (6.2) was designed. However, this particular polymer is quite rigid. R. Cohen [13] undertook a study to understand the role of the size of  $\kappa_1$ .

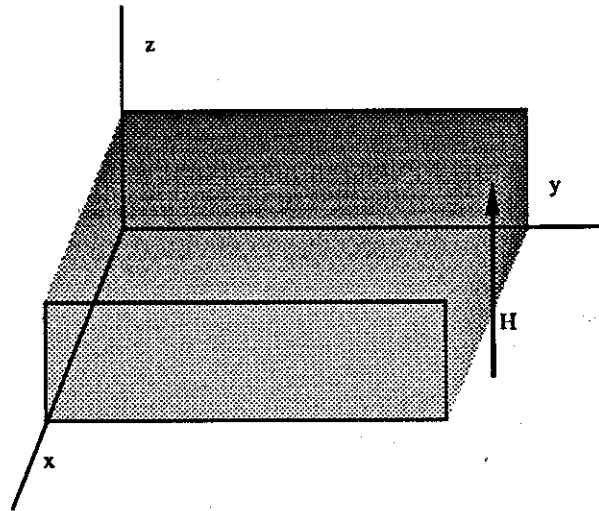


Fig. 8 Computational parallelepiped. The imposed magnetic field is in the  $z$  - direction.

What he found is illustrated in Plates 6 and 7. First he established an estimate for the critical field strength  $H_F$  for a three dimensional box, which is different from the essentially one dimensional configuration, with strong anchoring boundary conditions. The number  $H_F$  is generally less than  $H_1$ , the critical field strength based on the one dimensional Euler beam analysis, although they are very close when the Frank constants are about the same. The computation reveals the onset of a three dimensional periodic structure at about  $H_c = .75 H_F$ , [13].

Subsequent discussions with several experimentalists, especially J. L. Fergason, suggest that these instabilities may occur even in small molecule liquid crystals and that laboratory procedures are designed to suppress them.

A second motivation for investigating this phenomenon was the study of a Helfrich transition in cholesterics. Here the experimental arrangement is much the same, but the material is a cholesteric which means that the number  $q$  in (1.1) is not zero. In this situation, we may consider the competition among three items, the chirality  $q$ , the strong anchoring boundary condition, and the magnetic field strength  $H$ . Helfrich gave an analysis which predicts a two dimensional periodic instability in a thin film which arises from the interaction of  $H$  with the chirality occurring at a field strength less than that required for the Freederickz transition, cf. [12,17]. The experimental work of Hurault [37] and Rondelez and Hulin [48] confirmed the prediction. This was shown to be consistent with the variational principle in numerical experiments by S.-Y. Lin [42] and R. Cohen [13]. Cohen also gives an analysis of the problem.

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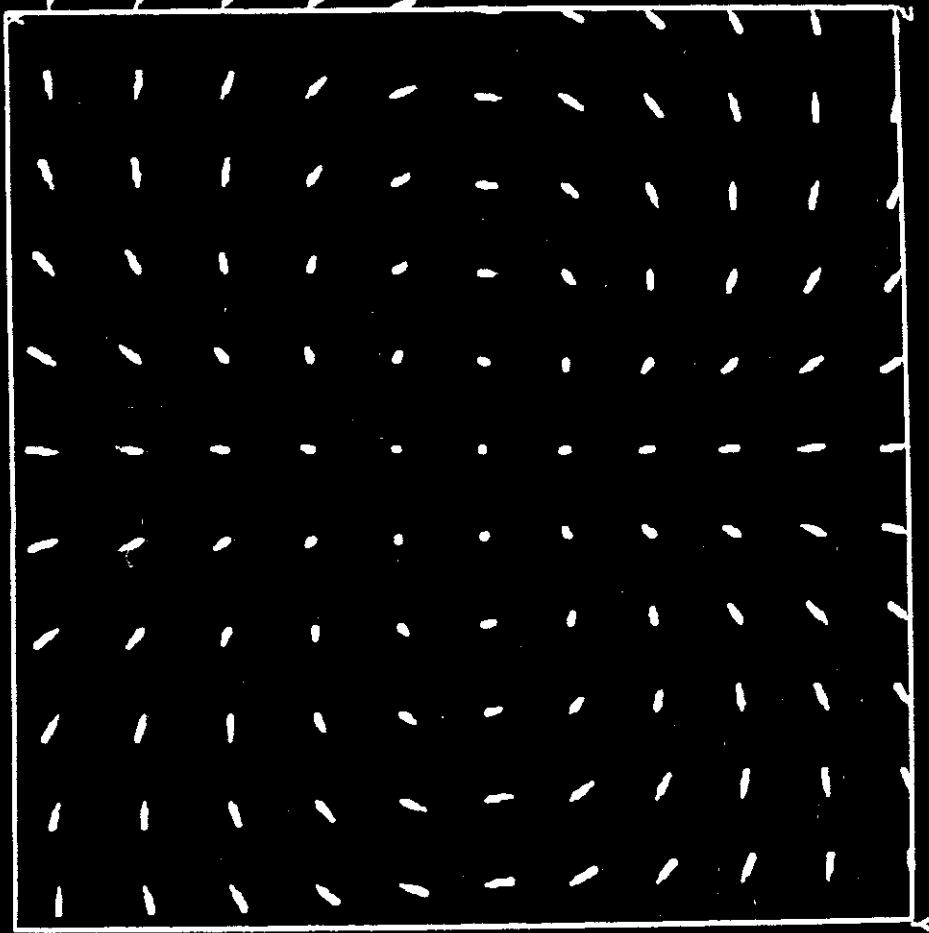


Plate 1

Projection of  $\eta_f$  for  $f(z) = z^2$  showing a dipole like singularity at  $a = (\frac{1}{2}, \frac{1}{2})$ .



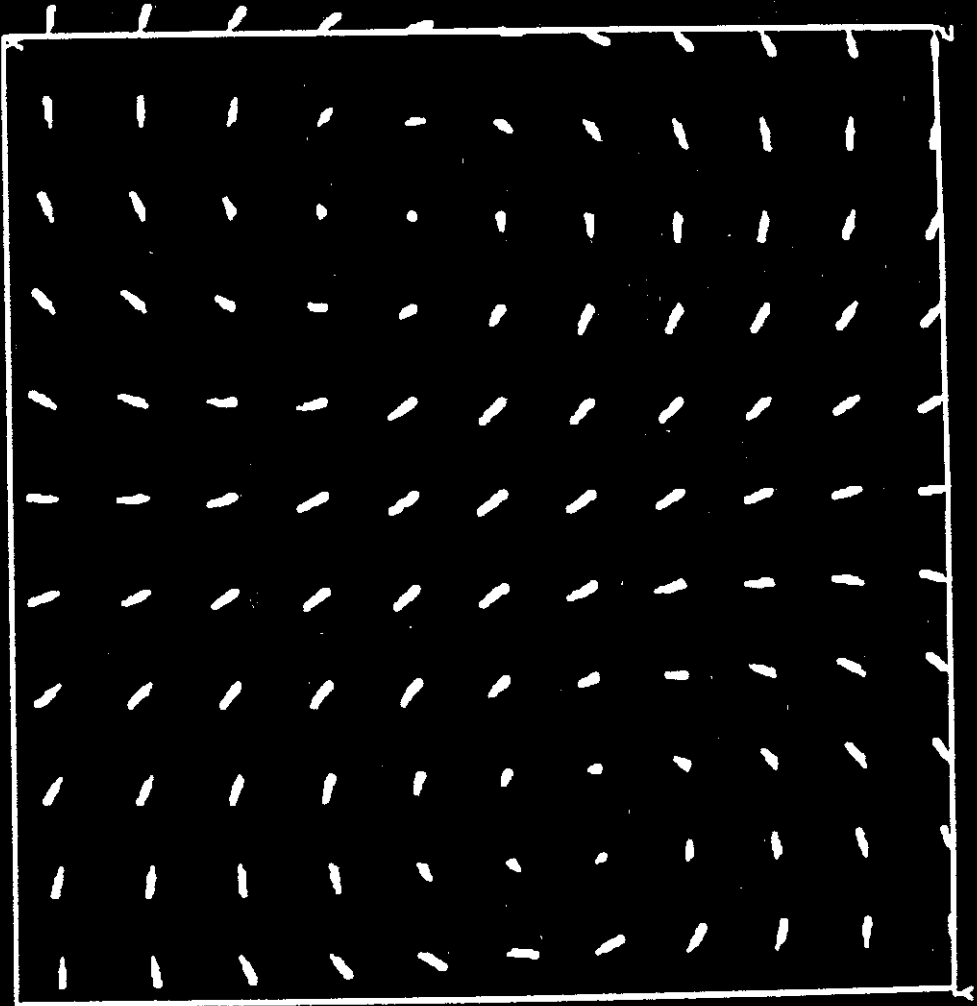


Plate 2 Projection of the converged solution with boundary data  $n_f$  for  $f(z) = z^2$  displaying two singularities of degree one. The initial data for the iterations was also  $n_f$ .

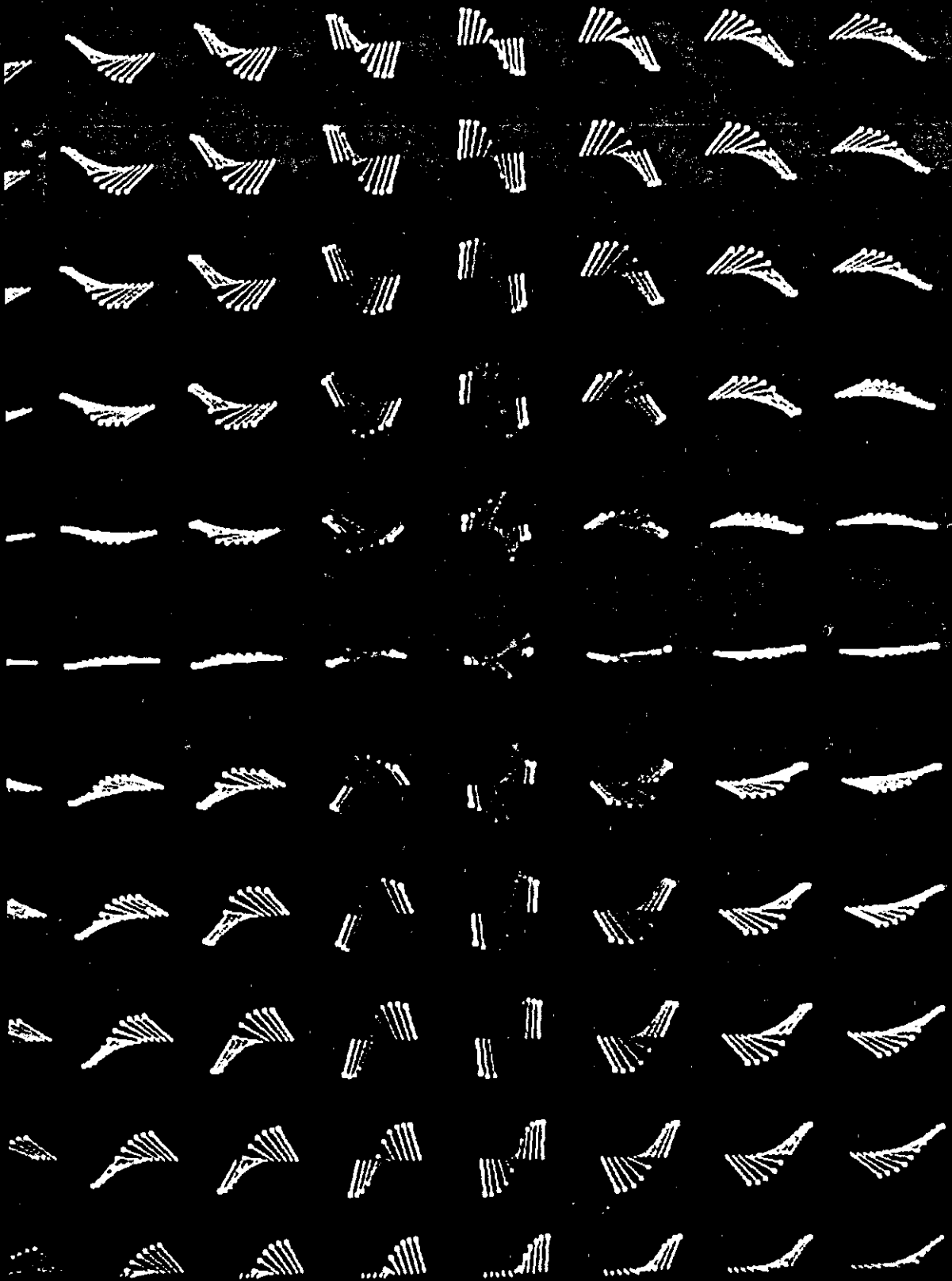


Plate 3

Magnification of the projection of  $\eta_f$  for  $f(z) = z^2$ , seen from  $(\frac{1}{2}, \frac{1}{2}, 2)$ , illustrating high oscillation of  $\eta_f$  near  $a = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ .

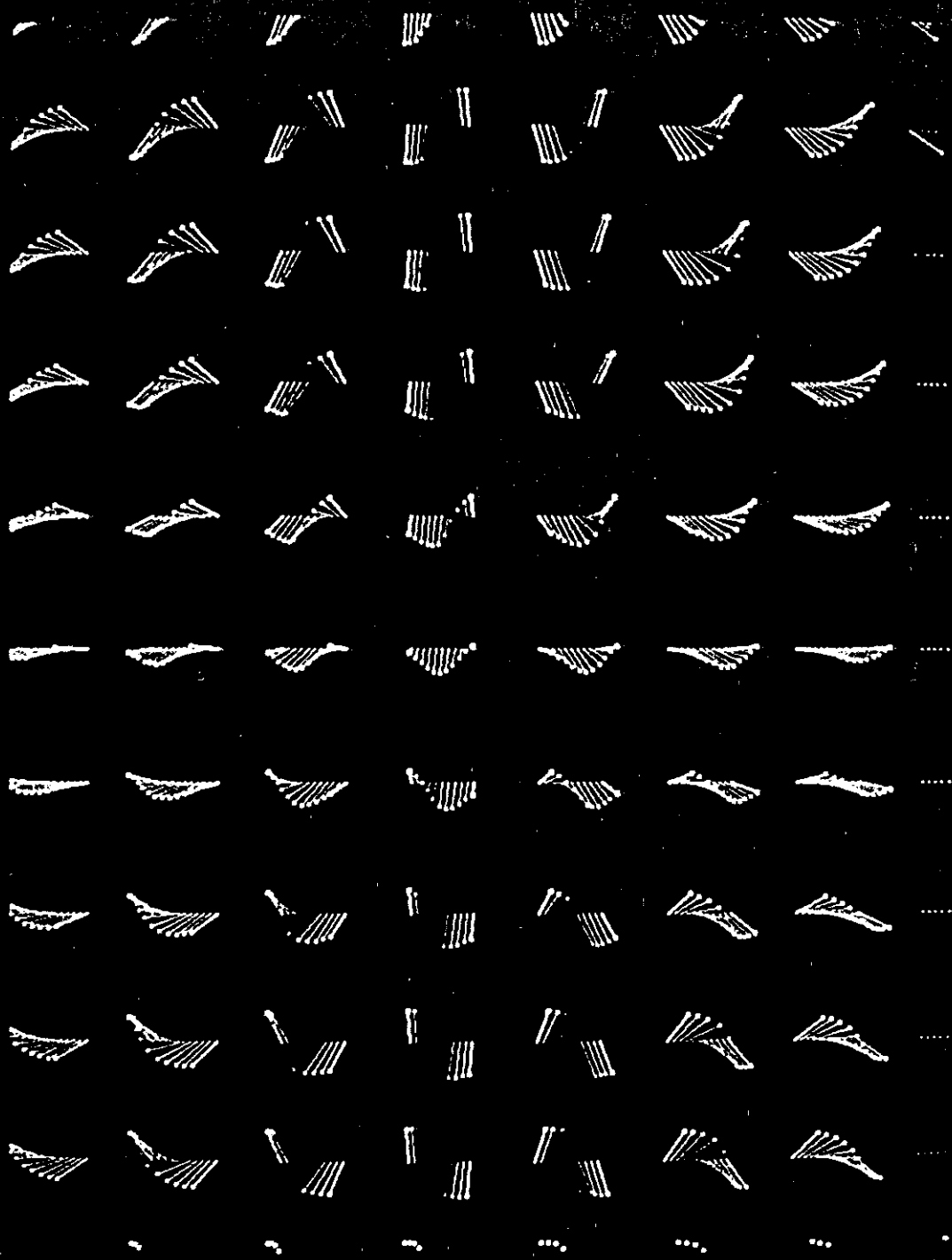


Plate 4

Magnification of the projection of the converged solution with boundary data  $\eta_f$  for  $f(z) = z^2$  illustrating oscillation near a pair of degree one defects.

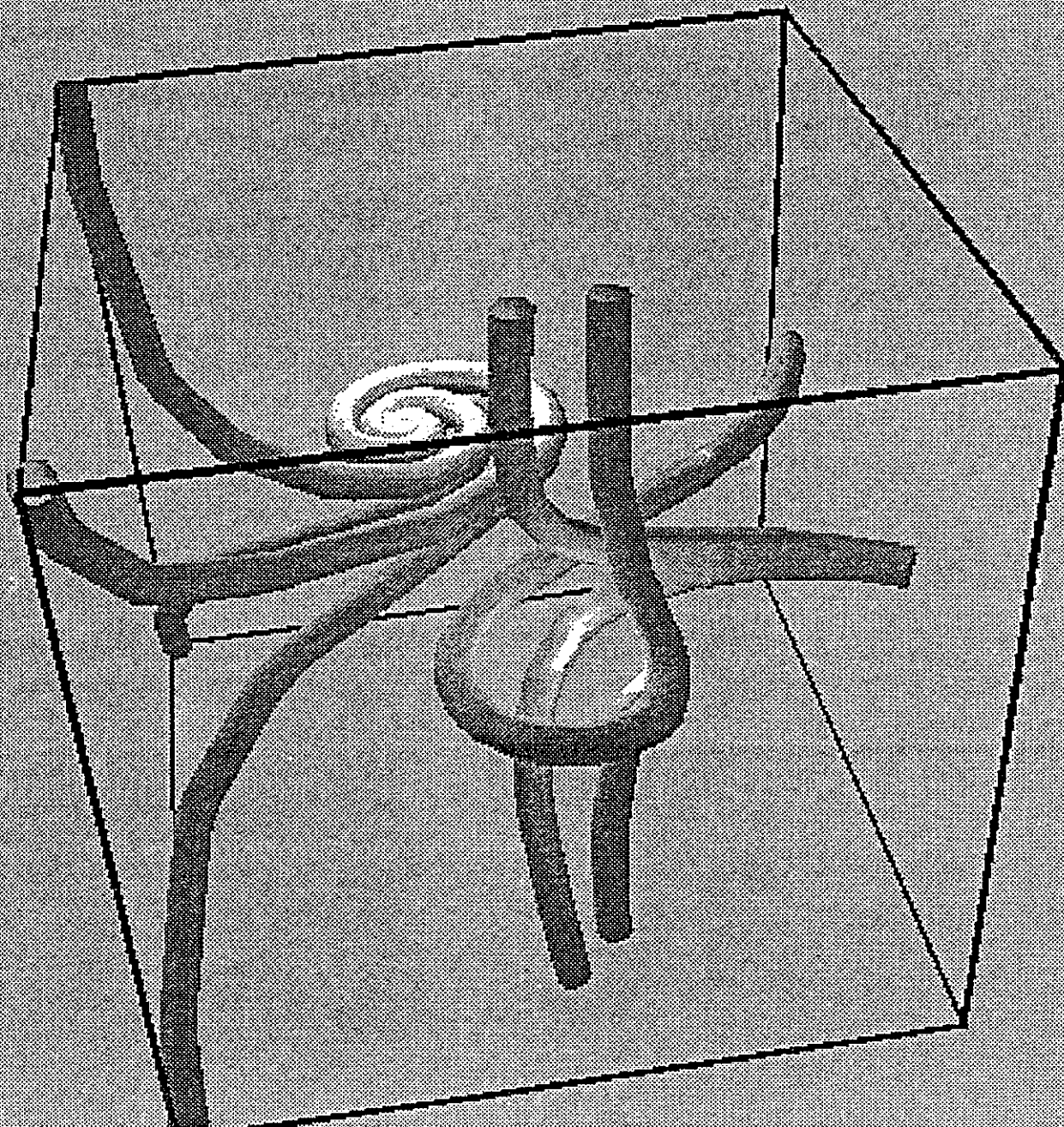


Plate 5

A view of the converged solution of Plates 2 and 4 prepared by tracking "stream tubes" of the director by Visual Edge Software, Ltd., cf. R. R. Dickinson and R. H. Bartels [18].

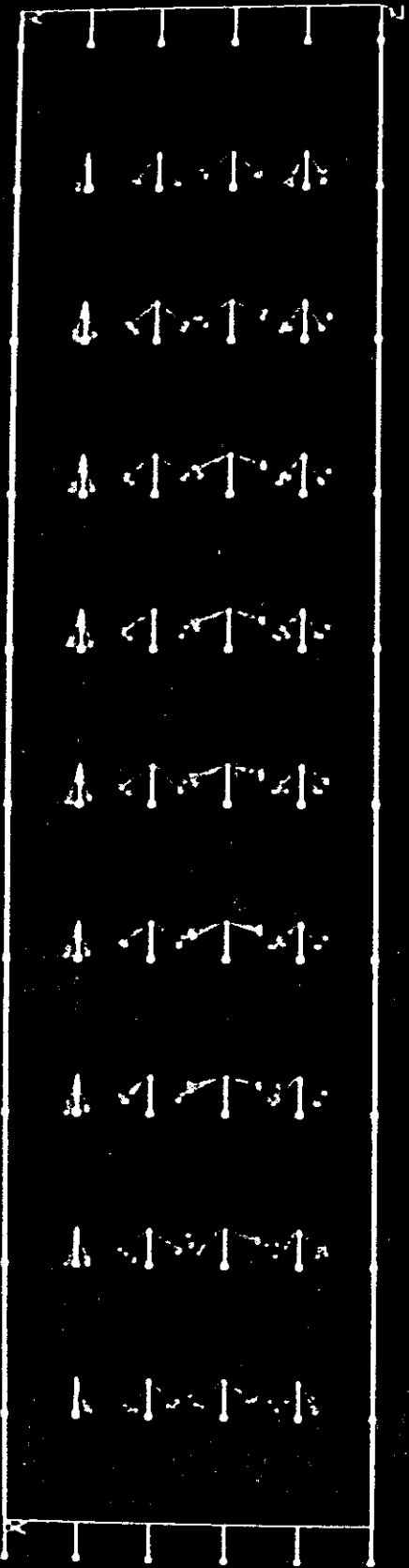


Plate 6  
 Converged solution near subcritical field strength for the Fredericckz transition showing the oscillations of the optic axis. The perspective is the same as Fig. 8.

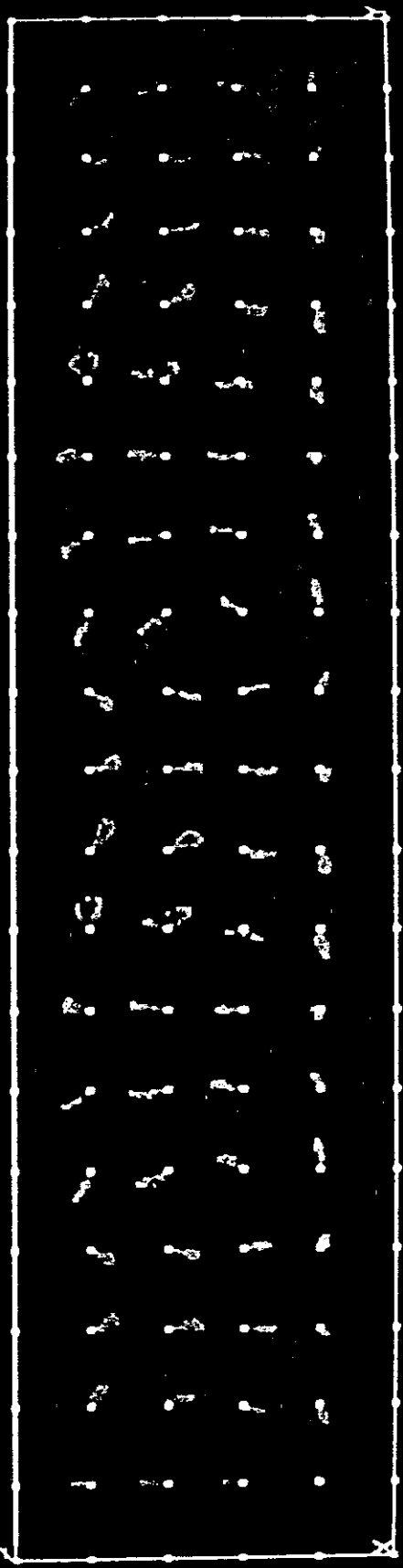


Plate 7 Projection on the  $y-z$  plane of the converged solution near subcritical field strength for the Freederickz transition displaying the periodic structure.

