A Remark about the Stability of Smooth Equilibrium Configurations of Static Liquid Crystals

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The William-Pieranski-Cladis experiment [7] is reviewed in the context of the equilibrium theory of liquid crystals. Static theory does not suffice to explain the apparent cancellation of singularities.

One observation in the William-Pieranski-Cladis experiment [7], discussed in [1], involves singularities of a nematic liquid crystal in a capillary tube where two point defects of opposite sign tend to persist along the axis of the tube. They observe that the singularities may gradually come together, apparently cancelling, rendering the configuration free of defects. Throughout, the director n is radially oriented at the surface of the tube.

Were one to view this from the context of the Ericksen-Leslie static theory [2], based on the Oseen-Frank bulk energy, one would be presented with a family of equilibrium configurations each of which exhibits defects subject to a boundary orientation that approaches a defect free configuration. In these remarks, we note a stability property of minimizers of the static bulk energy which would contradict such cancellation of defects, as observed in the William-Pieranski-Cladis experiment. Thus the explanation of this experimental phenomenon cannot rest on static theory alone. Our work does not preclude the possibility of cancellation of point defects in stationary configurations which are in local energy wells. However, our experience with variational problems of this nature leads us to believe that this is unlikely.

To further clarify the issues here, note that the existence of one static configuration without defects does not necessarily imply that all static configurations with the same boundary orientation are free of defects. This implication is unknown. On the other hand, Hardt and Lin have given in [3] examples of boundary orientations of degree zero [1] any of whose minimum energy configurations necessarily have defects.

Our study here also has some positive conclusions. For example, it may be used to show that some numerical schemes will explicit relatively large energy growth near singular points of a minimizing solution. We do not give details of this here since they are somewhat technical. There is some discussion in [3, §6]. Numerical research on these problems has been undertaken by Mitchell Luskin and his students at the University of Minnesota. We appreciate the remarks and encouragement of J.L. Ericksen, who introduced us to these problems. We also benefitted from discussions with participants of the 1985 I.M.A. workshop on Liquid Crystals.

Proceeding now with our argument, we recall that the Oseen-Frank free energy density is defined, for a unit vectorfield n, by

$$W(\nabla n, n) = \kappa_1(\operatorname{div} n)^2 + \kappa_2(n\cdot\operatorname{curl} n)^2 + \kappa_3|n\times\operatorname{curl} n|^2 + (\kappa_2+\kappa_4)[\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2].$$

On a region Ω, we will consider liquid crystal configurations n that are *local minima* of the energy, namely,

$$\int_{\mathbb{B}_r(a)} W(\nabla n, n)\,dx \le \int_{\mathbb{B}_r(a)} W(\nabla u, u)\,dx$$

whenever $\mathbb{B}_r(a) \subset \Omega$ and u is a unit vectorfield that coincides with n on $\partial\mathbb{B}_r(a)$. Our result is the following:

Let Ω *be a region containing a ball* $\mathbb{B}_{3\varepsilon} = \mathbb{B}_{3\varepsilon}(0)$. *Suppose that we are given a sequence* n_i, $i = 0, 1, 2, \cdots$, *of liquid crystal configurations on* Ω *in static equilibrium with the following properties:*

(a) *Each* n_i *is a local minimum of energy.*

(b) $n_i \to n_0$ *in* $L^2(\Omega)$ *as* $i \to \infty$.

(c) n_0 *is free of singularities in* Ω.

(d) n_i *may admit singularities in the ball* $\mathbb{B}_\varepsilon$, *but is free of singularities in* $\Omega \sim \mathbb{B}_\varepsilon$, for $i > 0$.

Then n_i *does not have any singularities when* i *is sufficiently large.*

Remarks. Convergence in the L^2 norm is frequently encountered in these problems. For example, a sequence of unit vectorfields having uniformly bounded energies contains a subsequence that converges in L^2.

The demonstration of the theorem is based on the following property [4, 2.5-2.6] of the normalized energy density for liquid crystals.

There exists a positive numbers $\sigma, C,$ *and* μ *so that if* n *is a local minimum of energy and if*

$$r^{-1}\int_{\mathbb{B}_r(a)} W(\nabla n, n)\,dx \leq \sigma \quad \textit{for some } r > 0, \tag{1}$$

then n *must be smooth on* $\mathbb{B}_{\frac{1}{2}r}(a)$ *and*

$$\rho^{-1}\int_{\mathbb{B}_\rho(a)} W(\nabla n, n)\,dx \leq C\rho^{\mu} \quad \textit{for } \rho \leq r .$$

Using this, one may actually deduce the smoothness of n_i on $\mathbb{B}_\varepsilon$, for i large, without assumption (d).[2] Here to simplify the exposition we retain assumption (d) and, moreover, treat only the equal constant case $\kappa = \kappa_1 = \kappa_2 = \kappa_3$, $\kappa_4 = 0$, so that

$$W(\nabla n, n) = \kappa|\nabla n|^2 .$$

LEMMA. *As* $i \to \infty$,

$$\int_{\mathbb{B}_{2\varepsilon}} |\nabla n_i|^2 dx \to \int_{\mathbb{B}_{2\varepsilon}} |\nabla n_0|^2 dx \quad \textit{and} \quad \int_{\mathbb{B}_{2\varepsilon}} |\nabla n_i - \nabla n_0|^2 dx \to 0 .$$

Proof. The lower semi-continuity of the energy functional means that

$$\int_{\mathbb{B}_{2\varepsilon}} |\nabla n_0|^2 dx \leq \liminf_{i\to\infty}\int_{\mathbb{B}_{2\varepsilon}} |\nabla n_i|^2 dx . \tag{2}$$

To show that

$$\int_{\mathbb{B}_{2\varepsilon}} |\nabla n_0|^2 dx \geq \limsup_{i\to\infty}\int_{\mathbb{B}_{2\varepsilon}} |\nabla n_i|^2 dx , \tag{3}$$

we may, if necessary, pass to a subsequence. In particular, since all of the functions n_i are, by [4, 2.6], analytic on $\Omega \sim \mathbb{B}_\varepsilon$, there is, by Ascoli's theorem, a subsequence, still denoted n_i, such that

$$n_i \to n_0 \quad \text{and} \quad \nabla n_i \to \nabla n_0 \quad \text{uniformly on } \mathbb{B}_{3\varepsilon} \sim \mathbb{B}_{2\varepsilon} . \tag{4}$$

In particular, for all i sufficiently large and some $K > 0$,

$$|n_i - n_0| \le \tfrac{1}{2} \quad \text{and} \quad |\nabla n_i| \le K \quad \text{on } \mathbb{B}_{3\varepsilon} \sim \mathbb{B}_{2\varepsilon} .$$

Now for any number t with $2\varepsilon < t < 3\varepsilon$, we choose a function $\eta : \mathbb{B}_t \to [0,1]$ with bounded derivative so that

$$\eta = \begin{cases} 1 & \text{on } \partial\mathbb{B}_t \\ 0 & \text{on } \mathbb{B}_{2\varepsilon} \end{cases} .$$

and set

$$u_i = v_i/|v_i| \quad \text{where} \quad v_i = \eta n_0 + (1-\eta) n_i ,$$

so that u_i is a unit vectorfield that coincides with n_i on $\partial\mathbb{B}_t$. Applying the chain rule rule, we find that

$$|\nabla u_i| = |v_i|^{-1}|\nabla v_i| + |v_i|^{-2}|v_i \cdot \nabla v_i| \le |v_i|^{-1}|\nabla v_i| + 4|v_i \cdot \nabla v_i| \tag{5}$$

because $\frac{1}{2} \le |v_i| \le 1$. Using the equation

$$\nabla v_i = \eta \nabla n_0 + (1-\eta)\nabla n_i + \nabla\eta \otimes (n_0 - n_i) ,$$

we estimate the first term

$$|v_i|^{-1}|\nabla v_i| \le \lambda|\nabla n_0| + 2\mu K + \mu|\nabla\eta||n_i - n| \tag{6}$$

where λ is the characteristic function of $\mathbb{B}_{2\varepsilon}$ and μ is the characteristic function of $\mathbb{B}_t \sim \mathbb{B}_{2\varepsilon}$. For the second term, we note that the constraint $|n_i| = 1$ implies $n_i \cdot \nabla n_i = 0$ and estimate

$$\begin{aligned} |v_i \cdot \nabla v_i| &\le \mu\big(|v_i \cdot \nabla n_i| + |v_i \cdot \nabla n_0| + |\nabla\eta||n_i - n_0|\big) \\ &\le \mu\big(|\nabla n_i| + |\nabla n_0| + |\nabla\eta|\big)|n_i - n_0| \le \mu\big(2K + |\nabla\eta|\big)|n_i - n_0| , \end{aligned} \tag{7}$$

where we have made the substitutions $v_i = n_i + (v_i - n_i)$, $v_i = n_0 + (v_i - n_0)$ and noted that $|v_i - n_i| \le |n_i - n_0|$ and $|v_i - n_0| \le |n_i - n_0|$. Combining (6) and (7) with (5) gives

$$|\nabla u_i|^2 \le \lambda |\nabla n_0|^2 + \mu\big(2K + (8K + 5|\nabla\eta|)|n_i - n_0|\big)^2 .$$

From the minimality of n_i we now deduce that

$$\int_{\mathbb{B}_t} |\nabla n_i|^2 dx \le \int_{\mathbb{B}_t} |\nabla u_i|^2 dx$$

$$\le \int_{\mathbb{B}_t} |\nabla n_0|^2 dx + \int_{\mathbb{B}_t \sim \mathbb{B}_{2\varepsilon}} \big(2K + (8K + 5|\nabla\eta|)|n_i - n_0|\big)^2 dx .$$

Letting $i \to \infty$, we infer from (4) that

$$\limsup_{i\to\infty} \int_{\mathbb{B}_{2\varepsilon}} |\nabla n_i|^2 dx \le \int_{\mathbb{B}_t} |\nabla n_0|^2 dx + 16\pi K^2 (t - 2\varepsilon)$$

for any t with $2\varepsilon < t < 3\varepsilon$. Then letting $t \to 2\varepsilon$ gives (3), which combined with (2), proves the first conclusion of the lemma.

To obtain the second, we observe that, on $\mathbb{B}_{2\varepsilon}$, the sequence of functions ∇n_i, being norm-bounded in the Hilbert space $L^2(\mathbb{B}_{2\varepsilon})$, has a weakly convergent subsequence whose limit must be ∇n_0. Thus, as $i \to \infty$,

$$\int_{\mathbb{B}_{2\varepsilon}} |\nabla n_i - \nabla n_0|^2 dx$$

$$= \int_{\mathbb{B}_{2\varepsilon}} \big[|\nabla n_i|^2 - |\nabla n_0|^2\big] dx - 2\int_{\mathbb{B}_{2\varepsilon}} \nabla n_0 \cdot (\nabla n_i - \nabla n_0)\, dx \quad \to \quad 0 - 0$$

by the first conclusion and this weak convergence. QED

Proof of main result. Since ∇n_0 is bounded on $\mathbb{B}_{2\varepsilon}$, we may choose a fixed positive number $r < \varepsilon$ so that

$$r^{-1} \int_{\mathbb{B}_r(a)} |\nabla n_0|^2 dx \le \tfrac{1}{4} K^{-1} \sigma \quad \text{for any } a \in \mathbb{B}_\varepsilon .$$

Moreover, the Lemma implies that, for i sufficiently large, independent of a,

$$r^{-1}\int_{\mathbb{B}_r(a)}|\nabla n_i|^2\,dx \le 2r^{-1}\int_{\mathbb{B}_r(a)}|\nabla n_i-\nabla n_0|^2\,dx + 2r^{-1}\int_{\mathbb{B}_r(a)}|\nabla n_0|^2\,dx$$

$$\le 2r^{-1}\int_{\mathbb{B}_{2\varepsilon}}|\nabla n_i-\nabla n_0|^2\,dx + \tfrac{1}{2}\kappa^{-1}\sigma \le \kappa^{-1}\sigma\ ;$$

hence, (1) is applicable, and n_i is smooth at a. QED

References

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Footnotes

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1 By degree zero, we mean topologically trivial, namely, there is some extension of the boundary orientation to a virtual director configuration in the domain, not necessarily a minimizer, which is free of defects.

2 This involves showing that the singularities of the n_i, which have one dimensional measure zero [4,2.6], may be controlled, as in [6,4.6], in establishing the L^2 convergence of the gradients of the n_i.