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David Kinderlehrer & Noel Walkington
Carnegie Mellon University

Biao Ou
University of Minnesota

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The elementary defects of the Oseen-Frank energy for a liquid crystal

David KINDERLEHRER, Biao OU, and Noel WALKINGTON

Résumé – Nous caractérisons tous les défauts élémentaires pour les cristaux liquides nématiques du type Oseen-Frank. Ce sont des solutions de la forme $Q\frac{x}{|x|}$, où $Q \in O(3)$. En plus des solutions traditionnelles nous trouvons une nouvelle solution quand les constantes élastiques d'Oseen-Frank verifient $k_1 = k_3$ et nous étudiions sa stabilité. Elle est stable si $k_2 \geq k_1 = k_3$ et instable si $k_2 \leq \frac{149}{184}k_1$. Nous avons vérifié le fait que l'on obtient bien toutes les solutions avec MAPLE.

The elementary defects of the Oseen-Frank energy for a liquid crystal

Abstract – All the elementary defects of the Oseen-Frank system for a nematic liquid crystal are characterized. These are solutions of the form $Q\frac{x}{|x|}$, where $Q \in O(3)$. In addition to the traditional solutions, a new one is found when the Oseen-Frank elastic constants satisfy $k_1 = k_3$, and its stability is investigated. It is stable for $k_2 \geq k_1 = k_3$ and unstable if $k_2 \leq \frac{149}{184}k_1$. That all solutions are known was verified by a symbolic computation (MAPLE).

Version abrégée en français -

1. La densité d'énergie d'Oseen-Frank exprime la densité d'énergie d'un cristal liquide nématique en fonction de ses directions optiques. Elle est donnée par:

$$2W(\nabla n,n) = k_1(\mathrm{div}\, n)^2 + k_2(n\cdot \mathrm{curl}\, n)^2 + k_3|n \wedge \mathrm{curl}\, n|^2 + \alpha(\mathrm{tr}(\nabla n)^2 - (\mathrm{div}\, n)^2),$$
$$|n| = 1. \qquad (1.1)$$

où $k_i > 0, i = 1,2,3,$ et α sont des constantes dépendant du matériau et de sa température. (1.1) est la forme quadratique en ∇n la plus générale satisfaisant les conditions d'invariance [4,6,7]:

$$W(Q\nabla nQ^T,Qn) = W(\nabla n,n), \quad Q \in SO(3), \text{ and } W(-\nabla n,-n) = W(\nabla n,n). \qquad (1.2)$$

Le configurations d'équilibre d'un cristal liquide vérifient le principe variationnel

$$\delta\int_\Omega W(\nabla n,n)\,dx = 0, \quad |n| = 1, \qquad (1.3)$$

et des conditions frontières. $\Omega \subset \mathbb{R}^3$ représente la région ocupée par le liquide. On peut trouver Ω et une donnée n sur $\partial\Omega$ (ceci grâce à des considèrations topologiques) tels que n ne puisse pas être regulière dans Ω mais ait une singularité ou un "defaut". La plus simple de ces defauts est donné par le champ de vecteurs $\frac{x}{|x|}$, qui est solution de (1.3) pour tout choix des constantes k_i et α.

Plus généralement on peut considèrer le problème: pour quelles constantes $k_i > 0$ et $Q \in SO(3)$

$$u(x) = Q\frac{x}{|x|} \tag{1.4}$$

est une solution de (1.3), et pour quelles valeurs de k_i celle-ci est elle stable? Les réponses à ces questions sont réumées dans la TABLE.

TABLE

constants	rotation Q	stability	instability
$k_1 = k_2 = k_3$	any Q	always	
$k_1 = k_3$	$Q = \pm 1$ and any 180° rotation	$k_2 \geq k_1$	$k_2 < \frac{149}{184} k_1$
any k_i, $i = 1,2,3$	$Q = \pm 1$	$8(k_2 - k_1) + k_3 \geq 0$	$8(k_2 - k_1) + k_3 < 0$

Dans le cas particulier où $k_1 = k_3$ alors (1.4) avec $Q = -1 + 2e \otimes e$, $|e| = 1$, une rotation de 180°, est solution de (1.3). Ceci ne semble pas connu. Nous montrons également que n est stable si

$$k_2 \geq k_1 = k_3 \qquad \text{et instable si} \quad k_2 < \frac{149}{184} k_1. \tag{1.6}$$

(1.6) résulte de l'utilisation d'une classe spéciale de variations dans (1.3) – cet argument a été employé précédement par Helein [10]. Nous n'avons pas pu faire mieux ni n'avons pas pu adapter notre argument de [12] pour montrer la stabilité de (1.5) quand (1.7) n'est plus vrai. Quand les k_i sont arbitraires, alors $\frac{x}{|x|}$ est une solution instable pour $8k_2 - k_1 + k_3 < 0$, (cf. Helein [10]) et (localement) stable pour $8k_2 - k_1 + k_3 > 0$, (cf. Cohen et Taylor [5], Kinderlehrer et Ou [12]). Si $k_1 = k_2 = k_3$, (1.1) se réduit à $W(\nabla n, n) = |\nabla n|^2$, l'intégrande d'une appplication harmonique d'une région $\Omega \subset \mathbb{R}^3$ a valeur dans $\mathbb{S}^2$. Dans ce cas (1.7) est une solution stable pour tout $Q \in SO(3)$ – ceci fut prouvé pour le première fois par Brezis, Coron, et Lieb [3] (voir également F.-H. Lin [13]). Nous avons vérifié sur MAPLE que notre table était complète: si u(x) vérifie (1.3) alors il apparait dans la table.

Le phénomène de stabilité pour les solutions de (1.3) avec défauts et les applications harmoniques singulières furent découverts par Hardt, Kinderlehrer, et Lin [9].

1. STATEMENT OF RESULT The Oseen-Frank energy density expresses the free energy density of a nematic liquid crystal in terms of its optic axis. It is given by

$$2W(\nabla n,n) = k_1 (\operatorname{div} n)^2 + k_2 (n \cdot \operatorname{curl} n)^2 + k_3 | n \wedge \operatorname{curl} n |^2 + \alpha (\operatorname{tr} (\nabla n)^2 - (\operatorname{div} n)^2),$$
$$| n | = 1. \qquad (1.1)$$

where $k_i > 0, i = 1,2,3,$ and α are (temperature dependent) material constants. (1.1) is the general expression quadratic in ∇n which fulfills the invariance conditions [4,6,7]

$$W(Q\nabla nQ^T,Qn) = W(\nabla n,n), \quad Q \in SO(3), \text{ and } \quad W(-\nabla n,-n) = W(\nabla n,n).$$

Equilibrium configurations of liquid crystals are subject to the variational principle

$$\delta \int_\Omega W(\nabla n,n)\, dx = 0, \quad | n | = 1, \qquad (1.3)$$

together with boundary conditions, where $\Omega \subset \mathbb{R}^3$ represents the region occupied by the fluid. Regions Ω and data for n on $\partial\Omega$ may be chosen so that, on the basis of topological considerations alone, n cannot be smooth in Ω, but must exhibit singularities or defects [9,11]. The simplest such defect is given by the vector field $\frac{x}{|x|}$, which is a solution of (1.3) for any choice of constants k_i and α.

More generally we may consider the question: for which constants $k_i > 0$ and $Q \in O(3)$ is

$$u(x) = Q\frac{x}{|x|} \qquad (1.4)$$

a solution of (1.3), and if so, for what range of the k_i is it stable? The results of our investigation are summarized in the TABLE. In particular, if $k_1 = k_3$, then

$$n(x) = Q\frac{x}{|x|}, \quad Q = -1 + 2e \otimes e, \ | e | = 1, \qquad (1.5)$$

a 180° rotation, is a solution of (1.3). This does not seem to be well known. We also show that it is stable if

$$k_2 \geq k_1 = k_3 \qquad \text{but unstable if} \qquad k_2 < \frac{149}{184} k_1. \qquad (1.6)$$

$(1.6)_1$ follows by optimizing the energy in (1.3) among a special class of variations, which is the same argument employed by Helein [10]. We have not been able to improve upon this nor have we been able to adapt our argument [12] to show the stability of (1.5) when $(1.6)_2$ does not hold. When the k_i are arbitrary, then $\frac{x}{|x|}$ is a solution which is unstable for $8(k_2 - k_1) + k_3 < 0$, Helein [10], and (locally) stable for $8(k_2 - k_1) + k_3 \geq 0$, Cohen and Taylor [5], Kinderlehrer and Ou [12]. If $k_1 = k_2 = k_3$, (1.1) reduces to $W(\nabla n,n) = | \nabla n |^2$, the integrand for harmonic mappings of a region $\Omega \subset \mathbb{R}^3$ into $\mathbb{S}^2$. Here (1.7) is a stable solution for any $Q \in O(3)$, which was first proved by Brezis, Coron, and Lieb [3], cf. also F.-H. Lin

[13]. By a MAPLE computation, we have verified that this table is complete: if $u(x)$ in (1.4) satisfies the equilibrium equation of (1.3), then it appears in the Table.

The phenomenon of stability for defects of solutions of (1.3) and singularities of harmonic mappings was discovered by Hardt, Kinderlehrer, and Lin [9].

2. EXPLANATION OF THE TABLE A vector field n of sufficient regularity, $n \in H^1(\Omega;\mathbb{R}^3)$ is adequate, is a solution of (1.3) provided it satisfies the Euler equation

$$-\operatorname{div}\frac{\partial W}{\partial \nabla n}(\nabla n,n) + \frac{\partial W}{\partial n}(\nabla n,n) + \lambda n = 0, \quad |n| = 1, \text{ in } \Omega, \tag{2.1}$$

where λ is the multiplier arising from the constraint $|n| = 1$. To compute (2.1) we exploit that the term involving α is a null-lagrangian and thus offers no contribution. (However α has interpretation as a surface quantity, cf. Allender, Crawford, and Doane [1].) Hence we may choose it at our convenience, which amounts to choosing it so we need not compute derivatives of $n \wedge \operatorname{curl} n$. Since, when $|n| = 1$,

$$|\nabla n|^2 = \operatorname{tr}(\nabla n)^2 + |\operatorname{curl} n|^2 \quad \text{and} \quad |\operatorname{curl} n|^2 = (n \cdot \operatorname{curl} n)^2 + |n \wedge \operatorname{curl} n|^2,$$

we select $\alpha = k_1$. This brings (1.1) to the form

$$2W(\nabla n,n) = k_3 |\nabla n|^2 + (k_1 - k_3)(\operatorname{div} n)^2 + (k_2 - k_3)(n \cdot \operatorname{curl} n)^2 \text{ with} \tag{2.2}$$

$$2W(\nabla n,n) = k_1 |\nabla n|^2 + (k_2 - k_1)(n \cdot \operatorname{curl} n)^2. \tag{2.3}$$

when $k_3 = k_1$. Let

$$Q_o = \operatorname{diag}(-1,-1,1) \quad \text{and} \quad n_o(x) = Q_o \frac{x}{|x|}. \tag{2.4}$$

Then $n_o \cdot \operatorname{curl} n_o = 0$. Since this term appears quadratically in (2.3), it does not contribute to (2.1) evaluated at n_o. On the other hand, n_o is clearly a solution to the Euler Equation corresponding to the first term in (2.3), cf. the Table. Thus n_o is an equilibrium solution of (1.3). Any other 180° rotation may be obtained from Q_o by conjugation and corresponds to a solution of (1.3) by use of the invariance (1.2).

In general, let u satisfy (1.4). Since such u is already a solution of the harmonic mapping system,

$$\Delta u + \lambda u = 0 \text{ in } \Omega,$$

as we noted above for n_o, (2.1) reduces to

$$-(k_1 - k_3)\nabla \operatorname{div} u - (k_2 - k_3)\operatorname{curl}(u \cdot \operatorname{curl} u)u - (k_2 - k_3)(u \cdot \operatorname{curl} u)\operatorname{curl} u + \mu u = 0 \tag{2.5}$$

Choosing coordinates so the axis of Q is (001), cf. (1.2), it suffices to check (2.5) on vector fields (1.4) for

$$Q = \begin{pmatrix} a & b & 0 \\ -b & a & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad a^2 + b^2 = 1. \tag{2.6}$$

MAPLE was used to find all parameters (k_1, k_2, k_3, a, b) such that (2.5) holds. No solutions other than the ones already discussed were found.

3. STABILITY OF AND THE RANGE OF INSTABILITY OF n_o Assume first that $k_2 \geq \alpha = k_1 = k_3$. Suppose that $u \in H^1(B_r;\mathbb{S}^2)$, $B_r \subset \Omega$, satisfies $u = n_o$ on ∂B_r. Since n_o is stable for the Dirichlet Integral,

$$\frac{\alpha}{2} \int_{B_r} |\nabla n_o|^2 \, dx \leq \frac{\alpha}{2} \int_{B_r} |\nabla u|^2 \, dx \quad \text{and}$$

$$0 = \frac{k_2 - \alpha}{2} \int_{B_r} (n_o \cdot \mathrm{curl}\; n_o)^2 \, dx \leq \frac{k_2 - \alpha}{2} \int_{B_r} (u \cdot \mathrm{curl}\; u)^2 \, dx,$$

hence

$$\int_{B_r} W(\nabla n_o, n_o) \, dx \leq \int_{B_r} W(\nabla u, u) \, dx \quad , \text{ for } u \in H^1(B_r;\mathbb{S}^2), \; u\big|_{\partial B_r} = n_o.$$

To determine instability, we optimize in a special class of variations, analogous to the proof for $x/|x|$ in [10]. Let B denote the unit ball in $\mathbb{R}^3$, $r = |x|$ and let $f \in C_o^\infty(0,1)$. Define the vector fields

$$\zeta(x) = (-f(r)x_2, f(r)x_1, 0) \quad \text{and}$$

$$n_\varepsilon = \frac{n_o + \varepsilon\zeta}{|n_o + \varepsilon\zeta|} = n_o + \varepsilon\zeta - \tfrac{1}{2}\varepsilon^2 |\zeta|^2 n_o + o(\varepsilon^2) \tag{3.1}$$

Obviously, for ε small, $n_\varepsilon \in H^1(B;\mathbb{S}^2)$. Using that

$$\Delta n_o + |\nabla n_o|^2 n_o = 0 \quad \text{and} \quad \zeta \cdot n_o = 0,$$

we calculate that

$$\int_B |\nabla n_\varepsilon|^2 \, dx = \int_B \{ |\nabla n_o|^2 + \varepsilon^2 |\nabla \zeta|^2 - \varepsilon^2 |\nabla n_o|^2 |\zeta|^2 \} \, dx + o(\varepsilon^2)$$

and that

$$\int_B (n_\varepsilon \cdot \mathrm{curl}\; n_\varepsilon)^2 \, dx = \varepsilon^2 \int_B (n_o \cdot \mathrm{curl}\; \zeta + \zeta \cdot \mathrm{curl}\; n_o)^2 \, dx + o(\varepsilon^2).$$

Thus, the energy of n_ε over B is

$$\int_B W(\nabla n_\varepsilon, n_\varepsilon) \, dx = \int_B W(\nabla n_o, n_o) \, dx + \frac{\varepsilon^2}{2} E + o(\varepsilon^2), \text{ where} \tag{3.2}$$

$$E = \int_B \{ \alpha(|\nabla\zeta|^2 - |\nabla n_o|^2 |\zeta|^2) + (k_2 - \alpha)(n_o\cdot\text{curl}\,\zeta + \zeta\cdot\text{curl}\,n_o)^2 \}\, dx \qquad (3.3)$$

To draw the conclusion that n_o is unstable for some range of k_2, we need only choose an f which renders (3.3) negative. Computing E explicitly, we find

$$E = \frac{8}{105}\pi \int_0^1 \{(19\alpha + 16k_2)(rf'(r))^2 - (80\alpha - 10k_2)f(r)^2\} r^2\, dr. \qquad (3.4)$$

Helpful here is the identity for bounded g,

$$\int_B g(r)x_3^k\, dx = 4\pi \int_0^1 g(r)\frac{r^{k+2}}{k+1}\, dr\ .$$

Now introduce the change of dependent variable $h(r) = r^2 f(r)$ for which

$$\int_0^1 (rf'(r))^2 r^2\, dr = \int_0^1 \{h'(r)^2 + 2r^{-2}h(r)^2\} r^2\, dr \ \text{, whence}$$

$$E = \frac{8}{105}\pi \int_0^1 \{(19\alpha + 16k_2)h'(r)^2 - 42(\alpha - k_2)r^{-2}h(r)^2\} r^2\, dr.$$

From [5,10,12], $\inf_{C_o^\infty(0,1)} \dfrac{\int_0^1 h'(r)^2\, dr}{\int_0^1 r^{-2}h(r)^2\, dr} = \dfrac{1}{4}$. Thus if

$$\frac{42(\alpha - k_2)}{19\alpha + 16k_2} > \frac{1}{4} \qquad (3.5)$$

we may find an $h(r)$, whence an $f(r) = h(r)/r^2$, which renders $E < 0$. Inspection shows that (3.5) is equivalent to $k_2 < \dfrac{149}{184}\alpha$.

4. ADDITIONAL REMARKS The quantity $n \cdot \text{curl}\, n$ which vanishes for our special solution is called the irregularity of the vector field. It vanishes if and only if $n = \nabla\varphi / |\nabla\varphi|$ for some function φ or n is perpendicular to a family of surfaces. This is equivalent to the compatibility condition $f_y + f_z g = g_x + g_z f$ for an integrable system of differential equations $z_x = f(x,y,z)$, $z_y = g(x,y,z)$, cf [15] appendix B as well as [2] on the Frobenius Theorem. For our n_o, it is easily seen that $\varphi(x) = -x_1^2 - x_2^2 + x_3^2$. More generally, all the axially symmetric harmonic mappings

discussed in [8] satisfy $n \cdot \text{curl}\, n = 0$. It follows both that n has the property (3.8) and that it is a solution of the liquid crystal system (2.1) for $k_1 = k_3$.

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DK and NW:
Department of Mathematics and
Center for Nonlinear Analysis
Carnegie Mellon University
Pittsburgh, PA 15213-3890
USA

BO:
School of Mathematics
University of Minnesota
206 Church St. SE
Minneapolis, MN 55455
USA