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Second Variation of Liquid Crystal Energy at x/|x|

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Abstract

A new and simplified proof of the sign of the second variation of the Oseen-Frank Energy in terms of the elastic constants is given. The proof relies on the frame indifference of the energy and a new expression for the second invariant null lagrangian as a surface integral.

keywords: second variation, liquid crystal, frame indifference, null lagrangian.

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1 Introduction

Equilibrium configuration of a nematic liquid crystal are generally assumed to be realized by minima, or at least stationary points of the Oseen Frank energy of its optic axis $u(x) = (u^1(x), u^2(x), u^3(x))$,

$$E(u) = \int_\Omega W(\nabla u, u)dx, \quad |u| = 1, \tag{1.1}$$

$$W(\nabla u, u) = \frac{1}{2}k_1(\operatorname{div} \mathrm{u})^2 + \frac{1}{2}\mathrm{k}_2(\mathrm{u} \cdot \operatorname{curl} \mathrm{u})^2 + \frac{1}{2}\mathrm{k}_3|\mathrm{u} \wedge \operatorname{curl} \mathrm{u}|^2, \tag{1.2}$$

where Ω is the domain in R^3 occupied by the material. [1] Above k_1, k_2, k_3 are positive constants. In view of the constranint $|u| = 1$, an equilibrium configuration will

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generally have defects, or singular points, where u fails to be continuous. The simplest example of a configuration with a defect is

$$n(x) = \frac{x}{|x|} = \nabla|x|, \tag{1.3}$$

which is stationary for all choices of k_1, k_2, k_3.

The issue we wish to consider is when $n(x)$ is stable among all possible choices of $u(x), |u(x)| = 1$, which, say, are defined in $|x| \leq 1$ and agree with n on $|x| = 1$. Let us formulate this by introducing

$$\begin{aligned} H^1(B, S^2) &= \{u \in H^1(B; R^3) : |u(x)| = 1 \quad \text{in} \quad B\} \quad \text{and} \\ \mathcal{A} &= \{u \in H^1(B, S^2) : \ u = n \quad \text{on} \quad S^2 = \partial B\}, \end{aligned} \tag{1.4}$$

where B denotes the unit ball in R^3, and $H^1(B; R^3)$ denotes the usual Sobolev space of R^3 valued functions with square integrable first derivatives.

S.-Y. Lin [LI] pointed out that $n(x)$ fails to minimize (1.1) in $\mathcal{A}$ if k_1 is too large, both by explicit construction of a trial vector field of lower energy and by computation of the minimizing configuration. F.Helein [H], independently, gave quantitative form to this fact by proving that $n(x)$ is not the minimum of E in $\mathcal{A}$ if

$$8(k_2 - k_1) + k_3 < 0. \tag{1.5}$$

Cohen and Taylor [CT] then proved the remarkable fact that n is stable, in a suitable sense, provided

$$8(k_2 - k_1) + k_3 \geq 0. \tag{1.6}$$

Our primary intention here is to give an elementary proof of the Cohen and Taylor result, whose proof is based on the spectral theory of the $\overline{\partial}$ operator on S^2. Pivotal to our argument is a new expression for the integral of the null lagrangian

$$\int_\Omega \operatorname{tr} \operatorname{adj} \nabla u dx = \frac{1}{2} \int_\Omega ((\operatorname{div} \mathrm{u})^2 - \operatorname{tr} (\nabla \mathrm{u})^2) \mathrm{dx} \tag{1.7}$$

as a surface integral.

One result relevant to our results which we would like to mention here is that if $k_1 \leq k_2$, then $n(x)$ is the unique minimizer of energy in $\mathcal{A}$ defined above. This is shown in [O1] by extending an earlier result of F.-H. Lin [L1] on harmonic maps.

We refer to [E1], [HK], [K], and [L2] for recent developments in liquid crystal theory.

We wish to thank J.L. Ericksen for much helpful guidance. We are indebted to G.Vergara Caffarelli for many discussions about boundary integrals for (1.7), including the extremely simple proof of LEMMA 4.2.

2 Second variation of the Oseen Frank energy

We review the second variation of the Oseen Frank energy at $n(x) = \frac{x}{|x|}$ as developed by Cohen and Taylor. We then explain our result. Let $v \in H^1(B; R^3) \bigcap L^\infty(B; R^3)$ have compact support and satisfy $v \cdot n = 0$. For λ small

$$v_\lambda = \frac{n + \lambda v}{|n + \lambda v|} \in \mathcal{A} \text{ and} \tag{2.1}$$

$$E(v_\lambda) = E(n) + \frac{1}{2}\lambda^2 E_n(v, v) + o(\lambda^2) \tag{2.2}$$

where

$$E_n(v,v) = \int_B \{k_1[(\mathrm{div}\, u)^2 - \frac{2}{|x|^2}|v|^2] + k_2|n \cdot \mathrm{curl}\, v|^2 + k_3|n \wedge \mathrm{curl}\, v|^2\}dx. \tag{2.3}$$

Our main objective is to prove this version of the result of Cohen and Taylor [CT]:

Theorem 2.1 *Let $v \in H^1(B; R^3) \bigcap L^\infty(B; R^3)$ satisfy $v \cdot n = 0$. Assume that $v \not\equiv 0$. Then*

$$E_n(v,v) > 0 \text{ when } 8(k_2 - k_1) + k_3 \geq 0$$

and

$$E_n(v,v) < 0 \text{ when } 8(k_2 - k_1) + k_3 < 0.$$

As noted in the introduction, the second part of this theorem is due to Helein [H].

As observed by Cohen and Taylor, the positivity of $E_n(v, v)$ when $8(k_2 - k_1) + k_3 \geq 0$ follows from the two inequalities

$$\int_B [(\mathrm{div\,v})^2 + |\mathrm{n}\cdot\mathrm{curlv}|^2]\mathrm{dx} \geq \int_{\mathrm{B}} \frac{2}{|\mathrm{x}|^2}|\mathrm{v}|^2\mathrm{dx}, \tag{2.4}$$

and

$$\int_B |n \wedge \mathrm{curl} v|^2 dx \geq \frac{1}{4}\int_B \frac{1}{|x|^2}|v|^2 dx, \tag{2.5}$$

$$\text{whenever } \ v \in H^1(B;R^3)\bigcap L^\infty(B;R^3) \text{ satisfies } \ v\cdot n = 0.$$

The inequality in (2.5) is strict if $v \not\equiv 0$.

The proof for this elementary but rather critical observation is simple. If $k_1 \leq k_2$, $E(n)(v,v)$ is lowered if k_2 in (2.3) is replaced by k_1, and the proof of the positivity simply follows the inequalities of (2.4) and (2.5); if $k_1 > k_2$, and $k_3 \geq 8(k_1 - k_2)$ then

$$\begin{aligned} E(n)(v,v) &\geq \int_B \{k_2(\mathrm{div\,v})^2 - \mathrm{k}_1\frac{2}{|\mathrm{x}|^2}|\mathrm{v}|^2 + \mathrm{k}_2|\mathrm{n}\cdot\mathrm{curl\,v}|^2 \\ &\quad +k_3|n \wedge \mathrm{curl\,v}|^2\}\mathrm{dx} \\ &= \int_B \{k_2[(\mathrm{div\,v})^2 + |\mathrm{n}\cdot\mathrm{curl\,v}|^2] + \mathrm{k}_3|\mathrm{n}\wedge\ \mathrm{curlv}|^2 \\ &\quad -k_1\frac{2}{|x|^2}|v|^2\}dx \\ &\geq \int_B \{k_2\frac{2}{|x|^2}|v|^2 + 8(k_1-k_2)\frac{1}{4}\frac{1}{|x|^2}|v|^2 \\ &\quad -k_1\frac{2}{|x|^2}|v|^2\}dx \\ &= \int_B [2k_1 + 2(k_1-k_2) - 2k_1]\frac{|v|^2}{|x|^2}dx \\ &= 0. \end{aligned}$$

3 Frame indifference

The energy density (1.1) is frame indifferent, which means that it is invariant under the change of variables

$$u'(x) = Qu(Q^T x), \ \ Q \in SO(3), \tag{3.1}$$

which transforms ∇u to $\nabla u' = Q\nabla u Q^T$. This was one of the bases for its derivation, cf.[F],[E]. In our proof we shall use the frame indifference of the quantities appearing in (2.3) as well, so we check that here. First of all note that for any vector valued function $u(x)$

$$\det(\lambda I - Q\nabla u Q^T) = \det(\lambda I - \nabla u), \quad -\infty < \lambda < +\infty. \tag{3.2}$$

Since

$$\det(\lambda I - \nabla u) = \lambda^3 - \operatorname{div} \mathrm{u}\lambda^2 + \frac{1}{2}((\operatorname{div} \mathrm{u})^2 - \operatorname{tr}(\nabla \mathrm{u})^2)\lambda - \det(\nabla \mathrm{u}), \tag{3.3}$$

the fundamental invariants $\operatorname{div} \mathrm{u}$, $(\operatorname{div} \mathrm{u})^2 - \operatorname{tr}(\nabla \mathrm{u})^2$, and $\det(\nabla u)$ are frame indifferent.

Now $\operatorname{curl} \mathrm{u}$ is the unique vector for which

$$\operatorname{curl} \mathrm{u} \wedge \xi = (\nabla \mathrm{u} - \nabla \mathrm{u}^{\mathrm{T}})\xi, \quad \xi \in \mathrm{R}^3. \tag{3.4}$$

Writing $\xi' = Q\xi$ and defining $u'(x) = Qu(Q^T x)$, as in (3.1) above, we have that

$$\operatorname{curl} \mathrm{u}' \wedge \xi' = \mathrm{Q}\operatorname{curl} \mathrm{u} \wedge \xi$$

so

$$|\operatorname{curl} \mathrm{u}' \wedge \xi'| = |\operatorname{curl} \mathrm{u} \wedge \xi|. \tag{3.5}$$

If ξ is a unit vector perpendicular to $\operatorname{curl} \mathrm{u}$, then ξ' is a unit vector perpendicular to $\operatorname{curl} \mathrm{u}'$, whence

$$|\operatorname{curl} \mathrm{u}'| = |\operatorname{curl} \mathrm{u}|.$$

If ξ is an arbitrary unit vector, then

$$|\xi \cdot \operatorname{curl} \mathrm{u}|^2 = |\operatorname{curl} \mathrm{u}|^2 - |\operatorname{curl} \mathrm{u} \wedge \xi|^2,$$

so

$$|\xi' \cdot \operatorname{curl} \mathrm{u}'|^2 = |\xi \cdot \operatorname{curl} \mathrm{u}|^2.$$

A special case of this is $\xi(x) = n(x)$ for which $n'(x) = n(x)$. This gives that

$$|n \cdot \operatorname{curl} \mathrm{u}'|^2 = |\mathrm{n} \cdot \operatorname{curl} \mathrm{u}|^2. \tag{3.6}$$

Thus each term in (2.3) is frame indifferent.

In this spirit, we do some computations along the positive x_3 axis to be used later.

Along the positive x_3 axis, $x = (0,0,r), n = x/|x| = (0,0,1)$. Exploiting $(n\cdot v) \equiv 0$, we have

$$x_i v_i = |x|(n \cdot v) \equiv 0,$$
$$\frac{\partial}{\partial x_j}(x_i v_i) = v_j + x_i \frac{\partial v_i}{\partial x_j} = 0 \text{ for } j = 1,2,3.$$

Writing them down explicitly,

$$\begin{aligned} v_3 &= 0, \\ v_1 + r\frac{\partial}{\partial x_1} v_3 &= 0, \\ v_2 + r\frac{\partial}{\partial x_2} v_3 &= 0, \\ v_3 + r\frac{\partial}{\partial x_3} v_3 &= 0. \end{aligned}$$

In summary,

$$\begin{aligned} (\nabla v) &= (\frac{\partial v}{\partial x}) \\ &= \begin{pmatrix} \frac{\partial v_1}{\partial x_1} & \frac{\partial v_1}{\partial x_2} & \frac{\partial v_1}{\partial x_3} \\ \frac{\partial v_2}{\partial x_1} & \frac{\partial v_2}{\partial x_2} & \frac{\partial v_2}{\partial x_3} \\ -\frac{v_1}{r} & -\frac{v_2}{r} & 0 \end{pmatrix} \\ &= \begin{pmatrix} a_1 & a_2 & \frac{\partial v_1}{\partial r} \\ b_1 & b_2 & \frac{\partial v_2}{\partial r} \\ -\frac{v_1}{r} & -\frac{v_2}{r} & 0 \end{pmatrix}. \end{aligned} \tag{3.7}$$

Therefore

$$\operatorname{curl} \mathrm{v} = (-\frac{\partial \mathrm{v}_2}{\partial \mathrm{r}} - \frac{\mathrm{v}_2}{\mathrm{r}}, \frac{\partial \mathrm{v}_1}{\partial \mathrm{r}} + \frac{\mathrm{v}_1}{\mathrm{r}}, \mathrm{b}_1 - \mathrm{a}_2) \tag{3.8}$$

and the following expressions for those quantities which are frame indifferent:

$$(\operatorname{div} \mathrm{v})^2 = (a_1 + b_2)^2; \tag{3.9}$$
$$|n \cdot \operatorname{curl} \mathrm{v}|^2 = (b_1 - a_2)^2; \tag{3.10}$$
$$|n \wedge \operatorname{curl} \mathrm{v}|^2 = (-\frac{\partial v_1}{\partial r} - \frac{v_1}{r})^2 + (\frac{\partial v_2}{\partial r} + \frac{v_2}{r})^2; \tag{3.11}$$
$$(\operatorname{div} \mathrm{v})^2 - \operatorname{tr}(\nabla \mathrm{v})^2 = \text{Twice the sum of the determinants of all}$$

$$
\begin{aligned}
& \text{the diagonal } 2\times 2 \text{ submatrices of } (\nabla v) \\
&= (2a_1b_2 - 2a_2b_1) + \frac{2}{r}v_1\frac{\partial v_1}{\partial r} + \frac{2}{r}v_2\frac{\partial v_2}{\partial r}; \qquad (3.12)
\end{aligned}
$$

$$|v|^2 = v_1^2 + v_2^2; \qquad (3.13)$$

$$\frac{\partial}{\partial r}|v|^2 = 2v_1\frac{\partial v_1}{\partial r} + 2v_2\frac{\partial v_2}{\partial r}. \qquad (3.14)$$

4 Proof of (2.4)

The inequality (2.4) is the more difficult to prove, so we shall focus first on it. In fact, we shall prove a better inequality..

PROPOSITION 4.1 *Let $v \in C^1(B;R^3)$ satisfy $v \cdot n = 0$. Then*

$$\int_{S_r} ((\mathrm{div\,v})^2 + (\mathrm{n}\cdot \mathrm{curl\,v})^2)\mathrm{dS_r} \geq \frac{2}{\mathrm{r}^2}\int_{\mathrm{S_r}} |\mathrm{v}|^2\mathrm{dS_r}, \quad 0 < \mathrm{r} < 1. \qquad (4.1)$$

where $S_r = \partial B_r$ and dS_r denotes the surface measure on S_r.

Integration of (4.1) yields (2.4) for smooth functions. We remove this restriction at the end of this section. The proof relies on two lemmas. The first of these is the interpretation of the null langrangian mentioned in the introduction.

LEMMA 4.2 *Let $v \in C^1(\overline{\Omega};R^3)$, where Ω is a domain with smooth boundary. Then*

$$
\begin{aligned}
& \frac{1}{2}\int_\Omega (\mathrm{div\,u})^2 - \mathrm{tr}\,(\nabla \mathrm{u})^2 \mathrm{dx} \\
&= \int_\Omega \mathrm{tr\ adj}\nabla u dx \\
&= \int_{\partial\Omega} \mathrm{adj}\nabla u \cdot x \otimes \nu dS, \qquad (4.2)
\end{aligned}
$$

where ν denotes the outward unit normal to Ω.

Proof of LEMMA 4.2. First suppose that $u \in C^\infty(\overline{\Omega};R^3)$.Then recalling that

$$\mathrm{div\,adj}\nabla\mathrm{u} = 0,$$

we have that

$$\begin{aligned}\int_\Omega \mathrm{adj}\nabla u \cdot x \otimes \nu dS &= \int_{\partial\Omega} (\mathrm{adj}\nabla u)_{ij} x_i \nu_j dS \\ &= \int_\Omega (\mathrm{adj}\nabla u)_{ij} \delta ij dx + \int_\Omega \frac{\partial}{\partial x_j}(\mathrm{adj}\nabla)_{ij} x_i dx \\ &= \int_\Omega (\mathrm{tr}\ \mathrm{adj}\nabla u) dx.\end{aligned}$$

The result now follows from approximation.

The lemma may be generalized in many directions, both to less smooth classes of functions and to other null langrangians. See section 8 for more discussion.

We apply the lemma. Assume that $v \in C^1(B; R^3)$. Introduce the (frame indifferent) expression

$$Tv = (\mathrm{div}\,\mathrm{v})^2 - \mathrm{tr}\,(\nabla \mathrm{v})^2 - \frac{1}{\mathrm{r}}\frac{\partial}{\partial \mathrm{r}}|\mathrm{v}|^2 \tag{4.3}$$

and note that if $v \cdot n = 0$, then

$$Tv(0,0,r) = 2(a_1 b_2 - a_2 b_1).$$

On the other hand, at $x = (0,0,r)$,

$$\begin{aligned}\mathrm{adj}\nabla v \cdot x \otimes \nu &= \mathrm{adj}\nabla v \cdot n \otimes n\, r, \quad n = (0,0,1), \\ &= (a_1 b_2 - a_2 b_1) r = \frac{1}{2} T v\, r.\end{aligned}$$

Hence

$$\int_{B_r} ((\mathrm{div} v)^2 - \mathrm{tr}(\nabla v)^2) dx = \int_{S_r} T v\, r dS_r \tag{4.4}$$

Finally, let us note that at $x = (0,0,r)$,

$$(\mathrm{div}\,\mathrm{v})^2 + (\mathrm{n} \cdot \mathrm{curl}\,\mathrm{v})^2 = (\mathrm{a}_1 + \mathrm{b}_2)^2 + (\mathrm{a}_2 - \mathrm{b}_1)^2 \geq 4(\mathrm{a}_1\mathrm{b}_2 - \mathrm{a}_2\mathrm{b}_1),$$

from which it follows that

$$(\mathrm{div}\,\mathrm{v})^2 + (\mathrm{n} \cdot \mathrm{curl}\,\mathrm{v})^2 \geq 2\mathrm{Tv}. \tag{4.5}$$

Hence PROPOSITION 4.1 for smooth function is a consequence of

LEMMA 4.3 *Let $v \in C_0^1(B;R^3)$ satisfy $v \cdot n = 0$. Then*

$$\int_{S_r} Tv\, dS_r = \frac{1}{r^2}\int_{S_r} |v|^2 dS_r, \quad 0 < r < 1. \tag{4.6}$$

PROOF: We may assume that $v = 0$ in a neighborhood of 0. Using (4.4),

$$\begin{aligned} &\int_{B_r} Tv\, dx \\ &= \int_{B_r} ((\mathrm{div\, u})^2 - \mathrm{tr}\,(\nabla \mathrm{u})^2)\mathrm{dx} - \int_{B_r} \frac{1}{\rho}\frac{\partial}{\partial \rho}|\mathrm{v}|^2 \mathrm{dx} \\ &= \int_{S_r} Tvr dS_r - \int_{B_r} \frac{1}{\rho}\frac{\partial}{\partial \rho}|v|^2 dx \end{aligned}$$

We calculate that

$$-\int_{B_r} \frac{1}{\rho}\frac{\partial}{\partial \rho}|v|^2 dx = \int_{B_r} \frac{1}{\rho^2}|v|^2 dx - \int_{S_r} \frac{1}{r}|v|^2 dS_r. \tag{4.7}$$

Placing this in the above and grouping the volume and surface terms separately gives that

$$\int_{B_r} \{Tv - \frac{1}{\rho^2}|v|^2\} dx = r\int_{S_r} \{Tv - \frac{1}{\rho^2}|v|^2\} dS_r. \tag{4.8}$$

Denote the left hand side of (4.7) by $f(r)$. Since v has compact support, (4.7) assumes the form

$$f(r) = r\frac{df(r)}{dr}, \quad f(1) = 0. \tag{4.9}$$

The solution of (4.8) is $f(r) = 0$, which is (4.6).

COMPLETION OF THE PROOF OF (2.4): We want to check that (1.4) is valid for $v \in H_0^1(B;R^3)$ with compact support. Suppose first that $v \in H_0^1(B;R^3)$ with $\mathrm{supp}\, v \subset B \setminus B_r$. Let $w_\epsilon \in C_0^\infty(B;R^3)$ be uniformly bounded, $\mathrm{supp}\, w_\epsilon \subset B \setminus B_r$ with $w_\epsilon \to v$ in $H_0^1(B;R^3)$. Then $v_\epsilon = w_\epsilon - (w_\epsilon \cdot n)n$ satisfies $v_\epsilon \cdot n = 0$ and

$$\|v_\epsilon - v\|_{L^2(B;R^3)} \le \|w_\epsilon - v\|_{L^2(B;R^3)}.$$

Moreover,

$$\int_B |\nabla(v_\epsilon - v)|^2 dx \le 2\int_B |\nabla(w_\epsilon - v)|^2 dx + \int_B |w_\epsilon - v|^2 |\nabla n|^2 dx.$$

Now for a subsequence of w_ϵ, not relabled,

$$w_\epsilon \longrightarrow v \quad \text{in B a.e.}$$

hence

$$|w_\epsilon - v|^2|\nabla n|^2 \longrightarrow 0 \quad \text{in B a.e.}$$

Moreover, since the w_ϵ are uniformly bounded,

$$|w_\epsilon - v|^2|\nabla n|^2 \leq C|\nabla n|^2 \in L^1(B).$$

Thus by Lebesque's Theorem,

$$\lim_{\epsilon \to 0} \int_B |w_\epsilon - v|^2|\nabla n|^2 dx = 0,$$

and (2.4) holds for $v \in H_0^1(B; R^3)$ with $\operatorname{supp} v \subset B \setminus B_r$. To remove the condition on the support of v, it suffices to replace v by $\eta^2 v, n = 1$ in $B \setminus B_r$ and $\eta = 0$ in $B_{r/2}$ and check that

$$\lim_{r \to 0} \int_B |\nabla(\eta^2 v - v)^2 dx = 0.$$

5 Proof of (2.5)

We begin by proving (2.5) for $v \in C_0^1(B \setminus B_r; R^3)$ satisfying $v \cdot n = 0$. Owing to the frame indifference of the integrand, it suffices to prove that along the positive x_3 axis

$$\int_0^1 |n \wedge \text{curl} v|^2 r^2 dr \geq \frac{1}{4} \int_0^1 \frac{1}{r^2}|v|^2 r^2 dr \tag{5.1}$$

and the inequality is strict if v does not vanish identically along the positive x_3 axis.

Let $g_i = rv_i$, $i = 1, 2$. From the calculations of (10),(12) along the positive x_3 axis,

$$\begin{aligned}
& \int_0^1 |n \wedge \text{curl} v|^2 r^2 dr \\
= & \int_0^1 [(\frac{\partial v_1}{\partial r} + \frac{v_1}{r})^2 + (\frac{\partial v_2}{\partial r} + \frac{v_2}{r})^2] r^2 dr \\
= & \int_0^1 [(\frac{\partial (rv_1)}{\partial r})^2 + (\frac{\partial (rv_2)}{\partial r})^2] dr
\end{aligned}$$

$$
\begin{aligned}
&= \int_0^1 [(\frac{\partial(g_1)}{\partial r})^2 + (\frac{\partial(g_2)}{\partial r})^2] dr \\
&\geq \frac{1}{4}\int_0^1 \frac{1}{r^2}[(g_1)^2 + (g_2)^2] dr \\
&= \frac{1}{4}\int_0^1 \frac{1}{r^2}[(rv_1)^2 + (rv_2)^2] dr \\
&= \frac{1}{4}\int_0^1 |v|^2 dr
\end{aligned}
$$

where we used Proposition 1 in the appendix to get the inequality above. We also use Proposition 1 to conclude that the inequality is strict if v does not vanish identically along the positive x_3 axis. The extension to general $v \in H_0^1(B;R^3)$ with compact support proceeds exactly as in the proof of (2.4). This completes the proof of THEOREM 2.1.

6 Optimality

Finally, we remark that inequalities (2.4) and (2.5) are optimal. In [H], Helein picked

$$v = (\chi(r)x_2, -\chi(r)x_1, 0), \quad r = |x|$$

to get the optimal choice in his proof that the second variation of $E(u)$ in (1) at $x/|x|$ is nonpositive if $8(k_2 - k_1) + k_3 < 0$. For such kind of v,

$$
\begin{aligned}
(\mathrm{div}v)^2 &= 0; \\
(\mathrm{div}v)^2 + |n \wedge \mathrm{curl}v|^2 &= \frac{4x_3^2}{r^2}\chi^2(r); \\
\frac{2}{|x|^2}|v|^2 &= \frac{2(x_1^2 + x_2^2)}{r^2}\chi^2(r).
\end{aligned}
$$

Thus for the two sides of the inequality (2.4),

$$
\begin{aligned}
\int_B [(\mathrm{div}v)^2 + |n \cdot \mathrm{curl}v|^2] &= \frac{4}{3}\int_B \chi^2(r)dx, \\
\int_B \frac{2}{|x|^2}|v|^2 dx &= \frac{4}{3}\int_B \chi^2(r)dx.
\end{aligned}
$$

Therefore (2.4) is in fact an equality. This calculation also shows that in (4.6), although the integrals of the two sides over a sphere are equal, their integrands are generally not. To be more specific, we easily verify it here by a direct computation.

$$\begin{aligned} Tv &= (\mathrm{div} v)^2 - \mathrm{tr}(\nabla v)^2 - \frac{1}{r}\frac{\partial(|v|^2)}{\partial r} \\ &= 2(\frac{\partial v_1}{\partial x_1}\frac{\partial v_2}{\partial x_2} - \frac{\partial v_2}{\partial x_1}\frac{\partial v_1}{\partial x_2}) - \frac{1}{r}\frac{\partial(|v|^2)}{\partial r} \\ &= 2(\chi^2 + \chi\chi'\frac{x_1^2 + x_2^2}{r}) \\ &\quad -\frac{1}{r}[2\chi\chi'(x_1^2 + x_2^2) + 2\chi^2\frac{x_1^2 + x_2^2}{r}] \\ &= 2\frac{x_3^2}{r^2}\chi^2(r), \end{aligned}$$

therefore for the two sides of (4.6),

$$\begin{aligned} r^2 Tv(r,\omega) &= 2\frac{x_3^2}{r^2}\chi^2(r), \\ |v|^2(r,\omega) &= \frac{x_1^2 + x_2^2}{r^2}\chi^2(r). \end{aligned}$$

Furthermore, the function χ in v can be chosen such that the left side of (2.5) can be less than the right side multiplied by any prescribed factor larger than one. We do not go to detail here, see [H] and/or the remark following the proof of our Proposition 1 in the appendix.

7 Appendix 1: A Sobolev type inequality

Proposition 1 *For a smooth function $g(t)$ with compact support in (0,1], the following inequality holds:*

$$\int_0^1 (g')^2 dt \geq \frac{1}{4}\int_0^1 \frac{g^2}{t^2} dt \tag{7.1}$$

and the equality holds only when $g \equiv 0$.

Proof: We notice that

$$\begin{aligned} \int_0^1 \frac{g^2}{t^2} dt &= \int_0^1 g^2 d(-\frac{1}{t}) \\ &= -\frac{g^2}{t}\Big|_0^1 + \int_0^1 2gg'/t\, dt \\ &\leq 2(\int_0^1 \frac{g^2}{t^2} dt)^{1/2}(\int_0^1 (g')^2 dt)^{1/2}. \end{aligned}$$

Squaring two sides above leads to (7.1).

From the proof, if (7.1) is an equality, g' has to be proportional to g/t. Only $g \equiv 0$ satisties this with the boundary condition $g(1) = 0$.

Remark 1: It's easy to verify that the proposition is equally true for nonsmooth, but absolutely continuous function g such that $|g| \leq ct$ for some constant c. The proof of (2.5) for general $v \in H^1 \bigcap L^\infty$ depends on this argument. Specifically in the proof of equality (5.1), $g_i = r\, v_i$, $|g_i| \leq cr$ since $v \in H_0^1 \bigcap L^\infty$.

Remark 2: 1/4 here is in fact the best coefficient in the following sense, for any constant $c > 1/4$, there is a smooth g with compact support in (0,1) such that

$$\int_0^1 (g')^2 dt \leq c \int_0^1 \frac{g^2}{t^2} dt. \tag{7.2}$$

The proof of this is also elementary.

Consider

$$c_\epsilon = \inf_{g \in H_0^1([\epsilon,1])} \int_0^1 (g')^2 dt / \int_0^1 \frac{g^2}{t^2} dt \quad \text{with} \quad 0 < \epsilon \ll 1.$$

c_ϵ is reached by a function g_ϵ which satisties

$$g_\epsilon'' + c_\epsilon \frac{g_\epsilon^2}{t^2} = 0, \quad g_\epsilon(\epsilon) = g_\epsilon(1) = 0$$

The ODE is solvable by the standard Euler method, c_ϵ is calculated as

$$c_\epsilon = [(\frac{2\pi}{-\ln \epsilon})^2 + 1]/4 \longrightarrow 1/4 \quad \text{as } \epsilon \to 0.$$

8 Appendix 2: A discussion on the null lagrangian energy

In [E2] there is a systematic discussion on the null lagrangian energies of liquid crystals. Here we are going to give a more geometrical understanding of the null lagrangian energy. In another sense, this is to put the simple proof of Lemma 4.2 in a larger context.

The first motivation of our study comes from the equality

$$\det(I+t\nabla f)=1+t\,\mathrm{div}f+\frac{t^2}{2}[(\mathrm{div}\nabla f)^2-\mathrm{tr}(\nabla f)^2]+\frac{t^3}{3}\det(\nabla f).$$

Obviously this equality suggests that all the three terms in the right side are null lagrangians, i.e, their integrations in a domain only depend on their values on the boundary.

In [BCL], an important role is played by the divergence of the vector function

$$(f\cdot\frac{\partial f}{\partial x_2}\wedge\frac{\partial f}{\partial x_3},f\cdot\frac{\partial f}{\partial x_3}\wedge\frac{\partial f}{\partial x_1},f\cdot\frac{\partial f}{\partial x_1}\wedge\frac{\partial f}{\partial x_2}).$$

Specifically, if $f=(f_1,f_2,f_3)$, $|f|=1$ and f only has finite singularities at P_i with degree d_i, then the aforementioned divergence is $\sum d_i\delta_{P_i}(x)$. A detailed proof has to employ the following identity of the diffential forms and the Stokes integration theorem:

$$\begin{aligned}&d(f_1df_2\wedge df_3+f_2df_3\wedge df_1+f_3df_1\wedge df_2)\\=\;&3df_1\wedge df_2\wedge df_3\\=\;&3\det(\nabla f)dx_1\wedge dx_2\wedge dx_3.\end{aligned}$$

Here we use $\wedge$ as the exterior product of differential forms (besides the exterior product of two vectors in R^3), and we use d as the exterior differentiation operator. We refer to [B] for an introduction to the calculus of the exterior differntiation.

Playfully, if we replace one of the f_i's in the above identity with x_i's, say the last ones, we find

$$\begin{aligned}&d(f_1df_2\wedge dx_3+f_2df_3\wedge dx_1+f_3df_1\wedge dx_2)\\=\;&df_1\wedge df_2\wedge dx_3+df_2\wedge df_3\wedge dx_1+df_3\wedge df_1\wedge dx_2\\=\;&1/2((\mathrm{div}(\nabla f)^2-\mathrm{tr}(\nabla f)^2)dx_1\wedge dx_2\wedge dx_3.\end{aligned}$$

The integration by Stokes theorem leads to something well known already. In fact, it is equivalent to writing

$$(\mathrm{div}f)^2-\mathrm{tr}(\nabla f)^2$$

$$= \frac{\partial f_i}{\partial x_i}\frac{\partial f_j}{\partial x_j} - \frac{\partial f_i}{\partial x_j}\frac{\partial f_j}{\partial x_i}$$
$$= \frac{\partial}{\partial x_i}(f_i\frac{\partial f_j}{\partial x_j} - f_j\frac{\partial f_i}{\partial x_j}),$$

then using the divergence theorem to express it as a boundary integral. Unfortunately, the formula as the surface integration does not provide much geometric insight into what it really is. In the proof of inequality (2.4) we were initially stalled at this point.

The difficulty encountered here was finally resolved by our observation that we should replace the *first* f_i's with x_i's, that is, we equally have

$$\begin{aligned} & d(x_1 df_2 \wedge df_3 + x_2 df_3 \wedge df_1 + x_3 df_1 \wedge df_2) \\ = \ & dx_1 \wedge df_2 \wedge df_3 + dx_2 \wedge df_3 \wedge df_1 + dx_3 \wedge df_1 \wedge df_2 \\ = \ & 1/2((\mathrm{div}(\nabla f)^2 - \mathrm{tr}(\nabla f)^2) dx_1 \wedge dx_2 \wedge dx_3. \end{aligned}$$

A salient feature of this equality is that here the *first* x_i's lead the two following f_i's instead of that the first f_i's lead one f_i's and one x_i's in the former identity. It was this symmetry that leads to the new expression.

Proposition 2 *Let $f = (f_1, f_2, f_3)$ be smooth on a smooth domain Ω. Denote ν as the outnormal of $\partial\Omega$ and e_1, e_2 as an orthonormal basis for the tangential plane at $x \in \partial\Omega$ such that (e_1, e_2, ν) forms a right handed basis for R^3. We have*

$$\int_\Omega [(\mathrm{div} f)^2 - \mathrm{tr}(\nabla f)^2] dx = 2\int_{\partial\Omega} x \cdot \frac{\partial f}{\partial e_1} \wedge \frac{\partial f}{\partial e_2} dS. \tag{8.1}$$

Proof: We use Stokes theorem on integration (cf. [B]).

$$\begin{aligned} & \int_\Omega [(\mathrm{div} f)^2 - \mathrm{tr}(\nabla f)^2] dx \\ = \ & 2\int_\Omega d(x_1 df_2 \wedge df_3 + x_2 df_3 \wedge df_1 + x_3 df_1 \wedge df_2) \\ = \ & 2\int_{\partial\Omega} (x_1 df_2 \wedge df_3 + x_2 df_3 \wedge df_1 + x_3 df_1 \wedge df_2) \\ = \ & 2\int_{\partial\Omega} (\begin{vmatrix} x_1 & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ x_2 & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ x_3 & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{vmatrix} dx_2 \wedge dx_3 + \begin{vmatrix} \frac{\partial f_1}{\partial x_1} & x_1 & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & x_2 & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & x_3 & \frac{\partial f_3}{\partial x_3} \end{vmatrix} dx_3 \wedge dx_1 \end{aligned}$$

$$+\begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & x_1 \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & x_2 \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & x_3 \end{vmatrix} dx_1 \wedge dx_2)$$

$$= 2\int_{\partial\Omega}(\begin{vmatrix} x_1 & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ x_2 & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ x_3 & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{vmatrix} \nu_1 + \begin{vmatrix} \frac{\partial f_1}{\partial x_1} & x_1 & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & x_2 & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & x_3 & \frac{\partial f_3}{\partial x_3} \end{vmatrix} \nu_2$$

$$+\begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & x_1 \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & x_2 \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & x_3 \end{vmatrix} \nu_3)dS$$

$$= 2\int_{\partial\Omega}(x_1 \begin{vmatrix} \nu_1 & \nu_2 & \nu_3 \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{vmatrix} + x_2 \begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \nu_1 & \nu_2 & \nu_3 \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{vmatrix}$$

$$+x_3 \begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \nu_1 & \nu_2 & \nu_3 \end{vmatrix})dS$$

where $(\nu_1, \nu_2, \nu_3) = \nu$ is the outnormal to $\partial\Omega$, dS is the area element of $\partial\Omega$. Let (e_1, e_2, ν) be a right handed basis for R^3, we have

$$\begin{vmatrix} \nu_1 & \nu_2 & \nu_3 \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{vmatrix} = \begin{vmatrix} 0 & 0 & 1 \\ \frac{\partial f_2}{\partial e_1} & \frac{\partial f_2}{\partial e_2} & \cdot \\ \frac{\partial f_3}{\partial e_1} & \frac{\partial f_3}{\partial e_2} & \cdot \end{vmatrix}$$

$$\begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \nu_1 & \nu_2 & \nu_3 \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{vmatrix} = \begin{vmatrix} \frac{\partial f_1}{\partial e_1} & \frac{\partial f_1}{\partial e_2} & \cdot \\ 0 & 0 & 1 \\ \frac{\partial f_3}{\partial e_1} & \frac{\partial f_3}{\partial e_2} & \cdot \end{vmatrix}$$

$$\begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \nu_1 & \nu_2 & \nu_3 \end{vmatrix} = \begin{vmatrix} \frac{\partial f_1}{\partial e_1} & \frac{\partial f_1}{\partial e_2} & \cdot \\ \frac{\partial f_2}{\partial e_1} & \frac{\partial f_2}{\partial e_2} & \cdot \\ 0 & 0 & 1 \end{vmatrix}$$

where "·" denotes an entry which is of no use.

From all of the calculations above, we get

$$\int_\Omega [(\mathrm{div} f)^2 - \mathrm{tr}(\nabla f)^2]dx = 2\int_{\partial\Omega} x\cdot\frac{\partial f}{\partial e_1}\wedge\frac{\partial f}{\partial e_2}dS. \tag{8.2}$$

Proposition 2 is proved.

As one might notice, the right side of (8.1) resembles strongly the expression $\int_{\partial\Omega} f\cdot\frac{\partial f}{\partial e_1}\wedge\frac{\partial f}{\partial e_2}dS$ in [BCL]. The proof of Lemma 4.2 is in fact a compact form of the above proof.

For liquid crytstals, the director vector u satisfy $|u| = 1$, therefore, both $\frac{\partial u}{\partial e_1}, \frac{\partial u}{\partial e_2}$ are perpendicular to u and

$$\frac{\partial u}{\partial e_1}\wedge\frac{\partial u}{\partial e_2} = uJ,$$

here J is the Jacobian of the map $u : \partial\Omega \to S^2$.

Proposition 3 *For liquid crystals, if u is the director vector field of the optic axises, and if there is no defect (or singular point) on $\partial\Omega$, then*

$$\int_\Omega [(\mathrm{div} u)^2 - \mathrm{tr}(\nabla u)^2]dx = 2\int_{\partial\Omega}(x\cdot u)JdS$$

where J is the Jacobian of the map $u : \partial\Omega \to S^2$, and dS is the area element on $\partial\Omega$.

Proof: Since we have assumed there is no defect or singular point on $\partial\Omega$, u can be approximated by smooth f's in Sobolev space $H^1(\Omega)$ with the same boundary values. ($|f|$ does not need to be $|f| = 1$). By Proposition 2 and the preceding remarks,

$$\int_\Omega [(\mathrm{div} u)^2 - \mathrm{tr}(\nabla u)^2]dx = 2\int_{\partial\Omega}(x\cdot u)JdS.$$

Some remarks to Proposition 3 might be interesting. If $\Omega = B$ and $u = x/|x|$ then $(x\cdot n) = 1, J = 1$ so the integration is 8π. If u is planar, i.e., if u takes on values in a grand circle of S^2, then $J \equiv 0$, so the integration is identically zero. Physically, it is an open problem how to measure the elastic constant associated with the null lagrangian energy in liquid crystals. (all of the other elastic constants have some experimental ways to measure them out.)

References

[B] W.H. Boothby, An Introduction to Differentiable Manifolds and Riemannian Geometry, Academic Press, New York, 1975

[BCK] H.Brezis, J.-M.Coron, E.Lieb, Harmonic Maps with defects. Comm. Math. Physics. 107(1986), pp.649-705.

[CT] R.Cohen, M.Taylor, Weak Stability of the map $x/|x|$ for liquid crystal. Preprint.

[E1] J.L.Ericksen, Equilibrium theory of liquid crystals, Advances in Liquid Crystals, vol.2, Brown,G.H.(ed), Academic Press 233-299, 1976

[E2] J.L.Ericksen, Nilpotent energies in liquid crystal theory, Arch. Rat. Mech. Anal. 10(1962) 189-196

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

[H] F. Helein, Minima de la fonctionelle energie libre des cristaux liquides, C.R.Acad.Sc.Paris 305(1987), 565-568.

[HK] R.Hardt D.Kinderlehrer, Mathematical question of liquid crystal theory, in Theory and Applications of Liquid Crystals, IMA vol.5, Springer, 1986

[HKL1] R.Hardt, D.Kinderlehrer, F.-H.Lin, Existence and partial regularity of static liquid crystal configurations. Comm.Math.Physics. 105 (1986), pp 547-570.

[HKL2] ..., Stable defects of minimizers of constrained variational problems. Ann.Inst. Henri Poincre, Analyse nonlineaire, 5, no.4 (1988), pp297-322.

[K] D.Kinderlehrer, Recent developments in liquid crystal theory,IMA preprint # 493

[KS] D.Kinderlehrer, G.Stampacchia, An Introduction to Variational Inequalities and Their Applications, Academic Press, 1980.

[L1] F.-H.Lin, A remark on the map $x/|x|$, C.R.Acad.Sc.Paris 305 (1987), 529-531.

[L2] F.-H.Lin, Nonlinear theory of defects in nematic liquid crystals - phase transition and flow phenomena, CPAM, oct.(1989)

[LI] S.-Y.Lin, Ph.D thesis, University of Minnesota, 1988.

[M] C.B. Morrey,JR., Multiple integrals in the calculus of variations, Springer-Verlag, 1966.

[O] C.W.Oseen, The theory of liquid crystals, Trans. Faraday Soc. 29(1933),883-889

[O1] B.Ou, Uniqueness of $x/|x|$ as a stable configuration in liquid crystals, preprint.

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