WEAK-STABILITY OF \( \frac{x}{\|x\|} \) AND
SYMMETRIES OF LIQUID CRYSTALS

DONG PYO CHI AND GIE HYUN PARK

A liquid crystal is mesomorphic phase of a material which is composed of rod-like molecules. Its physical behavior is interesting and some of which as we may see in LCD (liquid crystal displayer) is optically uniaxial.

To describe the liquid crystal configurations we observe that the orientation of molecules \( n(x) \) is well defined for every rod-like molecule \( x \in \Omega(\text{container}) \subset \mathbb{R}^3 \). Thus, assuming a liquid crystal is continuum, we may view \( n(x) \) as a map from \( \Omega \) to the unit sphere \( S^2 \subset \mathbb{R}^3 \). This leads to the Frank-Ossen model [dG], on which our discussion on the static liquid crystal configuration is based.

In this model, the deformation energy density of a liquid crystal is given by

\[
2W_{k_1,k_2,k_3,\alpha}(\nabla n, n) = k_1(\nabla \cdot n)^2 + k_2(n \cdot \nabla \times n)^2 + k_3\|n \times \nabla \times n\|^2 + \alpha(\text{tr}(\nabla n)^2 - (\nabla \cdot n)^2),
\]

where \( k_1, k_2, k_3 \) and \( \alpha \) are positive material constants, depending on temperature, pressure or other physical quantities. The first term in the right hand side of the above definition measures the deformation energy of spray type, the second of twist type, the third of bend type, and the final term measures the surface energy of the liquid crystal which depends only on the value of \( n \) at the boundary.

For some liquid crystals, the molecules at boundary orient to the normal direction to the boundary. This typical situation of prescribing the boundary data is called the strong anchoring in the liquid crystal literature.

The energy of the liquid crystal \( n \) in \( \Omega \) is given by

\[
W(n) = \int_{\Omega} W(\nabla n, n) dx.
\]

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When the constants $k_i$'s are all equal, the integrand is essentially $|\nabla n|^2$ disregarding uninteresting terms. This shows the strong relation of study of liquid crystal with harmonic mapping theory.

Since the equilibrium state of the liquid crystal corresponds to the minimizer of the energy functional we are obliged to study minimizers of $W$, and consequently we are led to the variational problem; Given $n_0$ defined on $\partial \Omega$ with $|n_0| = 1$, is there a map $n : \Omega \to S^2$ with $n|_{\partial \Omega} = n_0$ which is $W$-minimizing among the class of suitable maps?

In this note we restrict our attention to the case $\Omega = \text{the unit ball } \mathbf{B}$ in $\mathbb{R}^3$ and to studying the minimizer $n$ of $W$ with strong anchoring $n|_{\partial \mathbf{B}} = \|x\|$. Lin [L] showed that the homogeneous extension $n(x) = \frac{x}{\|x\|}$ is the unique minimizer for the constants $\min(k_2, k_3) > k_1$. Helein [H] proved that $n(x) = \frac{x}{\|x\|}$ is not a minimizer if $8(k_3 - k_1) + k_3 < 0$.

So we may ask on the range of constants $k_1, k_2, and k_3$ for which the map $n(x) = \frac{x}{\|x\|}$ is minimizing.

Here we ask a similar question; when a minimizer $n$ is stable in the sense that for any variation $n_t$ of $n$, $W(n) \leq W(n_t)$ for small $t$? We give a partial answer to this question. If $8k_3 > k_1$, then $n(x) = \frac{x}{\|x\|}$ is weakly-stable. In fact, if we restrict our admissible class of maps to the class of the rotationally symmetric maps, we can show that $n(x) = \frac{x}{\|x\|}$ is weakly-stable if and only if $8(k_2 - k_1) + k_3 > 0$.

In this context we study whether the minimizer is symmetric for a given symmetric boundary data for various symmetries.

1. Weak-Stability of $n_0(x) = \frac{x}{\|x\|}$

Our main concern in this section is when $n_0(x) = \frac{x}{\|x\|}$ is a minimizer of the energy functional $W$.

**Theorem 1.1** [L]. *In the cases $\min\{k_2, k_3\} \geq k_1$, $\frac{x}{\|x\|}$ is the unique minimizer of $W$.*

**Proof.** This is an immediate consequence of Lin's result [L] in the equal constant case.

There are some values of $k_1, k_2$ and $k_3$, for which $\frac{x}{\|x\|}$ is not a minimizer.
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**THEOREM 1.2 [H].** If $8(k_2 - k_1) + k_3 > 0$, $n_0 = \frac{x}{\|x\|}$ is not a minimizer.

**Proof.** Refer to [H] for details. Hélen proved this by perturbing $n_0$ by a map $u$ which is constructed using rotationally symmetric (see section 2 for the definition) functions $f_n$. In fact those $f_n$ satisfy

$$\frac{\int_0^1 r^2(f'_n)^2 dr}{\int_0^1 f_n^2 dr} \to \frac{1}{4} \text{ as } n \to \infty.$$

Expanding the variation $W(n_t)$ for a variation $n_t$ of $n$, by Taylor series, we have for small $t$

$$W(n_t) = W(n_0) + \left. \frac{d}{dt} W(n_t) \right|_{t=0} t + \frac{1}{2} \left. \frac{d^2}{dt^2} W(n_t) \right|_{t=0} t^3 + O(t^3).$$

There are two types of variations we may consider. So to speak, one is a variation of domain and another is that of image, i.e., one type of variation is $n_t = n \circ \nu_t$ for a one parameter family of diffeomorphisms $\nu_t : B \to B$ fixing boundary, and another is $n_t = \frac{n + tu}{\|n + tu\|}$ where $u : B \to \mathbb{R}^3$ is smooth and $u|_{\partial B} = 0$.

In this note we consider only the variation of image. We say that a map $n$ is weakly-stable if $\frac{d}{dt} W(n_t)\big|_{t=0} = 0$ and $\frac{d^2}{dt^2} W(n_t)\big|_{t=0} > 0$ for any non-trivial variation of image.

**THEOREM 1.3.** If $k_3 > 8k_1$, then $n_0 = \frac{x}{\|x\|}$ is weakly-stable.

The above Theorem 1.2, 1.3 and the Theorem 2.1 which will follow are related to the following fact.

**LEMMA 1.4.** $\inf \left\{ \frac{\int_0^1 r^2(u')^2 dr}{\int_0^1 u^2 dr} : u(0) = \text{bounded}, u(1) = 0 \right\} = \frac{1}{4}$.

**Proof.** Let $u(r) : [0,1] \to \mathbb{R}$ be a smooth map with $u(0) = \text{bounded}$ and $u(1) = 0$. Putting $u(r) = v(r^\frac{1}{2})$, we have

$$v(1) = 0, \quad \lim_{r \to \infty} v(r) = u(0)$$

and

$$\frac{\int_0^1 r^2(u')^2 dr}{\int_0^1 u^2 dr} = \frac{\int_1^\infty (v'(r))^2 dr}{\int_1^\infty v(r)^2 \frac{1}{r^2} dr}.$$
We now set \( v(r) = rf(r) \). Then \( f(1) = 0, f(r) = v(r)/r = O(r^{-1}) \) as \( r \to \infty \), and
\[
\frac{\int_1^\infty (v'(r))^2 \, dr}{\int_1^\infty v(r)^2 \frac{1}{r^2} \, dr} = \frac{\int_1^\infty r^2(f'(r))^2 \, dr}{\int_1^\infty f(r)^2 \, dr}.
\]
Thus the lemma will follow if we show that
\[
\inf \left\{ \frac{\int_1^\infty r^2(f'(r))^2 \, dr}{\int_1^\infty f(r)^2 \, dr} : f(1) = 0, f(r) = O(r^{-1}) \text{ as } r \to \infty \right\} = \frac{1}{4}.
\]
Now for any \( \eta > 0 \) and a smooth function \( u \) with \( \text{supp} u \subset (\eta, \infty) \), let \( u_\eta(r) = u(r/\eta) \), then \( \text{supp} u_\eta \subset (1, \infty) \) and
\[
\frac{\int_1^\infty r^2(u'_\eta)^2 \, dr}{\int_1^\infty u^2_\eta \, dr} = \frac{\int_0^\infty r^2(u')^2 \, dr}{\int_0^\infty u^2 \, dr}.
\]
So we have
\[
\inf \left\{ \frac{\int_1^\infty r^2(f'(r))^2 \, dr}{\int_1^\infty f(r)^2 \, dr} : f(1) = 0, f(r) = O(r^{-1}) \text{ as } r \to \infty \right\}
\]
\[
= \inf \left\{ \frac{\int_1^\infty r^2(u')^2 \, dr}{\int_1^\infty u^2 \, dr} : u \text{ has compact support in } (1, \infty) \right\}
\]
\[
= \inf \left\{ \frac{\int_0^\infty r^2(u')^2 \, dr}{\int_0^\infty u^2 \, dr} : u \text{ has compact support in } (0, \infty) \right\},
\]
which is known [SU, Lemma 1.3] to be \( \frac{1}{4} \).

The symmetries involved in the problem suggest that we should calculate in the spherical coordinates. In the spherical coordinates \( x^1 = r = \text{the radial distance}, x^2 = \theta = \text{the elevation angle from } z\text{-axes}, x^3 = \phi = \text{the azimuthal angle}, \) we have
\[
(1) \quad \nabla \cdot n = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 n_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta n_\theta) + \frac{1}{r \sin \theta} \frac{\partial n_\phi}{\partial \phi},
\]
\[ \nabla \times n = \left( \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\phi) - \frac{1}{r \sin \theta} \frac{\partial u_\theta}{\partial \phi} \right) e_r \\
+ \left( \frac{1}{r \sin \theta} \frac{\partial u_r}{\partial \phi} - \frac{1}{r} \frac{\partial}{\partial r} (ru_\phi) \right) e_\theta \\
+ \left( \frac{1}{r} \frac{\partial}{\partial r} (ru_\theta) - \frac{1}{r} \frac{\partial u_r}{\partial \theta} \right) e_\phi, \]

for \( n = ne + n_\theta e_\theta + n_\phi e_\phi \), where \( e_r, e_\theta \) and \( e_\phi \) are the orthonormal spherical coordinate vectors at the point with coordinate \((r, \theta, \phi)\).

For any variation \( n_t = n_{r,t}e_r + n_{\theta,t}e_\theta + n_{\phi,t}e_\phi \) of \( n_0(x) = x/\|x\| \), since \( \nabla \times n_0 = 0 \) and \( n_{r,t}\big|_{t=0} = \frac{d}{dt} n_{r,t}\big|_{t=0} = 0 \), the first derivative of the variation \( W(n_t) \) of the energy reads

\[ \frac{d}{dt} W(n_t)\big|_{t=0} = \int_B k_1 (\nabla \cdot n_0) \cdot (\nabla \cdot \dot{n}_t) \]

\[ = \int_B k_1 \left( \frac{2}{r} \right) (\nabla \cdot (n_{\theta,t}e_\theta + n_{\phi,t}e_\phi)) \]

\[ = \int_0^1 k_1 \left( \frac{2}{r} \right) \left( \int_{S^2} \nabla \cdot (n_{\theta,t}e_\theta + n_{\phi,t}e_\phi) d\xi \right) dr, \]

which is 0 by the divergence theorem.

The second derivative of the energy functional reads

\[ \frac{d^2}{dt^2} W(n_t)\big|_{t=0} \]

\[ = \int_B k_1 [(\nabla \cdot \dot{n}_t)^2 + (\nabla \cdot n_0) \cdot (\nabla \cdot \ddot{n}_t)] \]

\[ + k_2 (n \cdot \nabla \times \dot{n}_t)^2 + k_3 \|n \times \nabla \times \dot{n}_t\|^2 \]

Let

\[ u = u(r, \theta, \phi) = u_r(r, \theta, \phi)e_r + u_\theta(r, \theta, \phi)n_\theta e_\theta + u_\phi(r, \theta, \phi)n_\phi e_\phi \]

be a smooth map from \( \mathbb{B} \) to \( \mathbb{R}^3 \) with \( u|_{\partial \mathbb{B}} = 0 \). We consider the smooth perturbation \( n_t \) of \( n \) by \( u \), which can be written as

\[ n_t = \frac{n_0 + tu}{\|n_0 + tu\|} = \frac{(1 + tu_r)e_r + tu_\theta e_\theta + tu_\phi e_\phi}{\sqrt{(1 + tu_r)^2 + t^2 u_\theta^2 + t^2 u_\phi^2}}. \]
On the set
\[ A = \{(r, \theta, \phi), \ 0 \leq r \leq 1, \ 0 \leq \theta \leq \pi, \ 0 \leq \phi \leq 2\pi\}, \]
we have
\[ \hat{n}_t|_{t=0} = (0, u_\theta, u_\phi), \]
\[ \hat{n}_t|_{t=0} = (-u_\theta^2 - u_{\phi}^2, -2u_r u_\theta, -2u_r u_\phi). \]

Thus using (1) and (2), we calculate the second derivative of the energy functional
\[
\frac{d^2}{dt^2} W(n_t)|_{t=0} = \int_A \left\{ k_1 \left[ \frac{1}{\sin \theta} \left( \cos \theta u_\theta + \frac{\partial u_\phi}{\partial \theta} + \sin \theta \frac{\partial u_\phi}{\partial \theta} \right)^2 \right. \right.
\]
\[ - 4(\sin \theta u_\phi^2 + \sin \theta u_{\phi}^2 + u_r \frac{\partial u_\phi}{\partial \phi} + u_\phi \frac{\partial u_\phi}{\partial \phi} + \cos \theta u_\phi u_\theta \]
\[ + \sin \theta u_\theta \frac{\partial u_r}{\partial \theta} + \sin \theta u_r \frac{\partial u_\theta}{\partial \phi} + r \sin \theta u_\phi \frac{\partial u_\phi}{\partial r} + r \sin \theta u_\theta \frac{\partial u_\theta}{\partial r} ] \right\}
\[ + k_2 \frac{1}{\sin \theta} \left( \cos \theta u_\phi - \frac{\partial u_\theta}{\partial \phi} + \sin \theta \frac{\partial u_\phi}{\partial \theta} \right)^2 \]
\[ + k_3 \sin \theta (u_\phi^2 + u_\theta^2 + 2ru_\phi \frac{\partial u_\phi}{\partial r} + 2ru_\theta \frac{\partial u_\theta}{\partial r} \]
\[ + r^2 \left( \frac{\partial u_\phi}{\partial r} \right)^2 + r^2 \left( \frac{\partial u_\theta}{\partial r} \right) \} \right\} \right\} \}
\int_A \{ d\theta \sin \phi \}
\]

By deleting the terms whose contribution to the integration are zero, together with the integration by parts, we write this in a simpler form

(3)
\[
\frac{d^2}{dt^2} W(n_t)|_{t=0} = \int_A \left\{ k_1 \left[ \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \theta} \sin \theta u_\theta + \frac{\partial u_\phi}{\partial \phi} \right)^2 \right. \right.
\]
\[ + k_2 \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \theta} \sin \theta u_\phi - \frac{\partial u_\theta}{\partial \phi} \right)^2 \]
\[ + k_3 \sin \theta (r^2 \left( \frac{\partial u_\phi}{\partial r} \right)^2 + r^2 \left( \frac{\partial u_\theta}{\partial r} \right)^2 \)
\[ - 2k_1 \sin \theta (u_\phi^2 + u_\theta^2). \]
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**Proof of Theorem 1.3.** Using the Lemma 1.4 and considering the integration along the radial direction, we bound the third term in the above equation (3) from below by

$$k_3 \sin \theta (u_\phi^2 + u_\theta^2).$$

Therefore we have

$$\frac{d^2}{dt^2} W(n_t) |_{t=0} \geq \int_A k_1 \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \theta} \sin \theta u_\theta + \frac{\partial u_\phi}{\partial \phi} \right)^2 + k_2 \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \theta} \sin \theta u_\phi - \frac{\partial u_\theta}{\partial \phi} \right)^2$$

$$+ \left[ \frac{k_3}{4} - 2k_1 \right] \sin \theta (u_\phi^2 + u_\theta^2).$$

If $k_3 > 8k_1$, then the above terms are positive for any nontrivial perturbations. This means that $W(n_0) < W(n_t)$ for small $t$, i.e., $n_0 = \frac{x}{\|x\|}$ is a critical point of the functional $W$ for any variation of image.

2. Some symmetry breaking of liquid crystals

There are questions on the symmetry of a $W$-minimizer. Among them is whether a minimizer has a symmetry when its boundary data has it. In this section, we will show that some symmetries, rather simple ones, are not preserved in the sense that there are symmetric boundary data for which a minimizer is not symmetric.

We say that a map $n : B^3 \rightarrow S^2$ is axially symmetric if $n$ is obtained by rotating a map defined on the $xz$-plane into itself with respect to the $z$-axis.

Let a map $n : B^3 \rightarrow S^2$ be axially symmetric. In spherical coordinate, we have

$$n(r, \theta, \phi) = n_r(r, \theta, \phi)e_r + n_\theta(r, \theta, \phi)e_\theta + n_\phi(r, \theta, \phi)e_\phi = n_r(r, \theta)e_r + n_\theta(r, \theta)e_\theta.$$  

For this map the energy $W$ is given by

$$W(n) = \frac{1}{2} \int_A k_1 \frac{1}{r^2 \sin \theta} \left( \frac{\partial}{\partial r} (r^2 n_r \sin \theta) + \frac{\partial}{\partial \theta} (r n_\theta \sin \theta) \right)^2$$

$$+ k_2 \sin \theta \left( \frac{\partial}{\partial r} (r n_\theta) - \frac{\partial}{\partial \theta} (n_r) \right)^2.$$
We observe that $W(n)$ does not depend on $k_2$. Thus if $n$ is $W$-minimizing for $k_1, k_2$, and $k_3$ then $n$ is $W$-minimizing for $k_1, k_2$, and $k_3$ where $k_2 \geq k_2$.

Let $n$ be a $W$-minimizer with $n|_{\partial B} = n_0|_{\partial B}$ for

$$8(k_2 - k_1) + k_3 < 0, \quad k_3 \geq k_1.$$ 

In $n$ is axially symmetric, it is $W$-minimizing for $k_1, k_2, k_3$ such that $\min(k_2, k_3) \geq k_1$. Theorem 1.1 [L] implies that $n$ is equal to $n_0$. This contradicts to the Theorem 1.2 [H]. Thus $n$ is not axially symmetric.

We say that a map $n : B^3 \rightarrow S^2$ is rotationally symmetric if

$$r \circ \rho = \rho \circ n$$

for each rotation $\rho$ of $\mathbb{R}^3$ about the $z$-axis. Thus a rotationally symmetric map $n$ satisfies $n(r, \theta, \phi) = n(r, \theta)$.

It is not known whether the rotational symmetry is preserved for liquid crystals for any $k_1, k_2, k_3$. The energy $W$ of the map $n_0(x) = \frac{x}{\|x\|}$ is not stable under perturbation by an rotationally symmetric map for $8(k_2 - k_1) + k_3 < 0$, so that $n_0(x) = \frac{x}{\|x\|}$ is not a $W$-minimizer for $8(k_2 - k_1) + k_3 < 0$.

On the other hand we have;

**Theorem 2.1.** The map $n_0(x) = \frac{x}{\|x\|}$ is a weakly-stable point of $W$ among the rotationally symmetric maps iff $8(k_2 - k_1) + k_3 > 0$.

**Proof.** Let $u : B^3 \rightarrow S^2$ be a rotationally symmetric map with $u|_{\partial B^3} = 0$. For a perturbation $n_t$ of $n_0(x) = \frac{x}{\|x\|}$ by $u$, we calculate

$$\frac{d^2}{dt^2} W(n_t)|_{t=0}$$

$$= \int_A k_1 \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \theta} \sin \theta u_\theta \right)^2 + k_2 \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \theta} \sin \theta u_\phi \right)^2$$

$$+ k_3 \sin \theta (r^2 \left( \frac{\partial u_\phi}{\partial r} \right)^2 + r^2 \left( \frac{\partial u_\theta}{\partial r} \right)^2)$$

$$- 2k_1 \sin \theta (u_\phi^2 + u_\theta^2)$$
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by the equation (3). From the Lemma 1.4 and the Lemma 2.2 proved below, we have

\[
\frac{d^2}{dt^2} W(n_t) \bigg|_{t=0} \geq \int_A \left(2k_2 - 2k_1 + \frac{k_3}{4}\right) \sin \theta u_\phi^2 + \frac{k_3}{4} u_\theta.
\]

Thus if \( 8(k_2 - k_1) + k_3 > 0 \),

\[
\frac{d^2}{dt^2} W(n_t) \bigg|_{t=0} > 0,
\]

unless \( u_\phi = u_\theta = 0 \).

**Lemma 2.2.**

\[
\inf \left\{ \int_0^\pi \frac{1}{\sin \theta} \left( \frac{d^2 u}{d \theta^2} \right)^2 d \theta : u(0) = u(\pi) = 0 \right\} = 2.
\]

**Proof.** We get an Euler-Lagrange equation, by introducing a Lagrange multiplier \( \lambda \),

\[
d \left( \frac{1}{\sin \theta} \frac{du}{d \theta} \right) + \lambda \frac{1}{\sin \theta} u = 0, \quad u(0) = u(\pi) = 0,
\]

or

\[
\sin \theta \frac{d^2 u}{d \theta^2} - \cos \theta \frac{du}{d \theta} + \lambda \sin \theta u = 0, \quad u(0) = u(\pi) = 0.
\]

This equation has a solution

\[
\lambda = 2, \quad u = \sin^2 \theta,
\]

which is positive inside the domain \([0, \pi]\). Therefore the infimum corresponds to the first eigenvalue \( \lambda = 2 \).

Almgren and Lieb [AL] presented an example showing that the mirror symmetry through the \( xy \)-plane is not preserved for the case \( k_1 = k_2 = k_3 \). A map \( n \) is said to be **mirror symmetric** through the \( xy \)-plane if in Cartesian coordinate

\[
n(x, y, z) = (n_1(x, y, z), n_2(x, y, z), n_3(x, y, z))
\]

\[
= (n_1(x, y, -z), n_2(x, y, -z), n_3(x, y, -z))
\]

i.e.,

\[
\sigma \circ n = n \circ \sigma
\]

where \( \sigma \) is a reflection with respect to the \( xy \)-plane.
REMARK. The authors wish to thank H. Brézis for informing the work of Cohen and Taylor [CM], whose results are similar to ours proved with different methods.

Added in proof. Recently Biao Ou (Jour. Geo. Analy. Vol.2, No.2, 1992) showed that \( \|z\| \) is minimizing when \( k_2 \geq k_1 \).

References


Department of Mathematics
Seoul National University
Seoul 151–742, Korea

and

Department of Mathematics
Cheju National University
Cheju 690–756, Korea