A variational Problem for the Isotropic - Nematic Liquid crystals

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Outline

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What is a Liquid Crystal?

A liquid crystal

- is an intermediate state of matter between isotropic and solid phases
- has properties of both isotropic liquid and solid crystalline: flows like liquids, but retains orientational order
- is used in displays and optical switches etc

**Figure:** An array of microlenses (compound eyes) self assembled around a central pillar which could be used for three dimensional imaging Smectic C Liquid Crystal (U Penn group, 2015)
**Figure:** Applications of Liquid Crystals (Kang, Kyungbuk National Univ, 2016)
**Nematic Phases**

Assuming that molecules are rod-like (or uniaxial), nematic liquid crystal is described by the director $\mathbf{n}$, $|\mathbf{n}| = 1$.

*Figure*: Nematic (left), Chiral Nematic (right)
Figure: Uniaxial nematic(left), Biaxial nematic(right)
Uniaxial Nematic Liquid Crystal

The Oseen-Frank Energy functional which governs nematic liquid crystals is

$$\mathcal{W} = \int_\Omega F_{OF}$$

$$F_{OF} = K_1 (\nabla \cdot \mathbf{n})^2 + K_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3 |\mathbf{n} \times \nabla \times \mathbf{n}|^2 + (K_2 + K_4) (\text{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2)$$

$$\mathbf{n} : \Omega \to S^2$$

where $0 < K_2 + K_4 \leq \min\{K_1, K_3\}$, $K_4 \leq 0$
Related Works

The Order Tensor $Q$

Let $\Omega$ be a domain in $\mathbb{R}^3$ and fix $x \in \Omega$. Let $f$ be a probability density of molecular orientations satisfying $f(-\ell) = f(\ell)$ for all $\ell \in S^2$ and $\mu$ be the corresponding probability measure.

- The first moments of $f$ is $\int_{S^2} \ell f(\ell) d\ell = 0$
- The second moments $M$ is $\int_{S^2} \ell \otimes \ell f(\ell) d\ell$:
  $\text{tr}M = 1$, $M^T = M$, where $u \otimes v = (u_i v_j)_{i,j=1,2,3}$, $u, v \in \mathbb{R}^3$
- If $f = \frac{1}{4\pi}$ (molecules are equally distributed in all directions), then the second moments $M_0$ is $\frac{1}{3} I$.
- $Q = M - M_0$ is called the second order tensor: measures the second moments tensor associated with a given probability density deviates from its isotropic value (a measure of local degree of orientational order in liquid crystals)
- $\text{tr} \ Q = 0$
The Order Tensor $Q$

- $Q$ is a $3 \times 3$ symmetric matrix
  $\implies \exists$ an orthogonal matrix $\mathcal{O}$ such that $\mathcal{O}Q\mathcal{O}^T$ is diagonal.
- $\text{tr } Q = 0$
  $\implies Q = S_1 (m \otimes m - \frac{1}{3} I) + S_2 (n \otimes n - \frac{1}{3} I)$
  where $\{m, n, m \times n\}$ is an orthonormal basis (eigenvectors of $Q$) for $\mathbb{R}^3$.
- Three eigenvalues are
  $\frac{1}{3}(2S_1 - S_2), \ -\frac{1}{3}(S_1 + S_2), \ \frac{1}{3}(2S_2 - S_1)$.

Liquid crystal is uniaxial
  $\iff$ two eigenvalues are equal
Liquid Crystal is biaxial
  $\iff Q$ has three distinct eigenvalues
Classical Landau-de Gennes Theory

is a phenomenological model describing the state of a nematic liquid crystal by $Q$.

$$\mathcal{E}_{\text{LdG}}[Q] = \int F(Q, \nabla Q) d\mathbf{x}$$

Due to frame-indifference and material symmetry requirements,

$$F(Q, \nabla Q) = F(RQR^T, D^*)$$

where

$$D^*_{ijk} = R_{il}R_{jm}R_{kp}Q_{lm,p} \quad \forall R \in O(3)$$
\[ F(Q, \nabla Q) = f_{bulk}(Q) + F_e(Q, \nabla Q) \]

where \( f_{bulk} \) is a bulk energy density and \( F_e \) is an elastic free energy density.

\[ F_e(Q, \nabla Q) = L_1 Q_{ij,k} Q_{ij,k} + L_2 Q_{ij,j} Q_{ik,k} + L_3 Q_{ij,k} Q_{ik,j} + L_4 Q_{lk} Q_{ij,l} Q_{ij,k} \]

\[ f_{bulk}(Q) = \frac{1}{2} a_0 (T - T^*) \text{tr}(Q^2) - \frac{1}{3} b \text{tr}(Q^3) + \frac{1}{4} c [\text{tr}(Q^2)]^2 \]

+ higher order polynomial of \( \text{tr}(Q^2) \) and \( \text{tr}(Q^3) \)
If $Q_{ij} = s(n_i n_j - \frac{1}{3} \delta_{ij})$, then

$$Q_{ij,j}Q_{ik,k} = s^2[(\nabla \cdot n)^2 + |n \times \nabla \times n|^2]$$

$$Q_{ik,j}Q_{ij,k} = s^2[|n \times \nabla \times n|^2 + \text{tr}(\nabla n)^2]$$

$$Q_{ij,k}Q_{ij,k} = 2s^2[\text{tr}(\nabla n)^2 + (n \cdot \nabla \times n)^2 + |n \times \nabla \times n|^2]$$

$$Q_{lk}Q_{ij,l}Q_{ij,k} = 2s^3 \left[ \frac{2}{3}|n \times \nabla \times n|^2 - \frac{1}{3}\text{tr}(\nabla n)^2 - \frac{1}{3}(n \cdot \nabla \times n)^2 \right].$$

Letting $K_1 = s^2(L_1 + L_2 + 2L_3) - \frac{2}{3}s^3 L_4$, $K_2 = 2s^2 L_3 - \frac{2}{3}s^3 L_4$, $K_3 = s^2(L_1 + L_2 + 2L_3) + \frac{4}{3}s^3 L_4, K_4 = s^2(L_2 + 2L_3)$, we can obtain the Oseen-Frank energy

$$F_{OF} = K_1(\nabla \cdot n)^2 + K_2(n \cdot \nabla \times n)^2 + K_3|n \times \nabla \times n|^2$$

$$+(K_2 + K_4)[\text{tr}(\nabla n)^2 - (\nabla \cdot n)^2]$$
Elastic Energy

If $L_4 \neq 0$, then $\mathcal{L}$ may not be bounded from below: J. Ball and A. Majumdar constructed a sequence $Q$ such that

$$\mathcal{L}(Q) \to -\infty.$$ 

Let $L_4 = 0$. If either $L_1 > 0$, $L_1 + L_2 + L_3 > 0$ (W. Wei et al) or $L_1 + L_2 + L_3 > 0$, $L_2 + L_3 < 0$ (Bauman, Park, Phillips) or $L_1 > 0$, $-L_1 < L_3 < 2L_1$, $L_2 > -\frac{3}{5}L_1 - \frac{1}{10}L_3$ (Davis and Gartland), then $\mathcal{L}$ is coercive and thus there exist $0 < C < D$ such that

$$C\|\nabla Q\|_{L^2} \leq \int_{\Omega} F_e(Q, \nabla Q) dx \leq D\|\nabla Q\|_{L^2}.$$
Bulk Energy

If \( Q = S (n \otimes n - \frac{1}{3} I) \), then

\[
f_{\text{bulk}}(S) = f_{\text{bulk}}(Q) = \frac{1}{3} a S^2 - \frac{2b}{27} S^3 + \frac{c}{9} S^4, \quad a = a_0 (T - T^*) .
\]

Then there exist \( T^* < T^c < T^{**} \) such that

I. If \( T < T^* (a < 0) \), then the isotropic state is unstable (not a local minimizer) and nematic state is a global minimizer at some \( S^+ = \frac{b + \sqrt{b^2 - 24ac}}{4c} \).

II. If \( T^* < T < T^c \), then \( f_{\text{bulk}}(S) \) has still the global minimizer at \( S^+ \) and also a local minimizer at \( S = 0 \).

III. If \( T^c < T < T^{**} \), then \( f_{\text{bulk}}(S) \) has a local minimizer at \( S^+ \) and the global minimizer at \( S = 0 \).

IV. If \( T > T^{**} \), then \( f_{\text{bulk}}(S) \) has only the global minimizer at \( S = 0 \).
(J. Ball and A. Majumdar (2009): Consider the mean field Maier-Saupe free energy in the total energy

$$\psi(Q) = T \min_{\rho \in \mathcal{A}_Q} \int_{S^2} \rho(m) \ln \rho(m) \, dm - \kappa |Q|^2$$

$\mathcal{A}_Q$ is the set of all $\rho : S^2 \rightarrow \mathbb{R}$ satisfying

$$\rho \geq 0, \quad \int_{S^2} \rho(m) \, dm = 1, \quad Q = \int_{S^2} \left( m \otimes m - \frac{1}{3} \right) \rho(m) \, dm$$
(P. Zhang et al.): Let $B_Q$ be a symmetric traceless $3 \times 3$ matrix satisfying

$$\int_{S^2} \exp(B_Q(x) : m \otimes m) \, dn \int_{S^2} \left( m \otimes m - \frac{1}{3} I \right) \exp(B_Q(x) : m \otimes m) \, dm$$

$$= Q(x).$$

The generalized Landau-de Gennes energy is given by

$$\tilde{F}(Q, \nabla Q) = \int_{\Omega} \{ F_e(Q, \nabla Q) + \tilde{F}_b(Q) \} \, dx,$$

$$F_e = \frac{1}{2} \left( L_1 |\nabla Q|^2 + L_2 Q_{ij,j} Q_{ik,k} + L_3 Q_{ij,k} Q_{ik,j} + L_4 Q_{ij} Q_{kl,i} Q_{kl,j} \right),$$

$$\tilde{F}_b = k_B T c \left( Q : B_Q - \ln Z_Q - \gamma |Q|^2 \right)$$

Here $\gamma > 0$, $c > 0$, and $Z_Q = \int_{S^2} \exp(B_Q : m \otimes m) \, dm.$
In the case that $L_1 > 0$, $L_1 + L_2 + L_3 > 0$ and $L_4 = 0$,

1. The direct method of the calculus of variations guarantees the existence of minimizers for $\tilde{F}$ in the space

$$A = \left\{ Q \in W^{1,2}(\Omega, S_0) : Q = Q_0 \text{ on } \partial \Omega \right\},$$

where $Q_0$ is a smooth boundary data on $\partial \Omega$ and $S_0$ denotes the set of all symmetric traceless $3 \times 3$ matrices.

2. The global minimizers for modified bulk energies are uniaxial (Ball and Majumdar 2009, P. Zhang et al, 2015)
3. Modified bulk energies near the Isotropic-nematic phase transition are approximated by

\[ \frac{a}{2} trQ^2 - \frac{b}{3} trQ^3 + \frac{c}{4} (trQ^2)^2 + \text{higher order terms}. \]
For isotropic-Nematic Interface problems, we focus on a special form of the energy (Landau-de Gennes energy)

\[
\mathcal{F}(Q, \nabla Q) = \int_{\Omega} \frac{a}{2} \text{tr}Q^2 - \frac{b}{3} \text{tr}Q^3 + \frac{c}{4} (\text{tr}Q^2)^2 + f_{\text{bulk}}: \text{bulk energy} \\
+ \frac{1}{2} \left( L_1 |\nabla Q|^2 + L_2 Q_{ij,j}Q_{ik,k} + L_3 Q_{ij,k}Q_{ik,j} + L_4 Q_{ij}Q_{kl,i}Q_{kl,j} \right) dx.
\]

Here \(a, b, c\) are material-dependent and temperature-dependent nonnegative constants and \(L_i (i = 1, 2, 3, 4)\) are material dependent elastic constants.
Related Works

- **G. Di Fratta, A. Zarnescu, et al:** Half-Integer Point Defects in the Q-Tensor Theory of Nematic Liquid Crystals (J. of Nonlinear Sci., 2015)
- **D. Golovaty, J.A. Montero and P. Sternberg:** Dimension Reduction for the Landau-de Gennes Model in Planar Nematic Thin Films (J. of Nonlinear Sci., 2015)
- **Y. Hu, Y. Qu, P. Zhang:** On the Disclination Lines of Nematic Liquid Crystals (2015)
- **G. Canevari:** Biaxiality in the asymptotic analysis of a 2-D Landau-de Gennes model for liquid crystals (2014)
- **S. Alama, L. Bronsard, and X. Lamy:** Minimizers of the Landau-de Gennes energy around a spherical colloid particle (2015)
• D. Golovaty and J. A. Montero: On minimizers of a Landau-de Gennes energy functional on planar domains (ARMA, 2014)
• J. Ball and A. Majumdar: Nematic Liquid Crystals: From Maier-Saupe to a Continuum Theory (Molecular Crystals and Liquid Crystals., 2009)
• X. Lamy: Some properties of the nematic radial hedgehog in the Landau-de Gennes theory (JMAA 3013).
• There exist many others: sorry that I cannot list them all.
Background of the Isotropic-Nematic Interface

Based on the framework of the Ginzburg-Landau, de Gennes studied the interface between the isotropic and nematic phases (de Gennes 1971). With a special ansatz that de Gennes made on the variation of the order tensor, the biaxiality does not appear in the isotropic-nematic interface.

1. In the absence of the anisotropic energy ($L_2 = 0$), the de Gennes’ ansatz predicts that both the homeotropic and planar anchorings on the interface are possibly stable.
2. Popa-Nita et al (1997) investigated the isotropic-nematic interface by numerical and asymptotic analysis and showed that the de Gennes’ ansatz is valid when the bend and splay elastic energies dominate over the twist energy.
3. Numerical simulations (Kamil et al, 2010) give positive answer with the de Gennes ansatz in the absence of anisotropic elastic energy corresponding to $L_2$-term.

4. When the anisotropic energy presents ($L_2 \neq 0$), de Gennes argued energetically that the homeotropic anchoring is stable when $L_2 < 0$ while the planar anchoring is stable when $L_2 > 0$. It turns out that uniaxiality may lose in the interfacial profile.
Isotropic-Nematic Interface Problems

Assume that $L_3 = 0$.

$$\mathcal{F}[Q] = \int_{\Omega} \left\{ \frac{L_1}{2} |\nabla Q|^2 + \frac{L_2}{2} Q_{ij,j} Q_{ik,k} + F_b(Q) \right\} dx,$$

$$F_b(Q) = \frac{a}{2} tr(Q) - \frac{b}{3} tr(Q^2) + \frac{c}{4} [tr(Q^2)]^2.$$

where $\Omega$ is a bounded domain in $\mathbb{R}^3$.

Assume that $b^2 = 27ac$. Then the stable two constant states 0 and $s^+ (n \otimes n - \frac{1}{3}) (s^+ = \frac{b}{4c} )$ could coexist in the global minimizer.
Scalings: \( \tilde{x} = \frac{1}{\sqrt{L_1}} x \), \( \tilde{Q}(\tilde{x}) = Q(\sqrt{L_1} \tilde{x}) \)

\[
\frac{1}{3L_1 \sqrt{L_1}} F(Q, \nabla Q) = \int \frac{1}{\sqrt{L_1}} \Omega \frac{1}{6} (|\nabla \tilde{Q}|^2 + \frac{L_2}{L_1} \tilde{Q}_{ij,j} \tilde{Q}_{ik,k}) + F_b(\tilde{Q})) \, d\tilde{x}.
\]

we assume that the following limits exist

\[
\lim_{L_1 \to 0} \frac{2L_2}{3L_1} = L, \quad \lim_{L_1 \to 0} \frac{a}{L_1} = \tilde{a},
\]

\[
\lim_{L_1 \to 0} \frac{b}{L_1} = \tilde{b} \quad \lim_{L_1 \to 0} \frac{c}{L_1} = \tilde{c}
\]
Passing to the limit as $L_1 \to 0$, we obtain the following limiting energy functional (not relabelled) after removing the tilde

$$ F(Q, \nabla Q) = \int_{\mathbb{R}^3} \left\{ \frac{1}{6} |\nabla Q|^2 + \frac{L}{4} Q_{ij,j} Q_{ik,k} + F_b(Q) \right\} d\mathbf{x}. $$

After scaling if necessary, we take $a = \frac{1}{3}, b = 3, c = 1$ so that $f(n \otimes n - \frac{1}{3} I) = f(0) = 0$. Then energy functional takes the form

$$ F(Q, \nabla Q) = \int_{\mathbb{R}^3} \left\{ \frac{1}{6} |\nabla Q|^2 + \frac{L}{4} Q_{ij,j} Q_{ik,k} + \frac{1}{6} \text{tr} Q^2 - \text{tr} Q^3 + \frac{1}{4} (\text{tr} Q^2)^2 \right\} d\mathbf{x}. $$
The global minimizer for the case $L = 0$

We first investigate the global minimizer of the energy

$$\mathcal{F}_0(Q, \nabla Q) = \int_{\mathbb{R}} \left\{ \frac{1}{6} |Q'|^2 + \frac{1}{6} \text{tr}Q^2 - \text{tr}Q^3 + \frac{1}{4} (\text{tr}Q^2)^2 \right\} ds$$

with the boundary condition

$$Q(+\infty) = n \otimes n - \frac{1}{3} I, \quad Q(-\infty) = 0.$$
THEOREM (J. P., W. Wang, P. Zhang, Z. Zhang, Calc. Var. PDEs 2017). The global minimizer of $\mathcal{F}_0(Q, \nabla Q)$ must take the form

$$Q(s) = \frac{1}{2} (1 + \tanh(s - t))(n \otimes n - \frac{1}{3} I)$$

which is an uniaxial interfacial profile where $t$ is an arbitrary constant due to the translation.
In the case of $L \neq 0$, the one-dimensional Landau-de Gennes energy functional reads

$$
\mathcal{F}_L(Q, \nabla Q) = \int_{\mathbb{R}} \left\{ \frac{1}{6} |Q'|^2 + \frac{L}{4} \sum_{i=1}^{3} (Q'_{i3})^2 + \frac{1}{6} \text{tr}Q^2 - \text{tr}Q^3 + \frac{1}{4} (\text{tr}Q^2)^2 \right\} \, ds
$$

with the boundary condition

$$
Q(+\infty) = n \otimes n - \frac{1}{3} I, \quad Q(-\infty) = 0.
$$
Boundary Conditions

Unlike in the case of \( L = 0 \) the direction vector \( \mathbf{n} \) on the anchoring condition at \( +\infty \) makes a significant effect on the behavior of the global minimizers. There are three different types of the alignment director \( \mathbf{n} \) on the boundary

1. Homeotropic anchoring: \( \mathbf{n} \cdot (0, 0, 1) = 1 \);
2. Planar anchoring: \( \mathbf{n} \cdot (0, 0, 1) = 0 \);
3. Oblique (Tilt) anchoring: \( 0 < \mathbf{n} \cdot (0, 0, 1) < 1 \).
Without loss of generality, we look for minimizers of the form

\[
Q = \begin{pmatrix}
    -\frac{1}{3}(S + T) & 0 & 0 \\
    0 & -\frac{1}{3}(S - T) & 0 \\
    0 & 0 & \frac{2}{3}S
\end{pmatrix}
\]

with \(S(\infty) = 1, T(\infty) = S(-\infty) = T(-\infty) = 0\). Then the energy functional becomes

\[
\mathcal{F}_L(S, T) = \frac{2}{9} \int_{\mathbb{R}} \left( \frac{1}{2}(S')^2 + \frac{1}{6}(T')^2 + \frac{1}{6}(3S^2 + T^2) - S(S^2 - T^2) \\
+ \frac{1}{18}(3S^2 + T^2)^2 \right) ds
\]
Euler-Lagrange Equations

The corresponding Euler-Lagrange equations are

\[-\frac{1 + L}{2} S'' + \frac{S}{2} - \frac{3S^2}{2} + \frac{T^2}{2} + \frac{S(3S^2 + T^2)}{3} = 0, \quad -\infty < s < \infty,\]

\[-\frac{1}{6} T'' + \frac{T}{6} + ST + \frac{T(3S^2 + T^2)}{9} = 0, \quad -\infty < s < \infty\]

Note that a uniaxial state with \( T = 0 \) and \( S(z) = S^*(z/\sqrt{1 + L}) \) solves

\[-(1 + L)S'' + S - 3S^2 + 2S^3 = 0\]

where

\[S^*(\tau) = \frac{\exp(\tau - t)}{1 + \exp(\tau - t)}.\]
THEOREM (J.P., W. Wang, P. Zhang, Z. Zhang, Cal.Var.PDEs 2017). There exists a uniaxial equilibrium state of the energy functional $F_L$ which is stable with homeotropic anchoring when $L \leq 0$ and unstable (with homeotropic anchoring) when $L > 0$.

For any $P = (P_{ij}) \in C_c^\infty(\mathbb{R}, S_0)$, we calculate

$$\lim_{\xi \to 0} \frac{1}{\xi^2} (F_L(Q_0 + \xi P) - F_L(Q_0))$$

$$= \int_{\mathbb{R}} \left\{ \frac{1}{6} |P'|^2 + \frac{L}{4} ((P'_{13})^2 + (P'_{23})^2 + (P'_{33})^2) \\
+ \frac{1}{6} |P|^2 - 3 \text{tr}(Q_0 P^2) + \left( \frac{1}{2} |Q_0|^2 |P|^2 + (Q_0 : P)^2 \right) \right\} ds$$
Oblique Boundary Anchoring

For this, let us consider a special order tensor depending only on $z$ of the form

$$Q = \begin{pmatrix}
-\frac{(S+T)}{2} \cos^2 \theta + S \cos^2 \theta & 0 & -\frac{(3S+T)}{4} \sin 2\theta \\
0 & -\frac{(S-T)}{2} & 0 \\
-\frac{3(3S+T)}{4} \sin 2\theta & 0 & -\frac{(S+T)}{2} \sin^2 \theta + S \cos^2 \theta
\end{pmatrix}$$

with the boundary condition

$$S(-\infty) = T(\pm\infty) = 0, \ S(+\infty) = 1, \ \theta(+\infty) = \theta_0$$
Numerical Observation

- With the planar anchoring for $L > 0$, biaxial region appears in the interfacial profile.
- With the planar anchoring for $L < 0$, biaxial region appears in the interfacial profile.
- With the oblique anchoring for $L > 0$, biaxial region appears in the interfacial profile.
- With the oblique anchoring for $L < 0$, uniaxial profile is stable, which is similar to the homeotropic anchoring.
Thank you for your attention!