Uniaxial symmetry in nematic liquid crystals.

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Nematic liquid crystal

(O. Lavrentovitch / Kent State Univ.)
Outline

1. Model
2. Uniaxial equilibrium
3. Characterization in 2D
4. A model case in 3D: the hedgehog defect
5. Conclusion and perspectives
Orientational order in nematics

- rod-like molecules tend to align

\[ \lambda_1 + \lambda_2 + \lambda_3 = 0 \]

- order parameter (de Gennes) \( Q \)-tensor: symmetric traceless 3 \( \times \) 3 matrix

\[ S = \{ Q \in \mathbb{R}^{3\times3} : tQ = Q, \ tr(Q) = 0 \} \]

\[ \begin{align*}
\lambda_1 & \rightarrow \text{mean directions of alignment.} \\
\lambda_2 & \rightarrow \text{mean directions of alignment.} \\
\lambda_3 & \rightarrow \text{mean directions of alignment.}
\end{align*} \]

\[ \lambda_1 + \lambda_2 + \lambda_3 = 0 \]
Degrees of symmetry in $S$

- **Isotropic**
  - $Q = 0$
  - Full symmetry $G = SO(3)$

- **Uniaxial**
  - 2 equal eigenval.
  - Broken symmetry $H \approx O(2)$

- **Biaxial**
  - 3 distinct eigenval.
  - Broken symmetry $H \approx \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$

$$Q = s \left( n \otimes n - \frac{1}{3} I \right)$$

$s \in \mathbb{R}$ scalar order param.

$n \in \mathbb{S}^2$ director
Landau-de Gennes free energy

\[ Q(x) \in S \text{ describes local orientational order around } x \]

\[
\mathcal{F}(Q) = \int_{\Omega} \left[ \frac{L}{2} |\nabla Q|^2 + f_b(Q) \right]
\]

bulk free energy \( f_b(Q) = \varphi(\text{tr}(Q^2), \text{tr}(Q^3)) \)

( in the literature: \( f_b(Q) = -a|Q|^2 - b \text{ tr}(Q^3) + c|Q|^4 \) )

Equilibrium configuration

\[
|\mathcal{F}(Q + \delta Q) - \mathcal{F}(Q)| \ll \|\delta Q\|
\]

\[
L \Delta Q = 2(\partial_1 \varphi)Q + 3(\partial_2 \varphi) \left( Q^2 - \frac{|Q|^2}{3} I \right)
\] (E)
**Uniaxial equilibrium**

**Question**
Do there exist equilibrium configurations with uniaxial symmetry?

⇝ describe solutions of (E) satisfying the uniaxial *ansatz*

\[ Q(x) = s(x) \left( n(x) \otimes n(x) - \frac{1}{3} I \right) \]

**Biaxial escape**

Breaking of uniaxial symmetry: related to the presence of *defects*  
(Sonnet, Kilian, Hess ’95)
Principle of Symmetric Criticality (PSC)

$Q^{\text{sym}}$: configuration with symmetry.

\[ |\mathcal{F}(Q^{\text{sym}} + \delta Q^{\text{sym}}) - \mathcal{F}(Q^{\text{sym}})| \ll \|\delta Q^{\text{sym}}\| \]

\[
\Downarrow
\]

\[ |\mathcal{F}(Q^{\text{sym}} + \delta Q) - \mathcal{F}(Q^{\text{sym}})| \ll \|\delta Q\| \]

- tool to prove existence of symmetric equilibrium (plug symmetric ansatz into $\mathcal{F}$ and minimize...)
- Palais ’79 *Comm. Math. Phys.*
Application: the radial hedgehog

spherical droplet with radial anchoring:
- $\Omega = B_R$,
- radial Dirichlet boundary conditions

$PSC \iff \exists$ spherically symmetric equilibrium:

$$Q(x) = s(r) \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} I \right)$$ solution of (E)

Here, uniaxial symmetry = consequence of spherical symmetry
Uniaxial equilibrium

**Uniaxial equilibrium equations**

**no PSC** for uniaxial symmetry:

**equilibrium w.r.t. symmetry-preserving perturbations:**

**\( (S) \)**

\[
\begin{aligned}
\Delta s &= 3|\nabla n|^2 s + \frac{1}{L}(2s \partial_1 \varphi + s^2 \partial_2 \varphi) \\
\Delta n + 2(\nabla s \cdot \nabla)n &= -s|\nabla n|^2 n
\end{aligned}
\]

+ extra equation:

**equilibrium w.r.t. symmetry-breaking perturbations:**

**\( (SB) \)**

\[
2 \sum_{k=1}^{3} \partial_k n \otimes \partial_k n = |\nabla n|^2 (I - n \otimes n)
\]

\( \leadsto \) overdetermined...
Theorem (Characterization of 2D uniaxial equilibrium)

$Q$ equilibrium with uniaxial symmetry, $\partial_3 Q \equiv 0 \Rightarrow$ constant director

$$Q(x) = s(x) \left( n_0 \otimes n_0 - \frac{1}{3} I \right)$$
2D: ideas of proof

- (SB)

\[ \begin{align*}
\Rightarrow & \quad \left\{ \begin{array}{l}
\partial_1 n \cdot \partial_2 n = 0, \\
|\partial_1 n| = |\partial_2 n|
\end{array} \right. \\
\Rightarrow & \quad |\partial_1 n| = |\partial_2 n| \equiv \text{cste}
\end{align*} \]

- + (S)

- if $|\nabla n| \neq 0$, then $n : \mathbb{R}^2 \rightarrow S^2$ local parametrization

- in fact, up to rescaling, local isometry $\sim$ contradicts Gauss’ *Theorema egregium*
The hedgehog defect

\[ \Omega = B_R = \{ x \in \mathbb{R}^3 : |x| < R \} \]

radial anchoring:
\[ Q(x) = s_0 \left( \frac{x}{R} \otimes \frac{x}{R} - \frac{1}{3} I \right) \text{ for } |x| = R. \]

Theorem

Q equilibrium with uniaxial symmetry \Rightarrow \text{ spherically symmetric}

\[ Q(x) = s(r) \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} I \right) \]

Remark: Henao, Majumdar *SIAM J. Math. Anal.* ’12: similar result, for energy minimizers, in low temperature limit (Ginzburg Landau structure \( f_b = -\alpha |Q|^2 + \gamma |Q|^4 \))
Hedgehog: ideas of proof

- \sim Cauchy-Kovaleskaya: determine normal derivatives on the sphere surface, up to any order.
- difficulty:
  - boundary condition: order 0.
  - (S) of order 2.
  - (SB) of order 1, but boundary data is characteristic.
- using \( \partial_r^k (SB) \) for \( k \) up to 4 and \( \partial_r^k (S) \) for \( k \) up to 2:

\[
\partial_r n \equiv 0, \quad \partial_r s \equiv \text{cste} \quad \text{on the surface } |x| = R
\]
Conclusion and perspectives

- Constraint of uniaxial symmetry = very restrictive (satisfied only in presence of other symmetries)
- New light on ‘biaxial escape’
- Not only energy minimizers

- Radial hedgehog = only non trivial uniaxial solution?
- What about ‘approximately uniaxial’ configurations? Does equation (SB) play a role?
- More general elastic term? (SB) of 2nd order...