Uniaxial symmetry in nematic liquid crystals.

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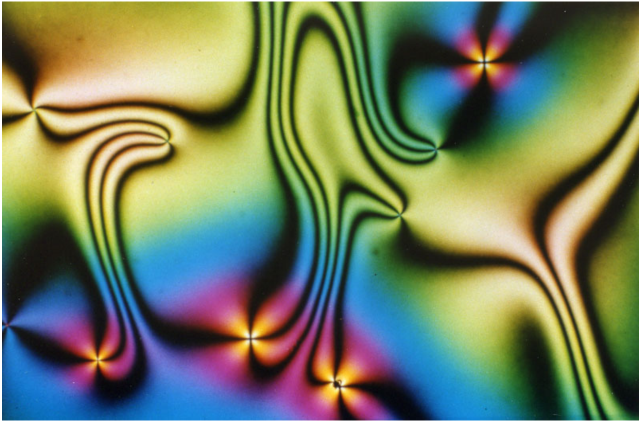
Nematic liquid crystal

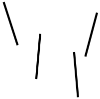


(O. Lavrentovitch / Kent State Univ.)

Outline

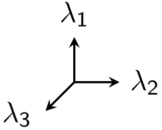
Orientational order in nematics

- rod-like molecules tend to align



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

$$\mathcal{S} = \left\{ Q \in \mathbb{R}^{3\times 3} \colon {}^{t}Q = Q,\ \mathrm{tr}(Q) = 0 \right\}$$

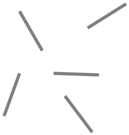


$\lambda_1 + \lambda_2 + \lambda_3 = 0$

- eigenframe $\rightsquigarrow$ mean directions of alignment.
- eigenvalues $\rightsquigarrow$ degrees of alignment.

Degrees of symmetry in $\mathcal{S}$

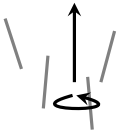
isotropic



$Q = 0$

full symmetry
$G = SO(3)$

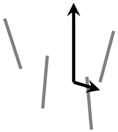
uniaxial



2 equal eigenval.

broken symmetry
$H \approx O(2)$

biaxial



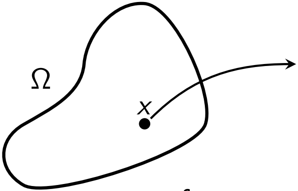
3 distinct eigenval.

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



$Q(x) \in \mathcal{S}$ describes local orientational order around x

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

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

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

Equilibrium configuration $\qquad |\mathcal{F}(Q + \delta Q) - \mathcal{F}(Q)| \ll \|\delta Q\|$

$$L\Delta Q = 2(\partial_1 \varphi) Q + 3(\partial_2 \varphi) \left(Q^2 - \frac{|Q|^2}{3} I \right) \qquad \text{(E)}$$

Uniaxial equilibrium

Question

Do there exist equilibrium configurations with uniaxial symmetry?

$\rightsquigarrow$ 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^{sym}: configuration with symmetry.

equilibrium w.r.t. symmetry-preserving perturbations

$$|\mathcal{F}(Q^{sym} + \delta Q^{sym}) - \mathcal{F}(Q^{sym})| \ll \|\delta Q^{sym}\|$$

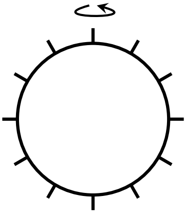
$$\Downarrow$$

equilibrium w.r.t. all perturbations

$$|\mathcal{F}(Q^{sym} + \delta Q) - \mathcal{F}(Q^{sym})| \ll \|\delta Q\|$$

- 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 $\Longrightarrow$ $\exists$ spherically symmetric equilibrium:

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

Here, uniaxial symmetry = consequence of spherical symmetry

Uniaxial equilibrium equations

no PSC for uniaxial symmetry:

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

$$(S) \qquad \begin{cases} \Delta s = 3|\nabla n|^2 s + \dfrac{1}{L}(2s\partial_1\varphi + s^2\partial_2\varphi) \\ s\Delta n + 2(\nabla s \cdot \nabla)n = -s|\nabla n|^2 n \end{cases}$$

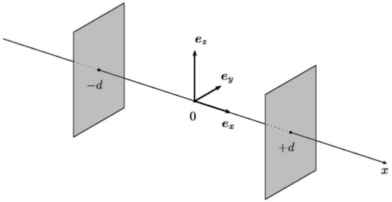
+ extra equation:

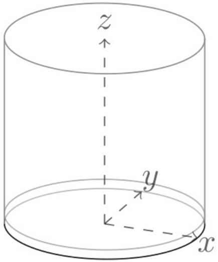
equilibrium w.r.t. **symmetry-breaking** perturbations:

$$(SB) \qquad 2\sum_{k=1}^{3} \partial_k n \otimes \partial_k n = |\nabla n|^2 (I - n \otimes n)$$

$\rightsquigarrow$ overdetermined...

Uniaxial equilibrium in 2D





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)

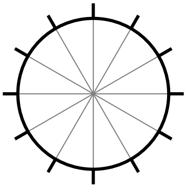
$$\rightsquigarrow \quad \begin{cases} \partial_1 n \cdot \partial_2 n = 0, \\ |\partial_1 n| = |\partial_2 n| \end{cases}$$

- + (S)

$$\rightsquigarrow \quad |\partial_1 n| = |\partial_2 n| \equiv \text{cste}$$

- if $|\nabla n| \neq 0$, then $n \colon \mathbb{R}^2 \to \mathbb{S}^2$ local parametrization
- in fact, up to rescaling, local isometry $\rightsquigarrow$ contradicts Gauss' *Theorema egregium*

The hedgehog defect



- $\Omega = B_R = \{x \in \mathbb{R}^3 \colon |x| < R\}$
- radial anchoring:
  $Q(x) = s_0 \left(\frac{x}{R} \otimes \frac{x}{R} - \frac{1}{3} I\right)$ for $|x| = R$.

Theorem

Q equilibrium with uniaxial symmetry $\Rightarrow$ **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 ∂_r^k(SB) for k up to 4 and ∂_r^k(S) for k up to 2:

$$\partial_r n \equiv 0, \quad \partial_r s \equiv \text{cste} \qquad \text{on the surface } |x| = R$$

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...