Laboratoire Jacques Louis Lions
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Biaxiality and asymptotic analysis of a 2D Landau-de Gennes model

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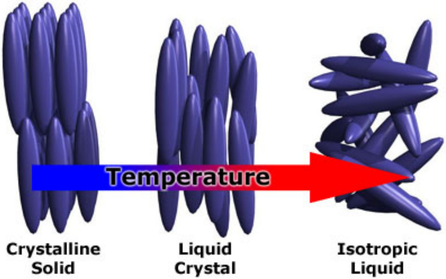
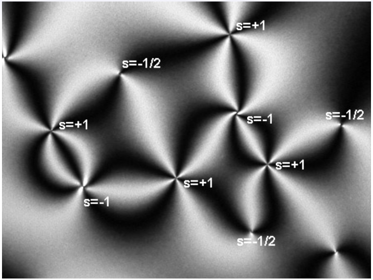
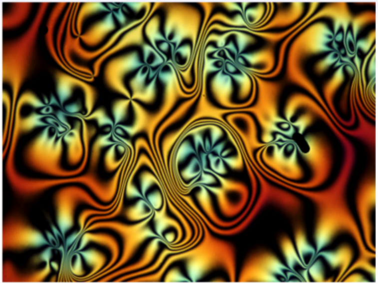
Introduction

Nematic liquid crystals are an intermediate phase of matter. They are composed by rigid, rod–shaped molecules which

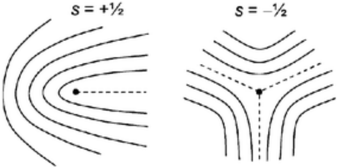
- can *flow* freely, as in liquid,
- but tend to align locally, recovering some *orientational order* (as in crystalline solid phases)







Examples of Schlieren textures.



Disclinations of strength $+1/2$ and $-1/2$.

Liquid crystal modeling: statistical mechanics

- Let $\mu\colon \mathscr{B}(S^2) \to [0,\ 1]$ be a probability on the sphere S^2.
  $\mu(A)$ is the probability that, at a given point, the molecules are pointing in a direction contained in $A \subset S^2$.

- Head–to–tail symmetry of molecules: $\mu(A) = \mu(-A)$ for all $A \in \mathscr{B}(S^2)$.

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- We consider the second–order momentum

$$Q := \int_{S^2} p^{\otimes 2}\, d\mu(p) - \frac{1}{3}\,\mathrm{Id}_3$$

  which is a symmetric traceless 3×3 matrix. Here

$$\left(p^{\otimes 2}\right)_{ij} := p_i p_j \qquad \text{for all } p \in S^2.$$

Liquid crystals modeling: Q–tensors

- We represent the local configurations by matrices:

$$\mathbf{S}_0 := \left\{ Q \in M_{3\times 3}(\mathbb{R}) \colon Q = Q^T, \, \operatorname{tr} Q = 0 \right\}.$$

- Each $Q \in \mathbf{S}_0$ can be written as

$$Q = s \left\{ \left(n^{\otimes 2} - \frac{1}{3} \operatorname{Id} \right) + r \left(m^{\otimes 2} - \frac{1}{3} \operatorname{Id} \right) \right\}$$

where (n, m) is an orthonormal pair in $\mathbb{R}^3$, $s \geq 0$ and $0 \leq r \leq 1$.

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  where (n, m) is an orthonormal pair in $\mathbb{R}^3$, $s \geq 0$ and $0 \leq r \leq 1$.
- The configurations are classified according to the eigenvalues of Q:
  - **isotropic**: $Q = 0$ ($s = 0$)
  - **uniaxial**: $Q \neq 0$ and two eigenvalues coincide ($s > 0$, $r \in \{0, 1\}$)
  - **biaxial**: all the eigenvalues are distinct ($s > 0$, $0 < r < 1$).
- For *uniaxial* configurations, n gives the local preferred orientation of the molecules.

The variational problem

- Let $\Omega \subseteq \mathbb{R}^2$ be a bounded, smooth domain, and $g : \partial\Omega \to \mathbf{S}_0$ a smooth boundary datum. Let

$$H^1_g(\Omega,\, \mathbf{S}_0) := \left\{ Q \in H^1(\Omega,\, \mathbf{S}_0) :\ \ Q|_{\partial\Omega} = g \right\}.$$

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- We consider the **Landau–de Gennes problem**

$$\min_{Q \in H^1_g(\Omega,\, \mathbf{S}_0)} E_\varepsilon(Q), \qquad E_\varepsilon(Q) := \int_\Omega \left\{ \frac{1}{2} \left|\nabla Q\right|^2 + \frac{1}{\varepsilon^2} f(Q) \right\} \qquad (\mathrm{P}_\varepsilon)$$

where ε^2 is an elastic constant ($\simeq 10^{-11}$ J/m) and f is the potential energy:

$$f(Q) := k - \frac{a}{2} \operatorname{tr} Q^2 - \frac{b}{3} \operatorname{tr} Q^3 + \frac{c}{4} \left(\operatorname{tr} Q^2 \right)^2$$

$a,\, b,\, c > 0$ and $k \in \mathbb{R}$ so that $\inf f = 0$.

The vacuum manifold

- The minimizers for f are exactly the elements of

$$\mathscr{N} := \left\{ s_* \left(n^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right) : n \in S^2 \right\},$$

for some constant $s_* = s_*(a,\ b,\ c)$. Notice that $n^{\otimes 2} = (-n)^{\otimes 2}$.

- $\mathscr{N}$ is a smooth submanifold of $\mathbf{S}_0$, called **vacuum manifold**. We have

$$\mathscr{N} \simeq \mathbb{RP}^2$$

($\mathbb{RP}^2$ is the quotient space of S^2, modulo the identification of antipodal points $n \sim -n$).

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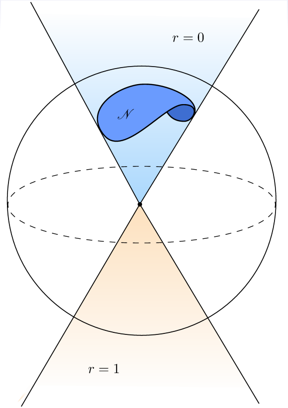
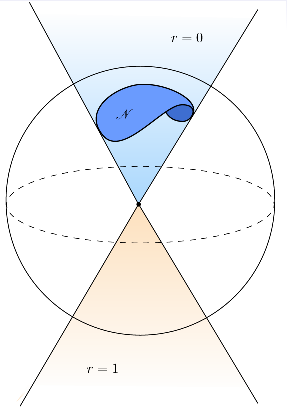
- $\varepsilon^{-2} f(Q)$ can be thought as a penalization term for the constraint $Q \in \mathscr{N}$.



Assume that $g(x) \in \mathscr{N}$ for all $x \in \partial\Omega$. It may be impossible to extend g continuously $\Omega \to \mathscr{N} \Rightarrow$ **Singularities**



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Question 1. Are the minimizers for Problem (P_ε) biaxial somewhere?

Question 2. How do minimizers behave as $\varepsilon \searrow 0$?

Biaxiality in the Q–tensor model

Should we expect biaxiality in minimizers of Problem (P_ε)?

- Numerics in 2D: **[Schopohl, Sluckin, '87]**.
- Numerics in 3D, biaxial torus: **[Gartland, Mkaddem, '99]**, **[Kralj, Virga, Zumer, '99]**, **[Kralj, Virga, '01]**.
- The uniaxial hedgehog is unstable in the low-temperature limit ($a \gg 1$): **[Gartland, Mkaddem, '99]**.
- Minimizers are either uniaxial everywhere, either biaxial a.e.: **[Majumdar, Zarnescu, '10]**.
- Minimizers are biaxial, in 3D, when $a \gg 1$: **[Henao, Majumdar, '12]**.

"Almost uniaxial" minimizers are not excluded.

Define the **biaxiality parameter** as

$$\beta(Q) = 1 - 6\frac{\left(\operatorname{tr} Q^3\right)^2}{\left(\operatorname{tr} Q^2\right)^3}\,, \qquad Q \in \mathbf{S}_0 \setminus \{0\}.$$

It holds that $0 \leq \beta(Q) \leq 1$, with $\beta(Q) = 0$ iff Q is uniaxial.

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Proposition 1 ([Majumdar, Zarnescu, '10])

Up to rescaling, f satisfies

$$\mu_1 (1 - |Q|)^2 + \sigma\beta(Q)\,|Q|^3 \le f(Q) \le \mu_2 (1 - |Q|)^2 + \sigma\beta(Q)\,|Q|^3$$

In addition, setting $t := ac/b^2$, we compute

$$\frac{\mu_1}{a}(t) \to \alpha > 0, \qquad \frac{\sigma}{a}(t) \to 0 \qquad \text{as } t \to +\infty. \tag{$\star$}$$

When $t \gg 1$, we expect biaxiality to be energetically convenient!

Assume that Ω is simply connected, and

(K1) g is a smooth curve $\partial\Omega \to \mathscr{N}$

(K2) g is non trivial, that is, g cannot be extended to a continuous map $\Omega \to \mathscr{N}$.

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Theorem 2

There exists $t_0 \geq 0$ and $\varepsilon_0 = \varepsilon_0(a,\, b,\, c)$ so that, if

$$t = \frac{ac}{b^2} \geq t_0 \qquad \textit{and} \qquad \varepsilon \leq \varepsilon_0,$$

then minimizers Q_ε for Problem (P_ε) *fulfill*

$$\min_{\overline{\Omega}} |Q_\varepsilon| > 0, \qquad \max_{\overline{\Omega}} \beta(Q_\varepsilon) = 1.$$

- No isotropic melting.
- In agreement with the numerical results **[Schopohl, Sluckin, ’87]**!

Sketch of the proof

- We know that $Q_\varepsilon \in C^\infty(\Omega, \mathbf{S}_0)$ (by elliptic regularity) and, by a comparison argument,
$$\|Q_\varepsilon\|_{L^\infty(\Omega)} \leq 1.$$
- By considering the topology of $\mathbf{S}_0$, one proofs
$$\min_{\overline{\Omega}} |Q_\varepsilon| > 0 \Rightarrow \max_{\overline{\Omega}} \beta(Q_\varepsilon) = 1$$
(the set $\{Q \in \mathbf{S}_0 \colon \ |Q| \geq \delta > 0, \ \beta(Q) \leq 1 - \delta\}$ retracts on $\mathscr{N}$).

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(the set $\{Q \in \mathbf{S}_0 \colon \ |Q| \geq \delta > 0, \ \beta(Q) \leq 1 - \delta\}$ retracts on $\mathscr{N}$).
- We write
$$2E_\varepsilon(Q_\varepsilon) = \lim_{t\to 0} \int_{\{|Q_\varepsilon|>t\}} \left\{ |\nabla |Q_\varepsilon||^2 + |Q_\varepsilon|^2 \left| \nabla \left(\frac{Q_\varepsilon}{|Q_\varepsilon|} \right) \right| + 2\varepsilon^{-2} f(Q_\varepsilon) \right\}$$

- Assume, by contradiction, that $\min_{\overline{\Omega}} |Q_\varepsilon| = 0$. Then, $\Gamma_t := \{|Q_\varepsilon| = t\} \neq \emptyset$ for a.e. $t \in (0, 1)$ and, applying the coarea formula,

$$2E_\varepsilon(Q_\varepsilon) = \int_0^1 dt \int_{\Gamma_t} d\mathcal{H}^1 \left\{ |\nabla |Q_\varepsilon|| + \frac{2f(Q_\varepsilon)}{\varepsilon^2 |\nabla |Q_\varepsilon||} + t^2 \left| \nabla \left(\frac{Q_\varepsilon}{|Q_\varepsilon|} \right) \right| \right\}$$

- Estimating the RHS with the help of Proposition 1 and **[Sandier, '98]**, we obtain

$$E_\varepsilon(Q_\varepsilon) \geq \kappa_* |\log \varepsilon| + \frac{\kappa_*}{2} \log \mu_1 - C_1$$

where $\kappa_* = \kappa_*(\Omega, g)$.

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  where $\kappa_* = \kappa_*(\Omega, g)$.

- For ε small enough, we construct a comparison map P_ε with

$$E_\varepsilon(P_\varepsilon) \leq \kappa_* |\log \varepsilon| + \frac{\kappa_*}{2} \log \sigma + C_2.$$

- We derive a contradiction due to $(\star)$: when $t \gg 1$

$$E_\varepsilon(P_\varepsilon) < E_\varepsilon(Q_\varepsilon).$$

The comparison map

How to construct the comparison map P_ε?

- By a topological argument, we reduce to the case $\Omega = B_1(0)$,

$$g(\theta) = s_* \left\{ n(\theta)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right\} \qquad \text{for } \theta \in [0,\, 2\pi]$$

where $n(\theta) = (\cos(\theta/2),\, \sin(\theta/2), 0)^T$.

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- We define P_ε by:

$$P_\varepsilon(\rho,\, \theta) = s_\varepsilon(\rho) \left\{ \left(n(\theta)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right) + r_\varepsilon(\rho) \left(m(\theta)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right) \right\}$$

  where $m(\theta) = (\sin(\theta/2),\, -\cos(\theta/2), 0)^T$, r_ε is a piecewise affine function such that

$$r_\varepsilon(\rho) = \begin{cases} 1 & \text{if } \rho = 0 \\ 0 & \text{if } \rho \geq \sigma^{-1/2}\varepsilon \end{cases}$$

  and s_ε is such that $|P_\varepsilon| = 1$.

Asymptotic analysis: a general setting

In what follows, we consider

$$u \in H^1_g(\Omega,\, \mathbb{R}^d) \mapsto E_\varepsilon(u) = \int_\Omega \left\{ \frac{1}{2} \left|\nabla u\right|^2 + \frac{1}{\varepsilon^2} f(u) \right\}, \qquad (\mathrm{P}'_\varepsilon)$$

where the unknown is a function $u\colon \Omega \to \mathbb{R}^d$.

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Assumptions on f:

(H1) $f \geq 0$ is smooth, $\mathscr{N} := f^{-1}(0) \neq \emptyset$ is a smooth, compact and connected manifold (without boundary).

(H2) For all $p \in \mathscr{N}$ and all normal vector $v \in \mathbb{R}^d$ to $\mathscr{N}$ at p,

$$\left. \frac{d^2}{dt^2} \right|_{t=0} f(p + tv) > 0.$$

(H3) For all $v \in \mathbb{R}^d$ with $|v| \geq 1$,

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$$f\left(\frac{v}{|v|}\right) < f(v).$$

Some (mild) assumption on the topology of $\mathscr{N}$ is also needed.

Statement of the results

We denote by u_ε the minimizers for $(\mathrm{P}'_\varepsilon)$.

Theorem 3

Assume that (K1)–(K2) and (H1)–(H3) are satisfied, let $\delta > 0$ be an arbitrarily small number. For ε small enough, there exists a finite number of balls $B_1, \ldots, B_k$ of radius $\lambda\varepsilon$, so that

$$\mathrm{dist}(u_\varepsilon(x), \mathscr{N}) \leq \delta \qquad \text{if } x \in \Omega \setminus \bigcup_{i=1}^{k} B_i.$$

- The balls B_i correspond, in the limit $\varepsilon \searrow 0$, to singularities of the limit map.
- In the Landau–de Gennes model, biaxiality is localized.

Theorem 4

Assuming (K1)–(K2), (H1)–(H3), there exists a subsequence $\varepsilon_n \searrow 0$, a finite set $X \subset \Omega$ and a function $u_0 \in C^\infty(\Omega \setminus X, \mathscr{N})$ so that

$$u_{\varepsilon_n} \to u_0 \qquad \textit{strongly in } H^1_{loc} \cap C^0(\Omega \setminus X, \mathbb{R}^d).$$

Moreover, on every ball $B \subset\subset \Omega \setminus X$ the map u_0 is minimizing harmonic, that is,

$$\frac{1}{2}\int_B |\nabla u_0|^2 = \inf\left\{\frac{1}{2}\int_B |\nabla v|^2 : v \in H^1(B, \mathscr{N}),\ v|_{\partial B} = u_0|_{\partial B}\right\}.$$

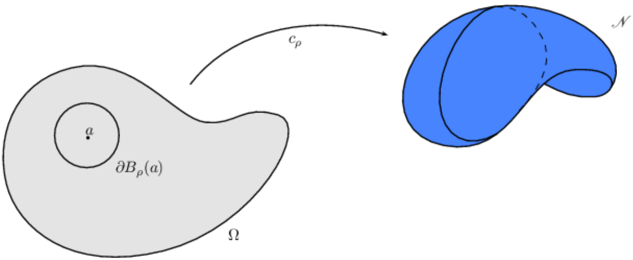
Remark: the map u_0 is *not* harmonic in Ω! In fact, u_0 has infinite energy, since

$$\frac{1}{2}\int_\Omega |\nabla u_\varepsilon|^2 \simeq \kappa_* |\log \varepsilon| + C.$$

- The energy of u_0 concentrates around the singularities.
- In case $\mathscr{N} \simeq \mathbb{RP}^2$, we can prove that $X = \{a\}$. Setting

$$c_\rho : \theta \in [0,\, 2\pi] \mapsto u_0\left(a + \rho e^{i\theta}\right),$$

along some subsequence $\rho_n \searrow 0$ there is uniform convergence of c_{ρ_n} to a geodesic in $\mathscr{N}$.



- As the boundary datum g is smooth, we can apply topological tools to our problem. The singularities which can possibly arise in u_0 are classified according the homotopic structure of $\mathscr{N}$ (see, e.g. **[Mermin, '79]**).

- By topological arguments, we can identify the best constant κ_* for the bound
$$\int_\Omega |\nabla u_\varepsilon|^2 \leq \kappa_* |\log \varepsilon| + C$$
then we use a comparison argument to prove it.

- The singularities of u_0 solve a minimization problem, which involves the homotopic invariants of $\mathscr{N}$.

Conclusions

- In the low temperature regime, minimizers Q_ε of Problem (P_ε) have no isotropic points.
- As $\varepsilon \to 0$, Q_ε converges to a map with a (unique) point defect a.
- Near a, the map Q_ε presents a region of maximal biaxiality.
  Outside, Q_ε looks "almost uniaxial".