Torus and split solutions of the Landau-de Gennes model for nematic liquid crystals

CY Days in Nonlinear Analysis

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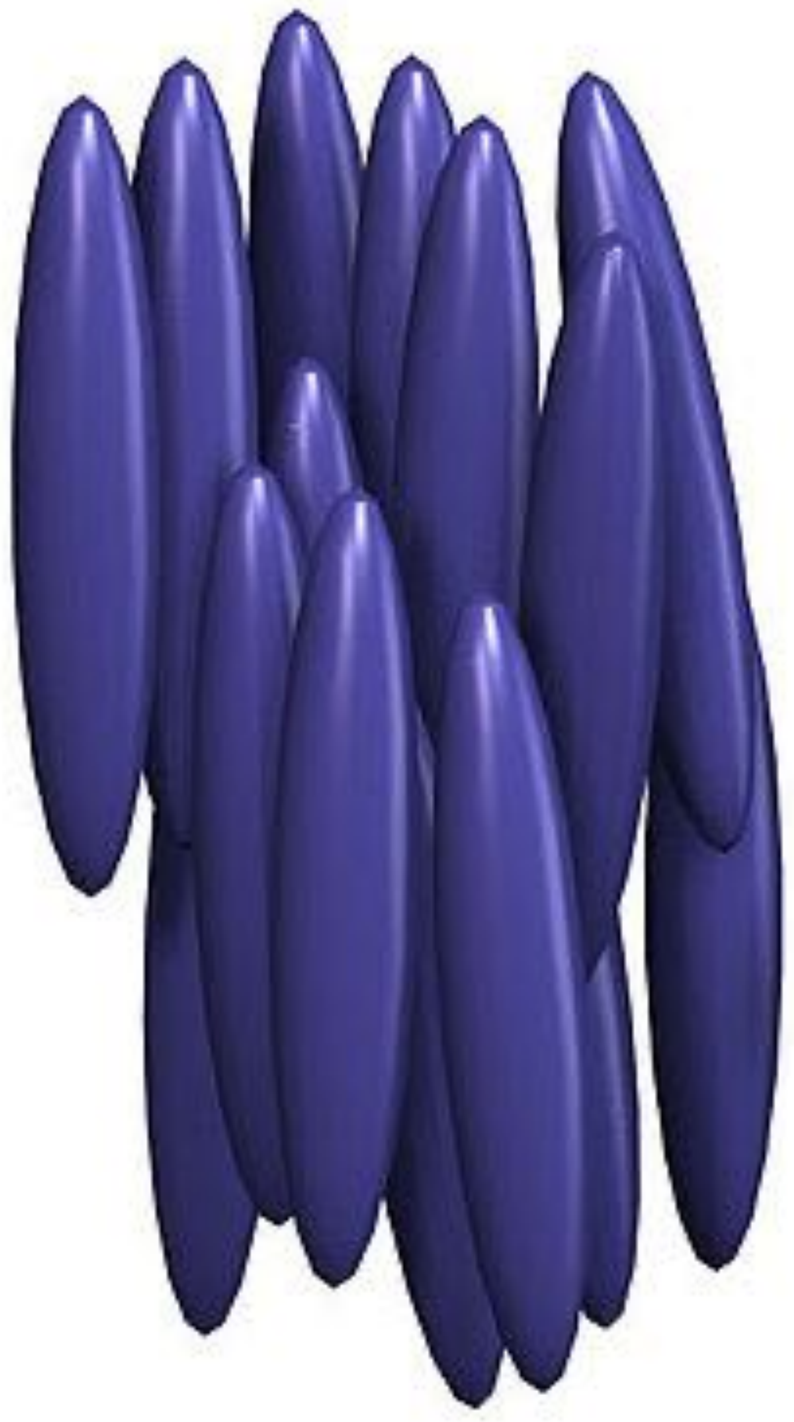
Nematic Liquid Crystals

State of matter : *between liquid and crystal solid*

Nematic phase : rod-like molecules

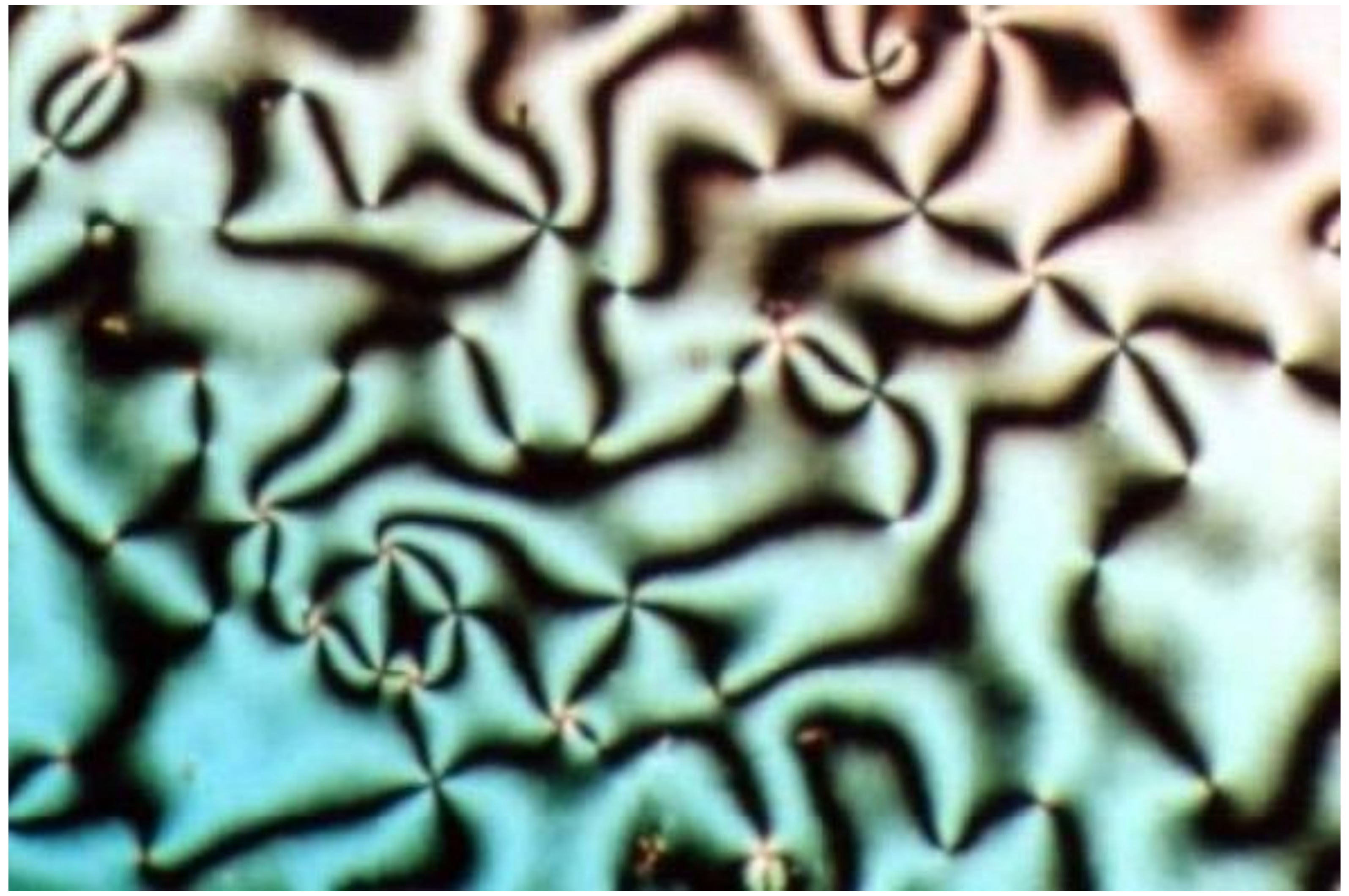
No position order for the center of mass, but directional order

Topological defects : threads (in greek "nema"), hedgehogs (points)



Three (local) phases :

- *Uniaxial* (one directional order)
- *Biaxial* (a secondary directional order)
- *Isotropic* (no directional order)



The Q-tensor model of Landau-de Gennes

Order parameter belongs to

$$\mathcal{S}_0 := \left\{ Q \in \mathcal{M}_{3\times 3}(\mathbb{R}) : Q = Q^t \,,\ \mathrm{tr}(Q) = 0 \right\} \simeq \mathbb{R}^5$$

(with Frobenius scalar product – $P : Q := \mathrm{tr}(PQ)$)

A given configuration contained in $\overline{\Omega} \subset \mathbb{R}^3$ is described through a mapping

$$Q : \overline{\Omega} \to \mathcal{S}_0$$

At a single point $x \in \overline{\Omega}$, **three possible phases :**

- *Isotropic :* $Q(x) = 0$
- *Uniaxial :* $Q(x)$ has a double eigenvalue
- *Biaxial :* $Q(x)$ has three distincts eigenvalues

The biaxiality parameter : (unusual one)

For $Q \in \mathcal{S}_0 \setminus \{0\}$,

$$\beta(Q) := \sqrt{6}\,\frac{\operatorname{tr}(Q^3)}{|Q|^3} \in [-1,1] \qquad \big(\ \beta(Q) = 3\sqrt{6}\det(Q)\ \big)$$

If $\sigma(Q) = \{\lambda_1, \lambda_2, \lambda_3\}$ with $\lambda_1 \le \lambda_2 \le \lambda_3$, then

- $\beta(Q) = 1 \iff \lambda_1 = \lambda_2 < \lambda_3 \iff Q$ **positive uniaxial**
- $\beta(Q) \in (-1,1) \iff \lambda_1 < \lambda_2 < \lambda_3 \iff Q$ **biaxial**
- $\beta(Q) = -1 \iff \lambda_1 < \lambda_2 = \lambda_3 \iff Q$ **negative uniaxial**
- $Q = 0 \iff \lambda_1 = \lambda_2 = \lambda_3 \iff Q$ **isotropic**

<u>**Uniaxial Matrices :**</u>

A matrix $Q \in \mathcal{S}_0 \setminus \{0\}$ is uniaxial iff

$$Q = s\left(\vec{n} \otimes \vec{n} - \frac{1}{3} I_d\right), \qquad s \in \mathbb{R} \setminus \{0\}, \quad \vec{n} \in \mathbb{S}^2$$

- Q positive uniaxial $\Leftrightarrow s > 0$
- Q negative uniaxial $\Leftrightarrow s < 0$

The Landau-de Gennes energy (*in the "one constant approximation"*)

For $Q \in H^1(\Omega; \mathcal{S}_0)$,

$$E_{LDG}(Q) := \int_\Omega \frac{L}{2} |\nabla Q|^2 \, dx + \int_\Omega F_{\text{bulk}}(Q) \, dx$$

where $0 < L < 1$ is the elasticity constant, and

$$F_{\text{bulk}}(Q) := -\frac{a^2}{2} \text{tr}(Q^2) - \frac{b^2}{3} \text{tr}(Q^3) + \frac{c^2}{4} \big(\text{tr}(Q^2)\big)^2$$

with $a \neq 0$, $b \neq 0$, $c \neq 0$ (material constants)

We set

$$\widetilde{F}(Q) := F_{\text{bulk}}(Q) - \min_{\mathcal{S}_0} F_{\text{bulk}} \geq 0$$

and

$$\widetilde{E}_{LDG}(Q) := \int_\Omega \frac{L}{2} |\nabla Q|^2 \, dx + \int_\Omega \widetilde{F}(Q) \, dx$$

The potential well :

$$\{\widetilde{F}=0\} = \left\{ Q = s^+\left(\vec{n}\otimes\vec{n} - \frac{1}{3}I_d\right) : \vec{n}\in\mathbb{S}^2 \right\} \subset s^+\sqrt{\frac{2}{3}}\,\mathbb{S}^4$$

with

$$s^+ := \frac{b^2+\sqrt{b^4+24a^2c^2}}{4c^2}$$

$\Longrightarrow$ up to the multiplicative factor $s^+\sqrt{\frac{2}{3}}$,

$$\{\widetilde{F}=0\} = \mathbb{R}P^2$$

that is,

$$\{\widetilde{F}=0\} = \textit{(smooth) embedding of } \mathbb{R}P^2 \textit{ in } \mathbb{S}^4 \textit{ (Veronese)}$$

The nematic droplet - Energy minimizers in the limit $L \to 0$

(Majumdar & Zarnescu 2010)

Assume $\Omega = B_1$, and consider the Dirichlet boundary condition

$$Q_{\mathrm{b}}(x) := s^+\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} I_d\right), \qquad x \in \partial B_1 \qquad (\textit{homeotropic})$$

If

$$Q_L \in \operatorname{argmin}\left\{ \widetilde{E}_{\mathrm{LDG}}(Q) : Q \in H^1(B_1; \mathcal{S}_0)\,,\ Q = Q_{\mathrm{b}} \text{ sur } \partial B_1 \right\},$$

then

$$Q_L \underset{L \to 0}{\longrightarrow} Q_*$$

with

$$Q_*(x) = s^+\left(\vec{n}_*(x) \otimes \vec{n}_*(x) - \frac{1}{3} I_d\right)$$

and

$$\vec{n}_* \in \operatorname{argmin}\left\{ \int_{B_1} |\nabla \vec{n}|^2\, dx : \vec{n} \in H^1(B_1; \mathbb{S}^2)\,,\ \vec{n}(x) = \frac{x}{|x|} \text{ sur } \partial B_1 \right\}$$

By a result due to *Almgren & Lieb (1988)*,

$$\vec{n}_*(x) = \frac{x}{|x|}$$

so that

$$Q_*(x) = s^+\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} I_d\right)$$

Observe that

$$Q_*(Rx) = RQ_*(x)R^t \qquad \forall R \in SO(3)\,, \forall x \in B_1 \setminus \{0\}$$

(equivariant radial symmetry)

The symmetry and uniaxiality questions

For $L > 0$ **fixed**,

1) Does Q_L present radial symmetry (equivariante) ?

$$Q_L(Rx) = RQ_L(x)R^t \quad \forall R \in SO(3)$$

2) Is Q_L uniaxial ? (with isotropic points)

The radially symmetric critical point

• There exists a unique radially symmetric critical point of E_{LDG} (*Ignat, Nguyen, Slastikov, Zarnescu 2014*)

$$Q_{\mathrm{rad}}(x) := f_L(|x|)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} I_d\right)$$

with $f_L(0) = 0$, $f_L(1) = s^+$, et $f_L \nearrow$

• Q_{rad} is the unique critical point which is uniaxial (*Lamy 2015*)

Hedgehog instability and the biaxial torus

In a certain regime of the parameters L, a, b, c,

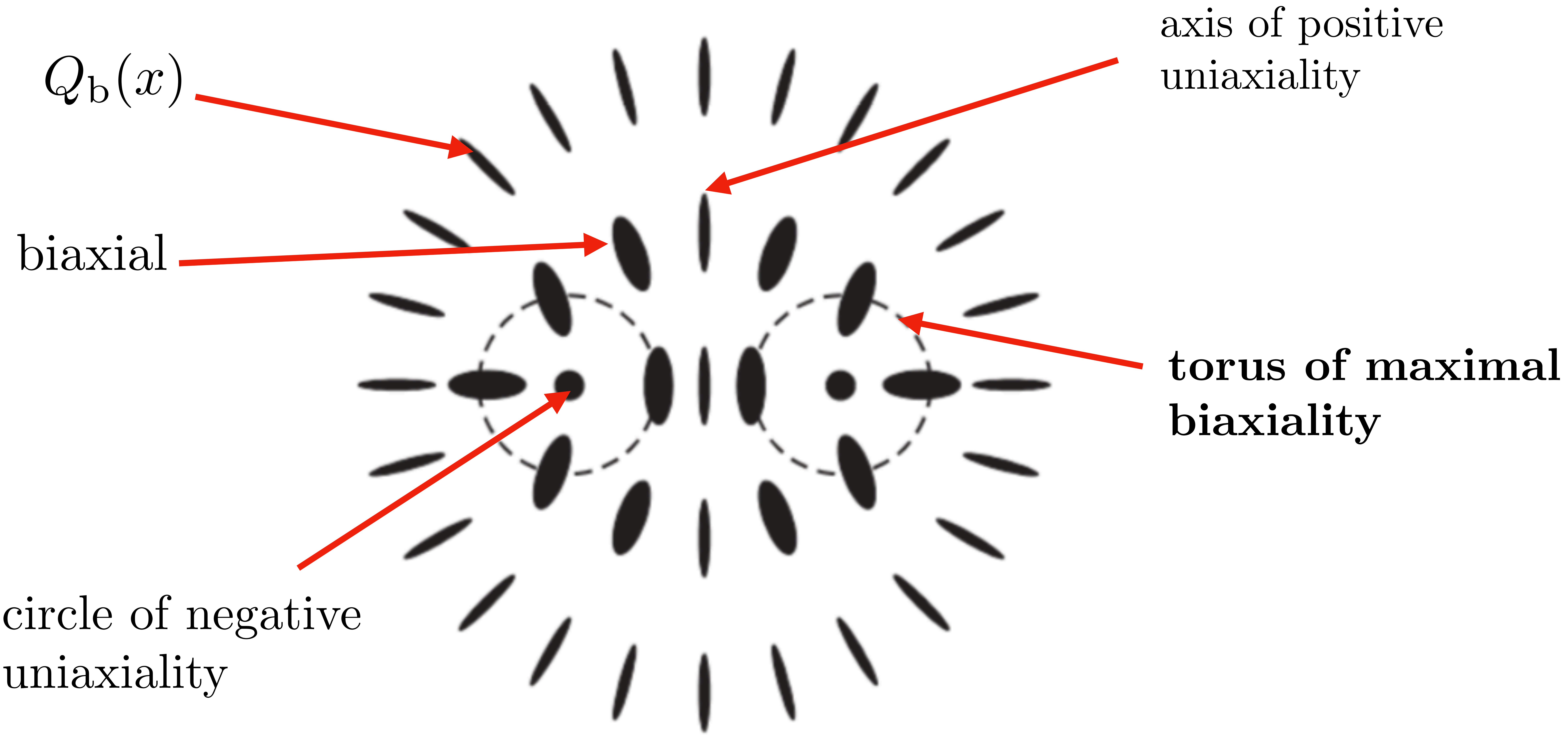
$$Q_{\text{rad}} \text{ is unstable}$$

Gartland & Mkaddem 1999, *Majumdar 2012*,
Ignat, Nguyen, Slastikov, Zarnescu 2015

$\Longrightarrow$ Full $SO(3)$-symmetry breaking + biaxial escape

Expected minimizer : *The biaxial torus*

$$(SO(2)) \text{ axial symmetry} + \text{No isotropic points}$$


$Q_{\mathrm{b}}(x)$
biaxial
axis of positive uniaxiality
torus of maximal biaxiality
circle of negative uniaxiality

Main objective :

Explain this structure, at least partially, by **topological arguments** ("easy" with axial symmetry)

$\Rightarrow$ prove the absence of the isotropic phase

Case 1 : With no symmetry ansatz

Case 2 : With axial symmetry

Analysis in the "Lyuksyutov regime" (of parameters)

The Lyutsukov regime

Renormalization et parameters réduction

Normalizing matrices by

$$\mathbf{Q} \leftarrow \frac{1}{s^+}\sqrt{\frac{3}{2}}\,Q\,,$$

the energy becomes

$$\widetilde{E}_{LDG}(Q) = \frac{2}{3}L(s^+)^2\mathcal{E}_{\lambda,\mu}(\mathbf{Q})$$

with

$$\mathcal{E}_{\lambda,\mu}(\mathbf{Q}) := \int_\Omega \frac{1}{2}|\nabla\mathbf{Q}|^2 + \lambda W(\mathbf{Q}) + \frac{\mu}{4}(1-|\mathbf{Q}|^2)^2\,dx$$

où

$$\lambda := \sqrt{\frac{2}{3}}\,\frac{b^2 s^+}{L} > 0\,, \qquad \mu := \frac{a^2}{L} > 0\,,$$

and

$$W(\mathbf{Q}) := \frac{|\mathbf{Q}|^3}{3\sqrt{6}}\big(1-\beta(\mathbf{Q})\big) + \frac{1}{12\sqrt{6}}(3|Q|^2+2|Q|+1)(|Q|-1)^2 \geq 0$$

$\Longrightarrow$ **We are interested in the regime** $\mu \to +\infty$ (with λ fixed)

The limiting effective energy is

$$\mathcal{E}_\lambda(Q) := \int_\Omega \frac{1}{2}|\nabla Q|^2 + \lambda W(Q)\, dx \quad \text{pour } Q \in H^1(\Omega; \mathbb{S}^4)$$

avec

$$W(Q) = \frac{1}{3\sqrt{6}}\big(1 - \beta(Q)\big) \qquad \forall Q \in \mathbb{S}^4$$

$\Longrightarrow$ By Ginzburg-Laudau type theories :

If any minimizer of $\mathcal{E}_\lambda$ are **smooth**, then

minimizers of $\mathcal{E}_{\lambda,\mu}$ **do not present the isotropic phase** for μ large enough.

Theorem

Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with $\partial\Omega$ of class C^3, and $Q_{\mathrm{b}} \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$.

Assume that any minimizer of $\mathcal{E}_\lambda$ over $H^1_{Q_{\mathrm{b}}}(\Omega; \mathbb{S}^4)$ is continuous on $\overline{\Omega}$.

If $Q_\mu \in H^1(\Omega; \mathcal{S}_0)$ minimizes $\mathcal{E}_{\lambda,\mu}$ over $H^1_{Q_{\mathrm{b}}}(\Omega; \mathcal{S}_0)$, then
$Q_\mu \in C^\omega(\Omega) \cap C^{1,\alpha}(\overline{\Omega})$ for every $\alpha \in (0,1)$.

Moreover, as $\mu \to +\infty$,

1) there exists a subsequence and Q_* minimizing $\mathcal{E}_\lambda$ over $H^1_{Q_{\mathrm{b}}}(\Omega; \mathbb{S}^4)$
such that $Q_\mu \to Q_*$ strongly $H^1(\Omega)$

2) $\mathcal{E}_{\lambda,\mu}(Q_\mu) \to \mathcal{E}_\lambda(Q_*)$ and $\mu \int_\Omega (1 - |Q_\mu|^2)^2 \, dx \to 0$

3) $|Q_\mu| \to 1$ uniformly on $\overline{\Omega}$

In particular, for every $\lambda \geq 0$, there exists $\mu_\lambda > 0$ such that

$$|Q_\mu| > 0 \text{ in } \overline{\Omega} \quad \text{whenever } \mu > \mu_\lambda$$

A first step toward the biaxial torus

Let us now consider

- Ω diffeomorphic to B_1
- $Q \in C^2(\partial\Omega; \mathbb{R}P^2)$ of the form

$$Q_{\mathrm{b}}(x) = \sqrt{\frac{3}{2}}\left(\vec{n}(x) \otimes \vec{n}(x) - \frac{1}{3} I_d\right)$$

with $\vec{n} \in C^2(\partial\Omega; \mathbb{S}^2)$ et $\deg(\vec{n}) = 1$

- $\mu > \mu_\lambda$ so that $|Q_\mu| > 0$ in $\overline{\Omega}$

Theorem Let $Q \in C^1(\overline{\Omega}; \mathbb{S}^4) \cap C^\omega(\Omega)$ such that $Q = Q_{\mathrm{b}}$ on $\partial\Omega$

1) The set of critical values of $\beta \circ Q$ is at most countable and it can accumulate only at 1. In addition, for every regular value $-1 < t < 1$, the surface $\{\beta \circ Q = t\} \subset \Omega$ is smooth and has a connected component of positive genus.

2) For every $-1 \leq t_1 < t_2 < 1$, the sets $\{\beta \circ Q \leq t_1\} \subset \Omega$ et $\{\beta \circ Q \geq t_2\} \subset \overline{\Omega}$ are non empty, compact, and non simply connected.

3) If $Q \in C^\omega(\overline{\Omega})$, then the set of singular values of $\beta \circ Q$ finite. Moreover, $\{\beta \circ Q = 1\} \subset \overline{\Omega}$ is non empty, compact, and non simply connected. In particular, $\{\beta \circ Q = 1\} \cap \Omega$ is non empty.

4) For every $-1 < t_1 < t_2 < 1$, if (t_1, t_2) does not contain any singular value, then $\{\beta \circ Q \leq t_1\}$ et $\{\beta \circ Q \geq t_2\}$ are mutually linked.

Rough idea of proof: positif genus statement

- Assume that $t \in (-1, 1)$ is a regular value of $\beta \circ Q$
- To make it simpler, assume that $\Sigma := \{\beta \circ Q = t\}$ is connected
- By contradiction, if Σ is a sphere, then

$$U := \{\beta \circ Q > t\} \simeq B_1 \setminus B_{1/2} \text{ is simply connected}$$

- there exists $v_3 \in C^1(\overline{U}; \mathbb{S}^2)$ such that $Q_\mu(x)v_3(x) = \lambda_3(x)v_3(x)\ \forall x \in \overline{U}$
- $v_3 = \pm\vec{n}$ on $\partial\Omega$, thus $\deg(v_3, \Sigma) = \pm 1$
- but $\lambda_1 < \lambda_2 < \lambda_2$ on Σ, hence there exists $v_1, v_2 \in C^1(\Sigma; \mathbb{S}^2)$ such that $Q_\mu(x)v_i(x) = \lambda_i(x)v_i(x)$
- $\{v_1(x), v_2(x)\}$ basis of $\{v_3(x)\}^\perp$ for every $x \in \Sigma$
- $\{v_1, v_2\}$ is a trivialization of $(\Sigma, T_{v_3}\mathbb{S}^2)$ **contradiction** since $\deg(v_3) \neq 0$.

Theorem

Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with $\partial\Omega$ of class C^3, and $Q_\mathrm{b} \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$. If Q minimizes $\mathcal{E}_\lambda$ over $H^1_{Q_\mathrm{b}}(\Omega; \mathbb{S}^4)$, then

1) $Q \in C^\omega(\Omega) \cap C^{1,\alpha}(\overline{\Omega})$ for every $\alpha \in (0,1)$.

2) If $\partial\Omega \in C^{k\vee 3,\alpha}$ and $Q_\mathrm{b} \in C^{k,\alpha}(\partial\Omega)$ with $k \geq 2$, then $Q \in C^{k,\alpha}(\overline{\Omega})$

3) If $\partial\Omega \in C^\omega$ et $Q_\mathrm{b} \in C^\omega(\partial\Omega)$, then $Q \in C^\omega(\overline{\Omega})$

Idea of proof

$\mathcal{E}_\lambda$ = lower order perturbation of the Dirichlet energy

$\Longrightarrow$ The general regularity theory for minimizing harmonic maps into a manifold applies (*Schoen & Uhlenbeck*)

$\Longrightarrow$ Q is smooth away from a finite number of singularities in Ω

"Blowing-up" the map Q near a singularity, we obtain a non trivial 0-homogeneous minimizing harmonic map from $\mathbb{R}^3$ into $\mathbb{S}^4$

By a result of *Schoen & Uhlenbeck*, all of them are trivial !

$\Longrightarrow$ Q has no singularities

Minimization under axial symmetry

• Now we assume that $\Omega \subset \mathbb{R}^3$ is **axially symmetric** with respect to the vertical axis (Ω still a topological ball)

• Identify rotations around the vertical axis with $\mathbb{S}^1$

• **Action of $\mathbb{S}^1$ on $\mathcal{S}_0$:**

$$Q \mapsto RQR^{\mathrm{t}}$$

$\Longrightarrow$ $\mathbb{S}^4$ is invariant under the action of $\mathbb{S}^1$ (and $\mathbb{R}P^2$ as well)

$\Longrightarrow$ $\mathcal{E}_\lambda(RQR^{\mathrm{t}}) = \mathcal{E}_\lambda(Q)$ for $Q : \Omega \to \mathbb{S}^4$

• **Equivariant map:** $Q : \Omega \to \mathbb{S}^4$ is $\mathbb{S}^1$-equivariant if

$$Q(Rx) = RQ(x)R^{\mathrm{t}} \quad \forall R \in \mathbb{S}^1$$

For $Q_{\rm b} \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ a given equivariant map, set

$$\mathcal{A}^{\rm sym}(\Omega, Q_{\rm b}) := \Big\{ Q \in H^1(\Omega; \mathbb{S}^4) : Q = Q_{\rm b} \text{ on } \partial\Omega\,,\ Q \text{ equivariant} \Big\}\,,$$

and consider

$$\min_{Q \in \mathcal{A}^{\rm sym}(\Omega, Q_{\rm b})} \mathcal{E}_\lambda(Q)$$

$\Longrightarrow$ Existence through the Direct Method (closed contraint)

$\Longrightarrow$ Solutions are critical points of $\mathcal{E}_\lambda$ ("Palais symmetric criticality principle")

$\Longrightarrow$ **Regularity of solutions ?**

Set

$$\mathbf{e}_0 := \frac{1}{\sqrt{6}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \in \mathbb{S}^4$$

$\mathbf{e}_0$ and $-\mathbf{e}_0$ are the only elements of $\mathbb{S}^4$ invariant under $\mathbb{S}^1$

$\Longrightarrow$ For $Q : \Omega \to \mathbb{S}^4$ continuous and equivariant,

$$Q(0,0,x_3) \in \{\pm \mathbf{e}_0\}$$

$\Longrightarrow$ If $\Omega = B_1$ and $Q_\mathrm{b}(0,0,\pm 1) = \pm \mathbf{e}_0$, then

$$\mathcal{A}^{\mathrm{sym}}(B_1, Q_\mathrm{b}) \cap C^0(\overline{\Omega}) = \emptyset\,.$$

Remark:

$\beta(\mathbf{e}_0) = +1 \implies \mathbf{e}_0 \in \mathbb{R}P^2$

$\beta(-\mathbf{e}_0) = -1 \implies -\mathbf{e}_0 \notin \mathbb{R}P^2$

Theorem

Let $\Omega \subset \mathbb{R}^3$ be an axially symmetric bounded open set with $\partial\Omega$ of class C^3, and $Q_{\rm b} \in C^{1,1}(\partial\Omega;\mathbb{S}^4)$ equivariant.

If Q minimizes $\mathcal{E}_\lambda$ over $\mathcal{A}^{\rm sym}(\Omega, Q_{\rm b})$, then

1) $Q \in C^\omega(\Omega \setminus \Sigma) \cap C^{1,\alpha}(\overline{\Omega} \setminus \Sigma)$ for every $\alpha \in (0,1)$ where $\Sigma \subset \Omega \cap \{\text{axe}-x_3\}$ is a finite set.

2) If $\partial\Omega \in C^{k\vee 3,\alpha}$ and $Q_{\rm b} \in C^{k,\alpha}(\partial\Omega)$ with $k \geq 2$, then $Q \in C^{k,\alpha}(\overline{\Omega} \setminus \Sigma)$

3) If $\partial\Omega \in C^\omega$ and $Q_{\rm b} \in C^\omega(\partial\Omega)$, then $Q \in C^\omega(\overline{\Omega} \setminus \Sigma)$

Moreover, for each $\bar{x} \in \Sigma$, there exists $Q_\alpha \in \{\pm R Q_* R^{\rm t} : R \in \mathbb{S}^1\}$ and $p > 0$ such that

$$\|Q^{\bar{x},\rho} - Q_\alpha\|_{C^2(B_2 \setminus B_1)} = O(\rho^p) \quad \text{as } \rho \to 0\,,$$

with $Q^{\bar{x},\rho}(y) := Q(\bar{x} + \rho y)$ and

$$Q_*(x) := \frac{1}{\sqrt{6}}\frac{1}{|x|}\begin{pmatrix} -x_3 & 0 & \sqrt{3}x_1 \\ 0 & -x_3 & \sqrt{3}x_2 \\ \sqrt{3}x_1 & \sqrt{3}x_2 & 2x_3 \end{pmatrix}$$

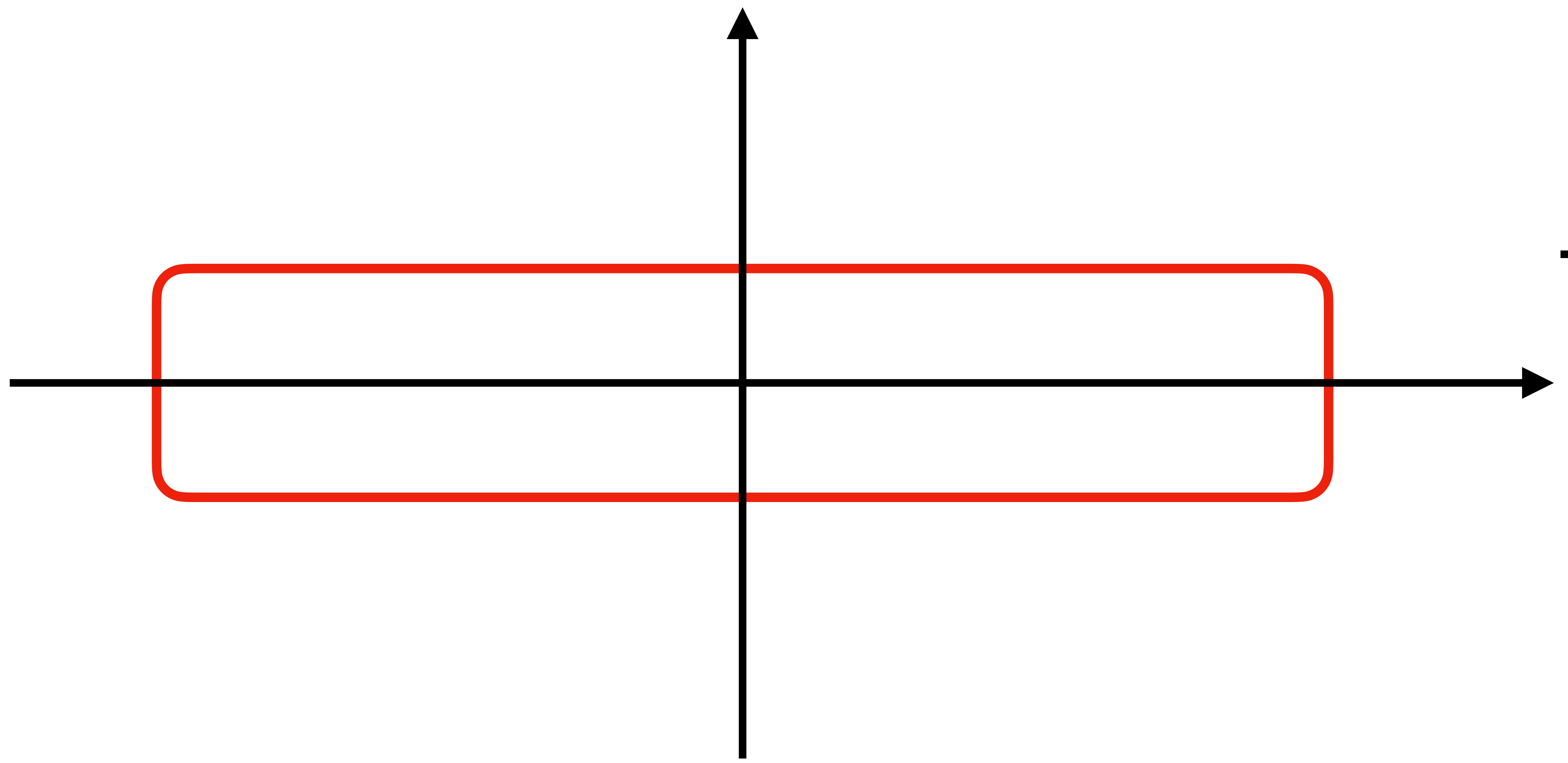
Homeotropic boundary condition in cylinders

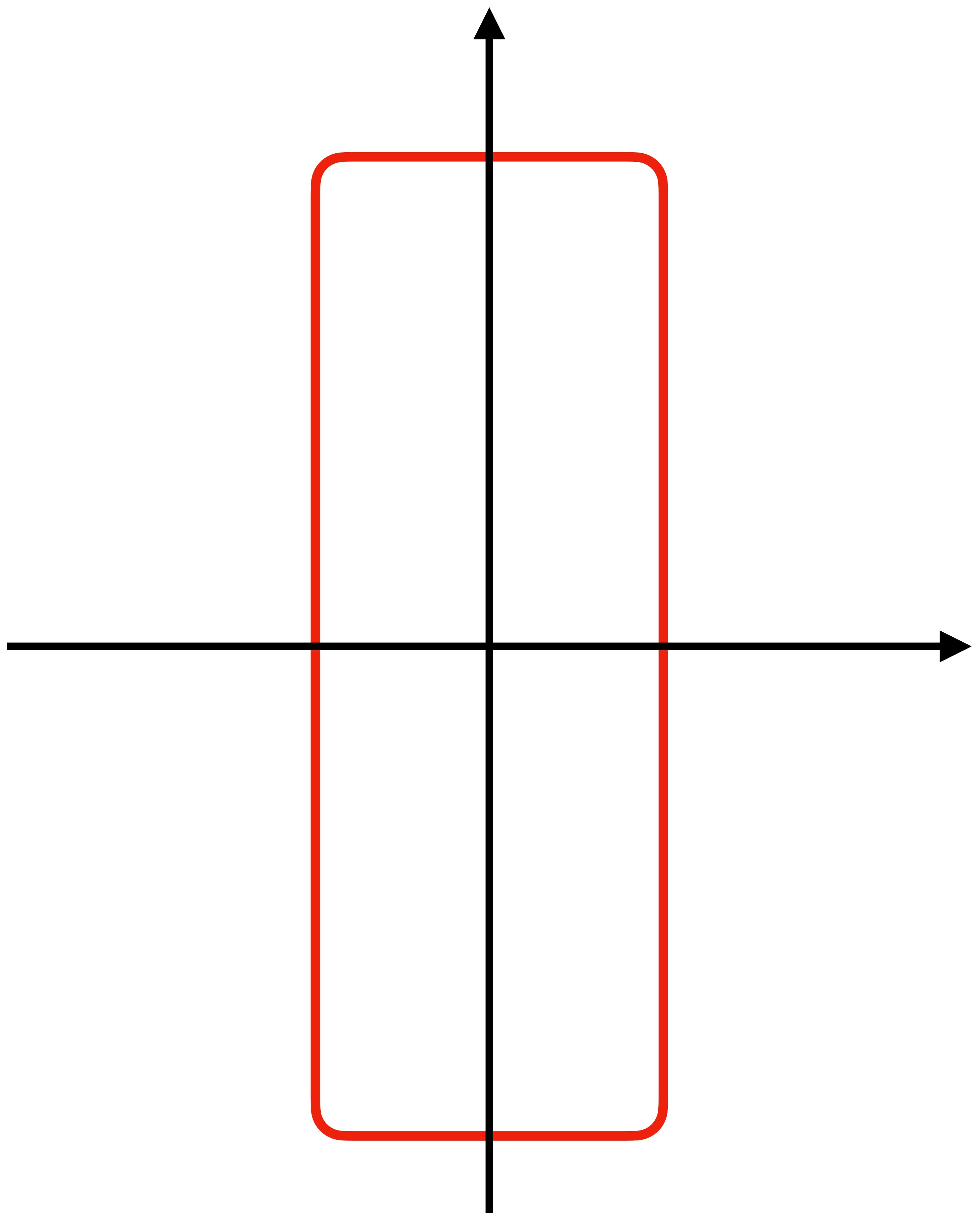
The boundary data Q_{b} is said to be *homeotropic* if

$$Q_{\mathrm{b}}(x) = \frac{\sqrt{3}}{\sqrt{2}}\left(\vec{n}(x) \otimes \vec{n}(x) - \frac{1}{3} I_d\right) \in \mathbb{R}P^2 \quad \text{for } x \in \partial\Omega$$

where $\vec{n}(x)$ denotes the unit normal.

Cylindrical domains:





h = height
ℓ = radius

$\Omega_{h,\ell}$

Theorem 1: large cylinders.

Let $\Omega_{h,\ell}$ a cylindrical domain and Q_{b} its homeotropic boundary data.

For $\lambda \geq 0$ et $h > 0$ fixed, if $\ell >> 1$ is large enough, then any solution of

$$\min_{\mathcal{A}^{\mathrm{sym}}(\Omega_{h,l},Q_{\mathrm{b}})} \mathcal{E}_\lambda$$

is smooth (i.e., $\Sigma = \emptyset$).

Theorem 2: thin and long cylinders.

Let $\Omega_{h,\ell}$ a cylindrical domain and Q_{b} its homeotropic boundary data.

There exists a critical value $\lambda_* > 0$ such that:

for $\lambda \geq 0$ and $0 < \ell < \sqrt{\lambda_*/\lambda}$ fixed, if $h >> 1$ is large enough, then any solution Q of

$$\min_{\mathcal{A}^{\mathrm{sym}}(\Omega_{h,l},Q_{\mathrm{b}})} \mathcal{E}_\lambda$$

is singular (i.e., $\Sigma \neq \emptyset$). Moreover, $\mathrm{Card}(\Sigma)$ is even and $\beta(Q) = -1$ in "most of the vertical axis".