The Well Order Reconstruction Solution for nematic liquid crystals in square domains

GIACOMO CANEVARI
with APALA MAJUMDAR *and* AMY SPICER

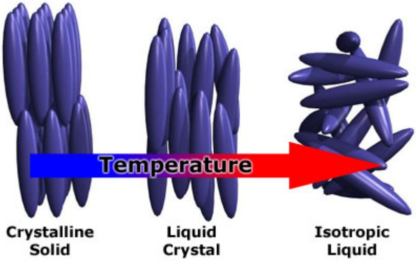
Partial Order in Materials: at the Triple Point of Mathematics, Physics and Applications

BIRS, November 2017

basque center for applied mathematics

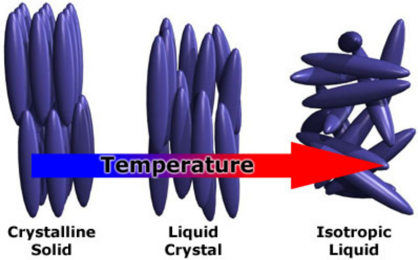
Liquid crystals

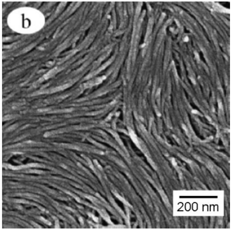
Liquid crystals are intermediate phases of matter between crystalline solids and the liquid phase.



Liquid crystals

Liquid crystals are intermediate phases of matter between crystalline solids and the liquid phase.



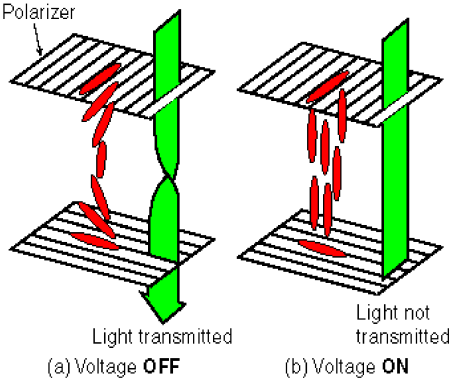


Carbon nanotubes as liquid crystals.
[Zhang, Kumar, '08]

Nematic liquid crystals:

- Rod-shaped molecules.
- The molecules can flow.
- Directional order, but no positional order.

- Anisotropic optical properties
- Confinement leads to pattern formation.



The order parameter: Q-tensors

- The material is represented by a symmetric, trace-free tensor field:

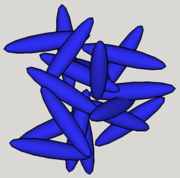
$$\Omega \subseteq \mathbb{R}^d \to \mathbf{S}_0 := \left\{ \mathbf{Q} \in \mathbb{R}^{3\times 3} \colon \mathbf{Q}^{\mathsf{T}} = \mathbf{Q},\ \operatorname{tr}\mathbf{Q} = 0 \right\}.$$

The order parameter: Q-tensors

- The material is represented by a symmetric, trace-free tensor field:

$$\Omega \subseteq \mathbb{R}^d \to \mathbf{S}_0 := \left\{ \mathbf{Q} \in \mathbb{R}^{3\times 3} \colon \mathbf{Q}^\mathsf{T} = \mathbf{Q}, \ \operatorname{tr} \mathbf{Q} = 0 \right\}.$$

▷ **Isotropic**: $\mathbf{Q}(\mathbf{x}) = 0$



$\mathbf{Q}(\mathbf{x}) = 0$

The order parameter: Q-tensors

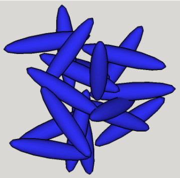
- The material is represented by a symmetric, trace-free tensor field:

$$\Omega \subseteq \mathbb{R}^d \to \mathbf{S}_0 := \left\{ \mathbf{Q} \in \mathbb{R}^{3\times 3} \colon \mathbf{Q}^\mathsf{T} = \mathbf{Q}, \ \mathrm{tr}\, \mathbf{Q} = 0 \right\}.$$

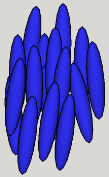
▷ **Isotropic**: $\mathbf{Q}(\mathbf{x}) = 0$

▷ **Uniaxial**: $\mathbf{Q}(\mathbf{x}) \neq 0$ and two eigenvalues coincide.

$$\mathbf{Q}(\mathbf{x}) = s(\mathbf{x}) \left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{1}{3} \, \mathrm{Id} \right)$$



$\mathbf{Q}(\mathbf{x}) = 0$



$\lambda_1 < \lambda_2 = \lambda_3$

The order parameter: Q-tensors

- The material is represented by a symmetric, trace-free tensor field:

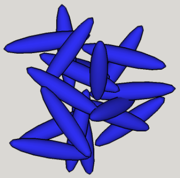
$$\Omega \subseteq \mathbb{R}^d \to \mathbf{S}_0 := \left\{ \mathbf{Q} \in \mathbb{R}^{3\times 3} \colon \mathbf{Q}^\mathsf{T} = \mathbf{Q}, \ \operatorname{tr} \mathbf{Q} = 0 \right\}.$$

▷ **Isotropic**: $\mathbf{Q}(\mathbf{x}) = 0$

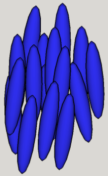
▷ **Uniaxial**: $\mathbf{Q}(\mathbf{x}) \neq 0$ and two eigenvalues coincide.

$$\mathbf{Q}(\mathbf{x}) = s(\mathbf{x}) \left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{1}{3} \operatorname{Id} \right)$$

▷ **Biaxial**: all the eigenvalues are distinct.

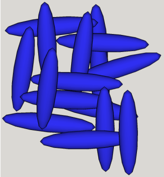


$\mathbf{Q}(\mathbf{x}) = 0$



$\lambda_1 < \lambda_2 = \lambda_3$

$$\xrightarrow{0 \leq \beta^2(\mathbf{Q}) \leq 1}$$



$\lambda_1 < \lambda_2 < \lambda_3$

The Landau-de Gennes energy

$$I[\mathbf{Q}] := \int_\Omega \left\{ \frac{L}{2} |\nabla \mathbf{Q}|^2 + f_b(\mathbf{Q}) \right\}$$

$$f_b(\mathbf{Q}) := \frac{A}{2} \operatorname{tr} \mathbf{Q}^2 - \frac{B}{3} \operatorname{tr} \mathbf{Q}^3 + \frac{C}{4} \left(\operatorname{tr} \mathbf{Q}^2 \right)^2$$

where B, C, L are positive material-dependent parameters; A also depends on the temperature.

The Landau-de Gennes energy

$$I[\mathbf{Q}] := \int_\Omega \left\{ \frac{L}{2} |\nabla \mathbf{Q}|^2 + f_b(\mathbf{Q}) \right\}$$

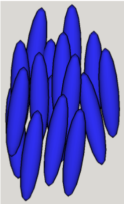
$$f_b(\mathbf{Q}) := \frac{A}{2} \operatorname{tr} \mathbf{Q}^2 - \frac{B}{3} \operatorname{tr} \mathbf{Q}^3 + \frac{C}{4} \left(\operatorname{tr} \mathbf{Q}^2 \right)^2$$

where B, C, L are positive material-dependent parameters; A also depends on the temperature.

- We work with $A < 0$.
- Energetically favorable configurations:

$$\mathscr{N} := \arg\min f_b = \left\{ s_+ \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \operatorname{Id} \right) : \mathbf{n} \in \mathbb{S}^2 \right\}$$

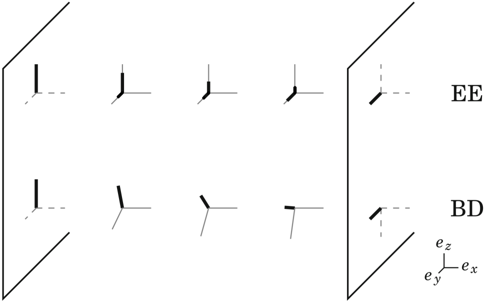
for $s_+ = s_+(A, B, C) > 0$.



A 1D problem

A layer of nematic material bounded by parallel plates, with competing BC.

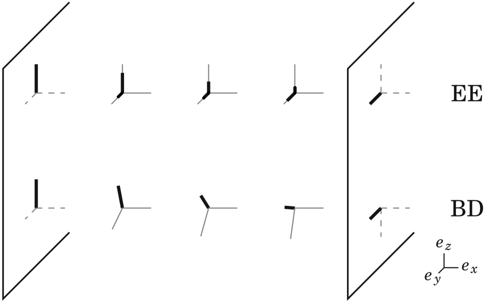
- **Eigenvalue exchange**
  - (i) Constant eigenframe
  - (ii) Negative uniaxiality in the middle
- **Bent director**

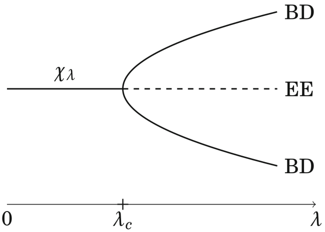


A 1D problem

A layer of nematic material bounded by parallel plates, with competing BC.

- **Eigenvalue exchange**
  - (i) Constant eigenframe
  - (ii) Negative uniaxiality in the middle
- **Bent director**



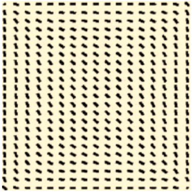


- $\lambda \propto$ cell width
- Pitchfork bifurcation

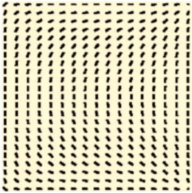
  [Palffy-Muhoray, Gartland, Kelly, '94; Bisi, Gartland, Rosso, Virga, '03; Lamy, '14]

The 2D problem: Planar bistable cell

Nematic-filled square well, of side length $\sqrt{2}\lambda$, with tangential BC.



Diagonal state

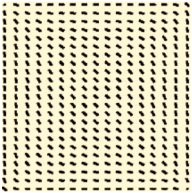


Rotating state

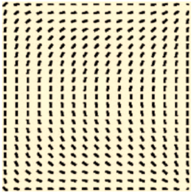
[Tsakonas, Davidson, Brown, Mottram, ’07; Luo, Majumdar, Erban, ’12. . .]

The 2D problem: Planar bistable cell

Nematic-filled square well, of side length $\sqrt{2}\lambda$, with tangential BC.



Diagonal state



Rotating state

Order reconstruction

[Tsakonas, Davidson, Brown, Mottram, '07; Luo, Majumdar, Erban, '12. . .]

[Kralj, Majumdar, '14]

Order reconstruction solution, for small λ:

(i) Constant eigenframe ($\hat{\mathbf{z}}$ is an eigenvector)

(ii) Negative uniaxial cross along the diagonals.

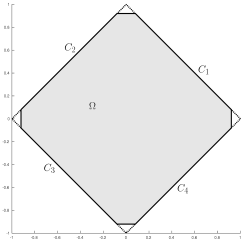
Setting of the problem

▷ **Scaling** $x \mapsto \lambda x$:

$$I[\mathbf{Q}] := \int_\Omega \left\{ \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{\lambda^2}{L} f_b(\mathbf{Q}) \right\}$$

$$f_b(\mathbf{Q}) := \frac{A}{2} \operatorname{tr} \mathbf{Q}^2 - \frac{B}{3} \operatorname{tr} \mathbf{Q}^3 + \frac{C}{4} \left(\operatorname{tr} \mathbf{Q}^2 \right)^2$$

▷ $\Omega \subseteq \mathbb{R}^2$ is a **truncated square** with side length $\sqrt{2}$.



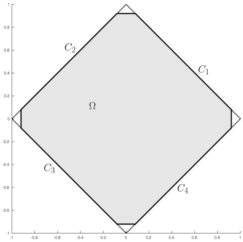
Setting of the problem

▷ **Scaling** $x \mapsto \lambda x$:

$$I[\mathbf{Q}] := \int_\Omega \left\{ \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{\lambda^2}{L} f_b(\mathbf{Q}) \right\}$$

$$f_b(\mathbf{Q}) := \frac{A}{2} \operatorname{tr} \mathbf{Q}^2 - \frac{B}{3} \operatorname{tr} \mathbf{Q}^3 + \frac{C}{4} \left(\operatorname{tr} \mathbf{Q}^2 \right)^2$$

▷ $\Omega \subseteq \mathbb{R}^2$ is a **truncated square** with side length $\sqrt{2}$.



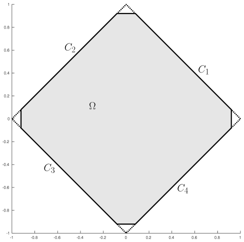
Setting of the problem

- ▷ **Scaling** $x \mapsto \lambda x$:

$$I[\mathbf{Q}] := \int_\Omega \left\{ \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{\lambda^2}{L} f_b(\mathbf{Q}) \right\}$$

$$f_b(\mathbf{Q}) := \frac{A}{2} \operatorname{tr} \mathbf{Q}^2 - \frac{B}{3} \operatorname{tr} \mathbf{Q}^3 + \frac{C}{4} \left(\operatorname{tr} \mathbf{Q}^2 \right)^2$$

- ▷ $\Omega \subseteq \mathbb{R}^2$ is a **truncated square** with side length $\sqrt{2}$.



Dirichlet boundary conditions:

- ▷ Uniaxial, tangent conditions on the long edges ($\mathbf{Q}_b(x, y) \in \mathscr{N}$).
- ▷ 'Artificial' conditions on the short edges ($\mathbf{Q}_b(x, y) \notin \mathscr{N}$).

Reducing to a scalar equation

We look for solutions to the Euler-Lagrange system

$$-\Delta\mathbf{Q} + \frac{\lambda^2}{L}\left(A\mathbf{Q} + B\mathbf{Q}^2 - \frac{B}{3}(\operatorname{tr}\mathbf{Q}^2)\operatorname{Id} - C(\operatorname{tr}\mathbf{Q}^2)\mathbf{Q}\right) = 0 \qquad \text{(EL)}$$

with constant eigenframe

$$\mathbf{n}_1 := \frac{1}{\sqrt{2}}(-1,\, 1,\, 0), \qquad \mathbf{n}_2 := \frac{1}{\sqrt{2}}(1,\, 1,\, 0), \qquad \hat{\mathbf{z}} := (0,\, 0,\, 1).$$

Reducing to a scalar equation

We look for solutions to the Euler-Lagrange system

$$-\Delta\mathbf{Q} + \frac{\lambda^2}{L}\left(A\mathbf{Q} + B\mathbf{Q}^2 - \frac{B}{3}(\operatorname{tr}\mathbf{Q}^2)\,\mathrm{Id} - C(\operatorname{tr}\mathbf{Q}^2)\mathbf{Q}\right) = 0 \qquad \text{(EL)}$$

with constant eigenframe

$$\mathbf{n}_1 := \frac{1}{\sqrt{2}}(-1,\,1,\,0), \qquad \mathbf{n}_2 := \frac{1}{\sqrt{2}}(1,\,1,\,0), \qquad \hat{\mathbf{z}} := (0,\,0,\,1).$$

Lemma

For $A = -B^2/(3C)$ *and an arbitrary* $\lambda > 0$*, a branch of solutions to* (EL) *is given by*

$$\mathbf{Q}(x,y) := q(x,y)(\mathbf{n}_1\otimes\mathbf{n}_1 - \mathbf{n}_2\otimes\mathbf{n}_2) - \frac{B}{6C}(2\hat{\mathbf{z}}\otimes\hat{\mathbf{z}} - \mathbf{n}_1\otimes\mathbf{n}_1 - \mathbf{n}_2\otimes\mathbf{n}_2),$$

where q *is a (classical) solution of*

$$-\Delta q + \frac{\lambda^2}{L}\left(2Cq^3 - \frac{B^2}{2C}q\right) = 0 \quad \text{on } \Omega. \qquad (\mathrm{AC}_\lambda)$$

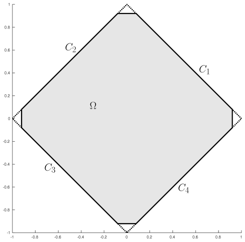
The OR solution corresponds to a critical point of

$$H[q] := \int_\Omega \left\{ |\nabla q|^2 + \frac{\lambda^2}{L} C \left(\frac{B^2}{4C^2} - q^2 \right)^2 \right\}$$

that satisfies the boundary condition

$$q(x, y) = q_{\rm b}(x, y) := \begin{cases} \frac{B}{2C} & \text{on } C_1 \cup C_3 \\ -\frac{B}{2C} & \text{on } C_2 \cup C_4 \\ g(y) & \text{on } S_1 \cup S_3 \\ g(x) & \text{on } S_2 \cup S_4 \end{cases}$$

and $q(x, y) = 0$ if $x = 0$ or $y = 0$.

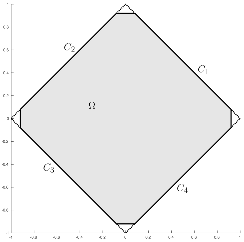


The OR solution corresponds to a critical point of

$$H[q] := \int_\Omega \left\{ |\nabla q|^2 + \frac{\lambda^2}{L} C \left(\frac{B^2}{4C^2} - q^2 \right)^2 \right\}$$

that satisfies the boundary condition

$$q(x, y) = q_{\mathrm{b}}(x, y) := \begin{cases} \dfrac{B}{2C} & \text{on } C_1 \cup C_3 \\ -\dfrac{B}{2C} & \text{on } C_2 \cup C_4 \\ g(y) & \text{on } S_1 \cup S_3 \\ g(x) & \text{on } S_2 \cup S_4 \end{cases}$$



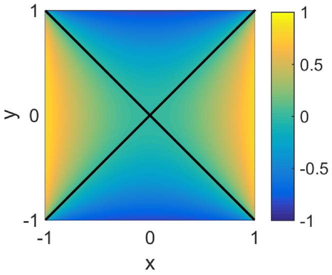
and $q(x, y) = 0$ if $x = 0$ or $y = 0$.

The datum $g\colon [-\varepsilon, \varepsilon] \to \mathbb{R}$ is chosen in such a way that

$$-g'' + \frac{\lambda^2}{L}\left(2Cg^3 - \frac{B^2}{2C} g\right) \geq 0 \quad \text{on } (0, \varepsilon), \qquad g(0) = 0, \quad g(\varepsilon) = \frac{B}{2C}$$

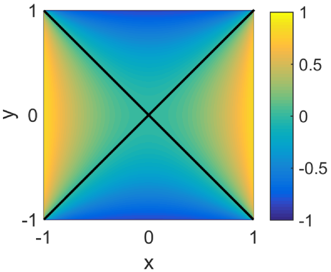
and $g(s) = -g(-s)$ for $s < 0$.

- For $\lambda \ll 1$, there exists a unique critical point of H that satisfies the boundary condition.
- The unique critical point is the global minimiser $q_{\min}$ of H.

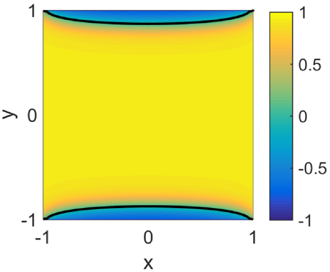


$$\frac{2C\lambda^2}{L} = 0.05$$

- For $\lambda \ll 1$, there exists a unique critical point of H that satisfies the boundary condition.
- The unique critical point is the global minimiser $q_{\min}$ of H.
- As $\lambda \gg 1$, the minimisers $q_{\min}$ develop transitions layers near the boundary.
  - ▷ Asymptotic analysis of minimisers as $\lambda \nearrow +\infty$ **[Modica, Mortola, '77; Sternberg, '88; Fonseca, Tartar, '89; ...]**



$$\frac{2C\lambda^2}{L} = 0.05$$



$$\frac{2C\lambda^2}{L} = 200$$

The saddle solution to Allen Cahn

A solution $q_{s,\lambda}$ to (AC_λ) that satisfies $q_{s,\lambda}(x, y) = 0$ if $xy = 0$ exists for any $\lambda > 0$.

- Analysis on $\mathbb{R}^2$ **[Dang, Fife, Peletier, '92; Schatzman, '95. . .]**

The saddle solution to Allen Cahn

A solution $q_{s,\lambda}$ to (AC_λ) that satisfies $q_{s,\lambda}(x, y) = 0$ if $xy = 0$ exists for any $\lambda > 0$.

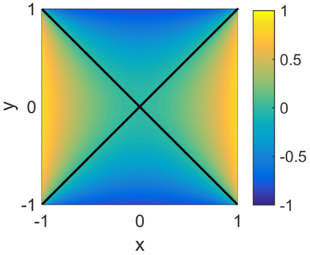
- Analysis on $\mathbb{R}^2$ **[Dang, Fife, Peletier, '92; Schatzman, '95. . .]**
- **Existence**: solve (AC_λ) on $Q := \Omega \cap (0, +\infty)^2$ with B.C.

  $$q(x, y) = 0 \quad \text{if } x = 0 \text{ or } y = 0,$$

  then extend $q_{s,\lambda}$ by odd reflection.
- **Uniqueness** as in **[Dang, Fife, Peletier, '92]**.
- **Sign of derivatives**:

  $$\frac{\partial q_{s,\lambda}}{\partial x} > 0, \quad \frac{\partial q_{s,\lambda}}{\partial y} > 0 \qquad \text{on } Q$$

  (based on comparison principle).



Stability of the saddle solution

Is $q_{s,\lambda}$ stable, i.e. is the second variation

$$\delta^2 H[\eta] := \frac{d^2}{dt^2}_{|t=0} H[q_{s,\lambda} + t\eta] = \int_\Omega \left\{ |\nabla\eta|^2 + \frac{\lambda^2}{L}\left(6Cq_{s,\lambda}^2 - \frac{B^2}{2C}\right)\eta^2 \right\}$$

non-negative for any $\eta \in H^1_0(\Omega)$?

- For $\lambda \ll 1$, $q_{s,\lambda}$ is a minimiser, hence is stable.
- For $\lambda \gg 1$, $q_{s,\lambda}$ is *not* stable (**[Schatzman, '95]**: infinite domain, $\lambda = +\infty$).

Stability of the saddle solution

Is $q_{s,\lambda}$ stable, i.e. is the second variation

$$\delta^2 H[\eta] := \frac{d^2}{dt^2}_{|t=0} H[q_{s,\lambda} + t\eta] = \int_\Omega \left\{ |\nabla\eta|^2 + \frac{\lambda^2}{L}\left(6Cq_{s,\lambda}^2 - \frac{B^2}{2C}\right)\eta^2 \right\}$$

non-negative for any $\eta \in H_0^1(\Omega)$?

- For $\lambda \ll 1$, $q_{s,\lambda}$ is a minimiser, hence is stable.
- For $\lambda \gg 1$, $q_{s,\lambda}$ is *not* stable (**[Schatzman, '95]**: infinite domain, $\lambda = +\infty$).

Lemma

Define

$$\mu(\lambda) := \inf_{\substack{\eta \in H_0^1(\Omega) \\ \int_\Omega \eta^2 = 1}} \int_\Omega \left\{ |\nabla\eta|^2 + \frac{\lambda^2}{L}\left(6Cq_{s,\lambda}^2 - \frac{B^2}{2C}\right)\eta^2 \right\}.$$

Then $\mu'(\lambda) < 0$.

A bifurcation result

Let λ_c the unique value of λ s.t. $\mu(\lambda_c) = 0$.

Theorem

A pitchfork bifurcation arises at $\lambda = \lambda_c$, that is, in a neighbourhood of $(\lambda_c, q_{s,\lambda_c})$ the equation (AC_λ) has only two branches of solutions:

$$q = q_{s,\lambda} \quad \textit{or} \quad \begin{cases} \lambda = \lambda(t) \\ q = q_{s,\lambda(t)} + t\eta_{\lambda_c} + O(t^2), \end{cases}$$

where $\eta_{\lambda_c} \not\equiv 0$ is a solution of

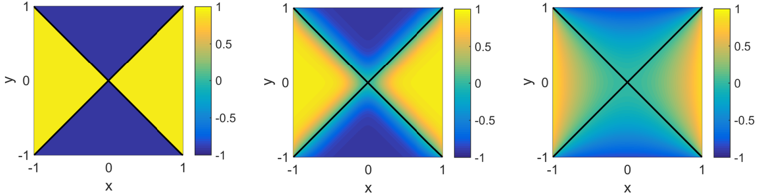
$$-\Delta\eta_{\lambda_c} + \frac{\lambda_c^2}{L}\left(6Cq_{s,\lambda_c}^2 - \frac{B^2}{2C}\right)\eta_{\lambda_c} = 0 \quad \textit{on } \Omega.$$

- ▷ From an abstract bifurcation result **[Crandall, Rabinowitz, '73]**.
- ▷ Relies on $\mu'(\lambda) > 0$, as in **[Lamy, '14]**.

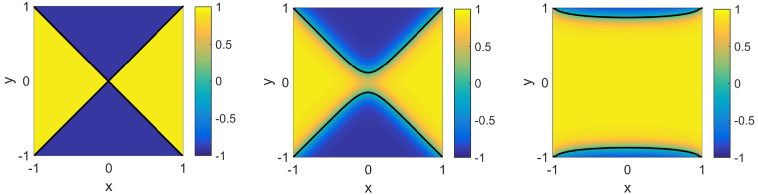
Numerics

Finite-difference approximation of the gradient flow

$$\frac{\partial q}{\partial t} - \Delta q + \frac{\lambda^2}{L}\left(2Cq^3 - \frac{B^2}{2C}q\right) = 0, \qquad t = \frac{20\bar{t}L}{\gamma\lambda^2}.$$

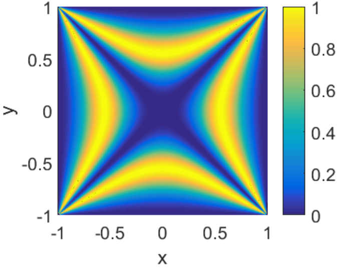


$2C\lambda^2L^{-1} = 0.05$, $t = 0$ | $t = 0.5$ | $t = 2$



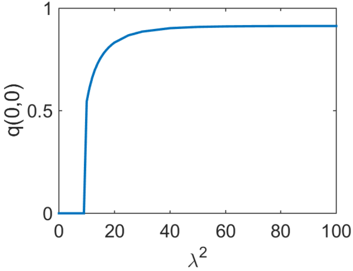
$2C\lambda^2L^{-1} = 200$, $t = 0$ | $t = 0.5$ | $t = 2$

$\beta^2(\mathbf{Q})$



$2C\lambda^2L^{-1} = 0.35 \times 10^{-2}$, $t = 2$

$q(0,\ 0)$ vs. $2C\lambda^2L^{-1}$

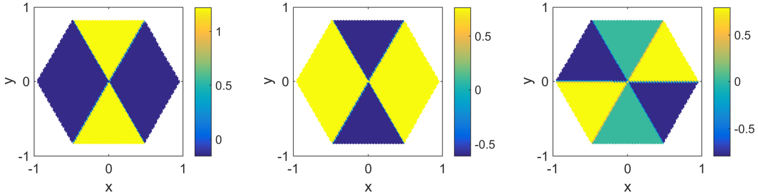


$$\lambda_c^2 \approx \frac{5L}{C}$$

Numerics on an hexagon

Finite-difference approximation of the Landau-de Gennes gradient flow

$$\frac{\partial \mathbf{Q}}{\partial t} - \Delta \mathbf{Q} + \frac{\lambda^2}{L}\left(-\frac{B^2}{3C}\mathbf{Q} + B\mathbf{Q}^2 - \frac{B}{3}(\mathrm{tr}\,\mathbf{Q}^2)\,\mathrm{Id} - C(\mathrm{tr}\,\mathbf{Q}^2)\mathbf{Q}\right) = 0$$



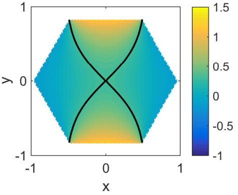
Q_{11} $\qquad$ Q_{22} $\qquad$ $Q_{12} = Q_{22}$

Initial condition:

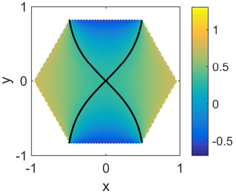
(i) Constant eigenvector $\hat{\mathbf{z}}$

(ii) 6-fold symmetry.

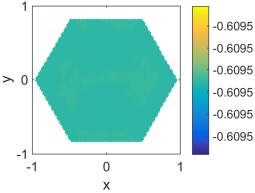
Numerical solution for $2C\lambda^2 L^{-1} = 10^{-6}$, $t = 2$:



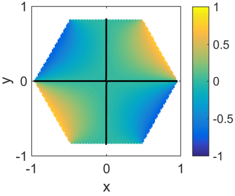
Q_{11}, contours at $B/6C$



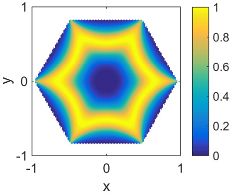
Q_{22}, contours at $B/6C$



$Q_{33} \approx -B/3C$

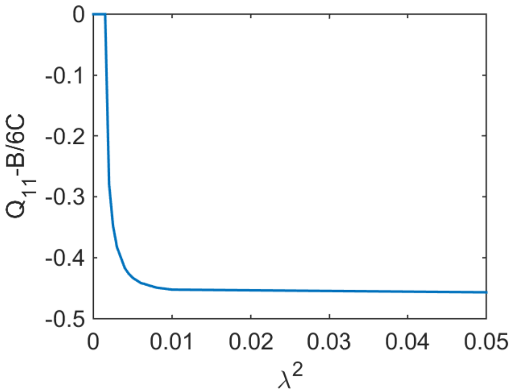


$Q_{12} = Q_{21}$, contours at 0



$\beta(\mathbf{Q})$

$$Q_{11}(0,\,0) - \frac{B}{6C} \text{ vs. } \lambda^2 L^{-1}$$



$$\lambda_c^2 \approx \frac{7L}{C}$$

Conclusions

- A special solution to the Landau-de Gennes system on a square:
  - ▷ constant eigenframe + uniaxial cross along the diagonals.
- Existence and qualitative properties for an arbitrary length size λ.
- Stability analysis:
  - ▷ Global stability for small length side, $\lambda^2 \lesssim L/C$
  - ▷ Instability for large length side, with a pitchfork bifurcation at $\lambda = \lambda_c$.
- Numerics on a square and an hexagon
- Stabilisation?