Nematic Order Reconstruction Solutions for Square Wells in the Landau-de Gennes theory

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A bit about myself…

- 2002 – 2006

Ph.D. in Applied Mathematics, University of Bristol

CASE studentship with Hewlett Packard Laboratories
Title: Liquid crystals and tangent unit-vector fields in polyhedral geometries

Jonathan Robbins, Maxim Zyskin; Chris Newton (HP)

- 2006 – 2012: University of Oxford

Oxford Centre for Nonlinear Partial Differential Equations

Oxford Centre for Collaborative Applied Mathematics

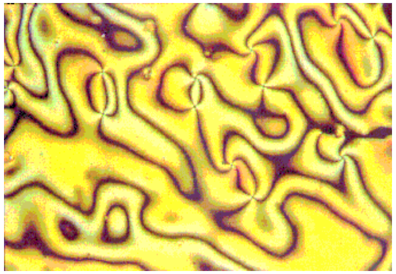
Keble College, University of Oxford

- 2012 – present: University of Bath, United Kingdom

(Visiting) affiliation with OCIAM (Mathematical Institute, University of Oxford)
And Advanced Studies Centre

Research themes

• Foundational aspects of continuum liquid crystal theories
e.g. Oseen-Frank theory, Landau-de Gennes theory



• theory of defects/singularities

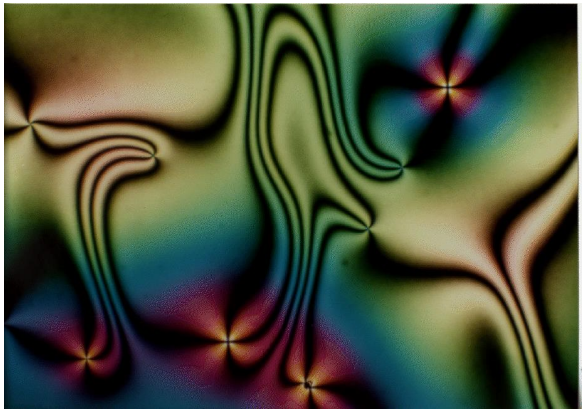
• analogies with other variational theories in materials science e.g. Ginzburg-Landau theory of superconductivity

A.Majumdar, A.Pisante & D.Henao 2014 Uniaxial versus Biaxial Character of Nematic Equilibria. http://arxiv.org/abs/1312.3358

D. Henao & A.Majumdar 2012 Symmetry of uniaxial global Landau-de Gennes minimizers in the theory of nematic liquid crystals. SIAM Journal on Mathematical Analysis 44-5, 3217-3241.

A.Majumdar & A.Zarnescu, 2010 The Landau-de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond. Archive of Rational Mechanics and Analysis, 196, 1, 227--280.

A.Majumdar, 2010 Equilibrium order parameters of liquid crystals in the Landau-de Gennes theory.
European Journal of Applied Mathematics,21 , 181-203.

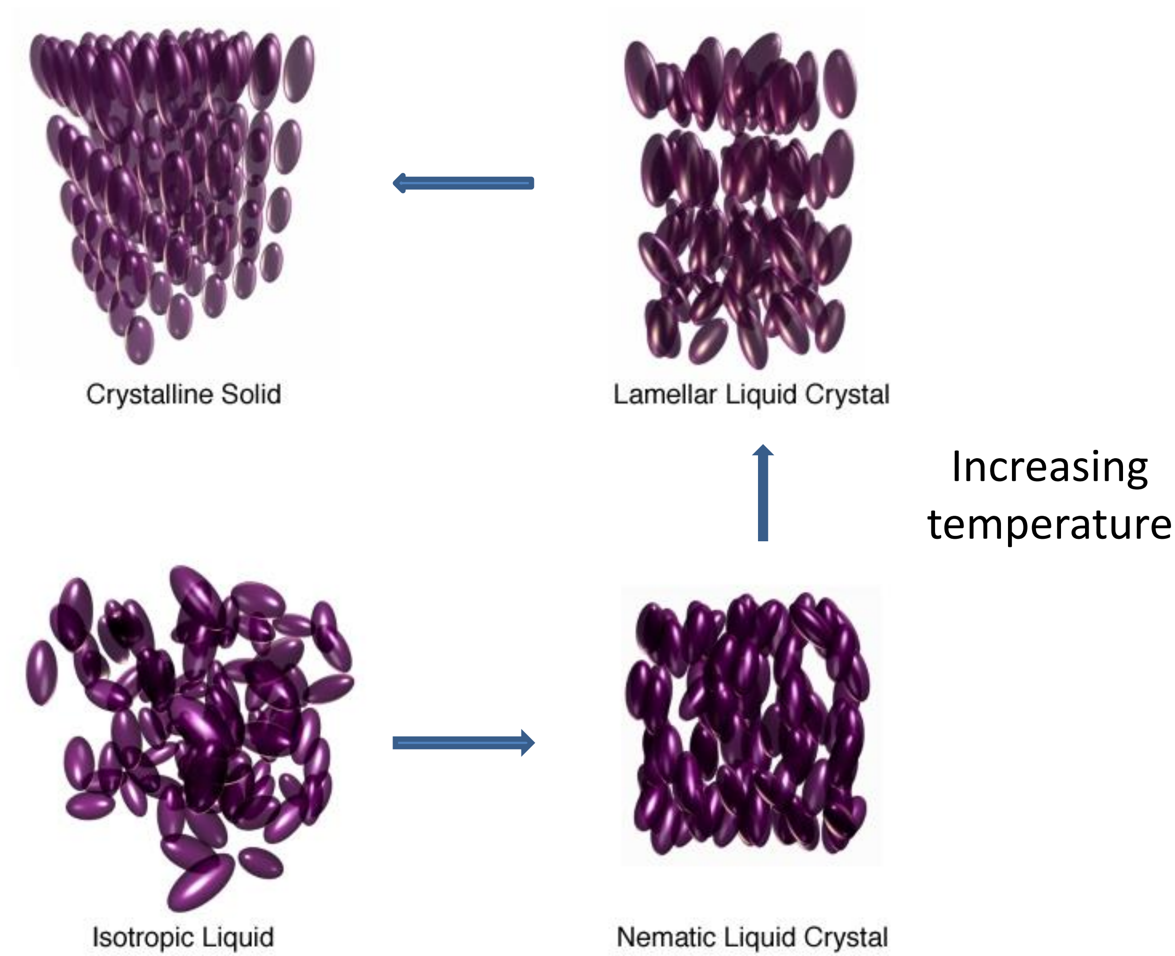


Point defects in liquid crystals.

(www.lci.kent.edu/defect.html)

Liquid Crystals – what are they?

- Mesogenic phases of matter

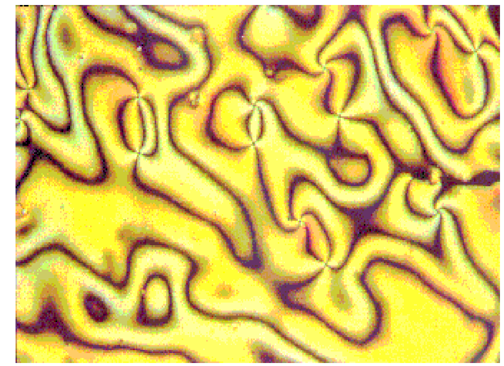


- Intermediate between solids and liquids

Liquid Crystals – what are they?

• `Cloudy liquids' discovered by the biochemist, Friedrich Reinitzer in 1888

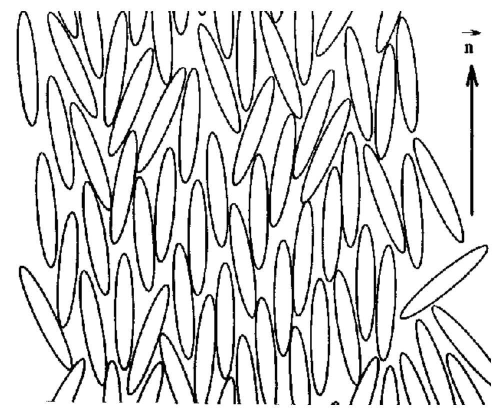
• anisotropic soft matter intermediate between solids and liquids



Nematic Liquid Crystals

- simplest liquid crystalline phase

- anisotropic liquids with special directions



Nematic – Greek word for `thread'

Research themes

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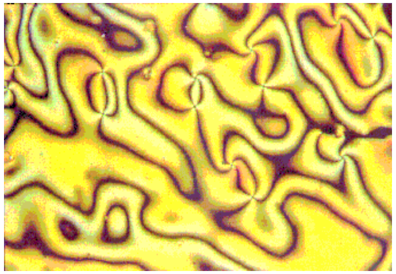
e.g. Oseen-Frank theory, Landau-de Gennes theory



• theory of defects/singularities

• uniaxial/biaxial character of equilibria

• analogies with other variational theories in materials science e.g. Ginzburg-Landau theory of superconductivity

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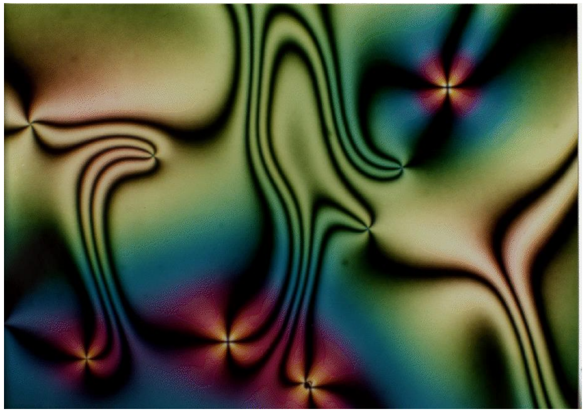

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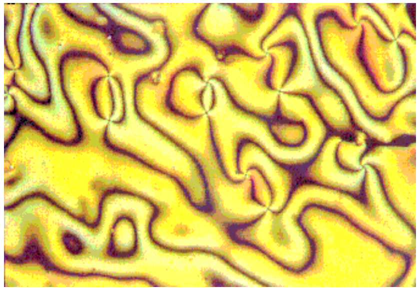
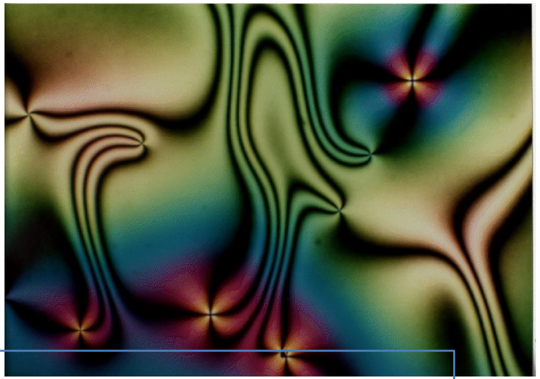
Research themes continued

• Multiscale approaches to liquid crystal modelling



▪ mean-field to continuum : propose a new bulk potential that interpolates between the Maier-Saupe and the Landau-de Gennes theory.

Advantages:
• retain mean-field level of information
• account for spatial inhomogeneities



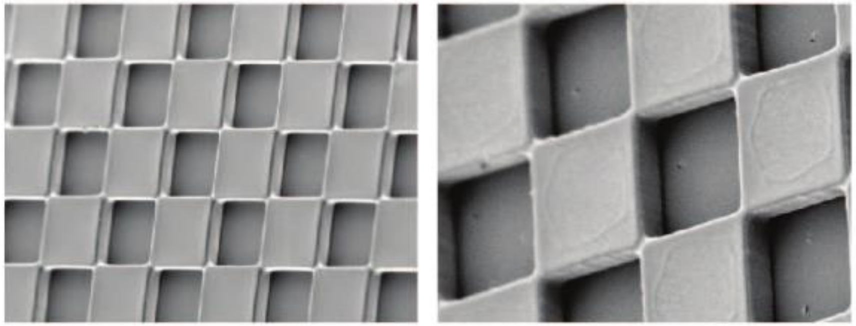
▪ Coupling between lattice-based molecular theories and continuum liquid crystal theories
e.g. Coupling between Lebwohl-Lasher lattice model and Oseen-Frank and Landau-de Gennes theories

See the following paper for a mean-field to continuum analysis:
J.Ball & A.Majumdar, 2010 Nematic liquid crystals : from Maier-Saupe to a continuum theory. Molecular Crystals and Liquid Crystals, 525, 1—11.
Other relevant papers: C.Luo, A.Majumdar & R.Erban 2012 Multistability in planar liquid crystal wells. Physical Review E, 85, Number 6, 061702.
Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Research themes continued

• Modelling of liquid crystal devices manufactured by industry

• Bistable liquid crystal displays
e.g. Planar Bistable Nematic Device
Post Aligned Bistable Nematic Device (Hew Packard)



Tsakonas, Davidson, Brown, Mottram 2007

• Mechanisms that can induce bistability
• stable equilibria
• dynamics/switching mechanisms

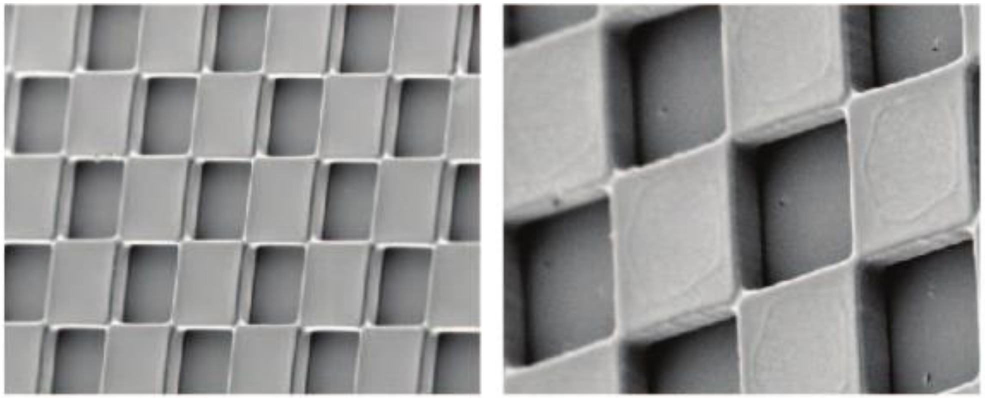
A.Majumdar, C.Newton, J.Robbins, M.Zyskin: Physical Review E, 75, 051703—051714 .

Raisch, A. and Majumdar, A., 2014. Order reconstruction phenomena and temperature-driven dynamics in a 3D zenithally bistable device. *EPL (Europhysics Letters)*, 107 (1), 16002.

Kusumaatmaja, H. and Majumdar, A., 2015. Free energy pathways of a multistable liquid crystal device. *Soft Matter*, 11 (24), pp. 4809-4817.

Majumdar, A., Ockendon, J., Howell, P. and Surovyatkina, E., 2013. Transitions through critical temperatures in nematic liquid crystals. *Physical Review E*, 88 (2), 022501.

From Diagonal and Rotated Solutions to Order Reconstruction Solutions in Nematic Square Wells



Tsakonas, Davidson, Brown, Mottram , Appl. Phys. Lett. 90, 111913 (2007)

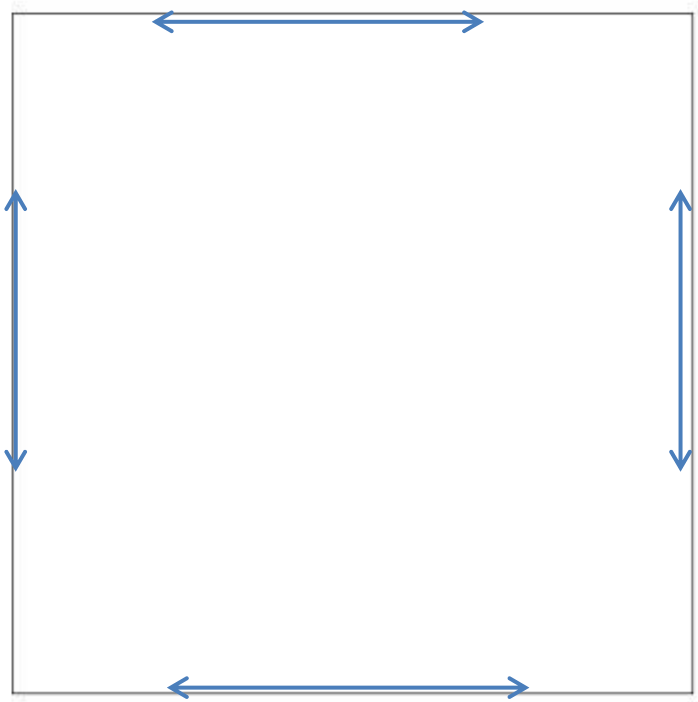
- Micro-confined liquid crystal system:

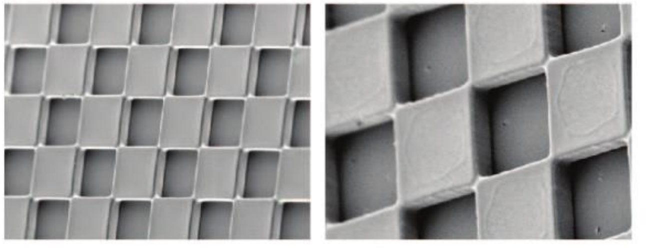
- Array of liquid crystal-filled square / rectangular wells with dimensions between 20×20×12 microns and 80×80×12 microns.

- Surfaces treated to induce planar or tangential anchoring

Boundary Conditions :

• Top and bottom surfaces treated to have tangent boundary conditions – liquid crystal molecules in contact with these surfaces are in the plane of the surfaces.





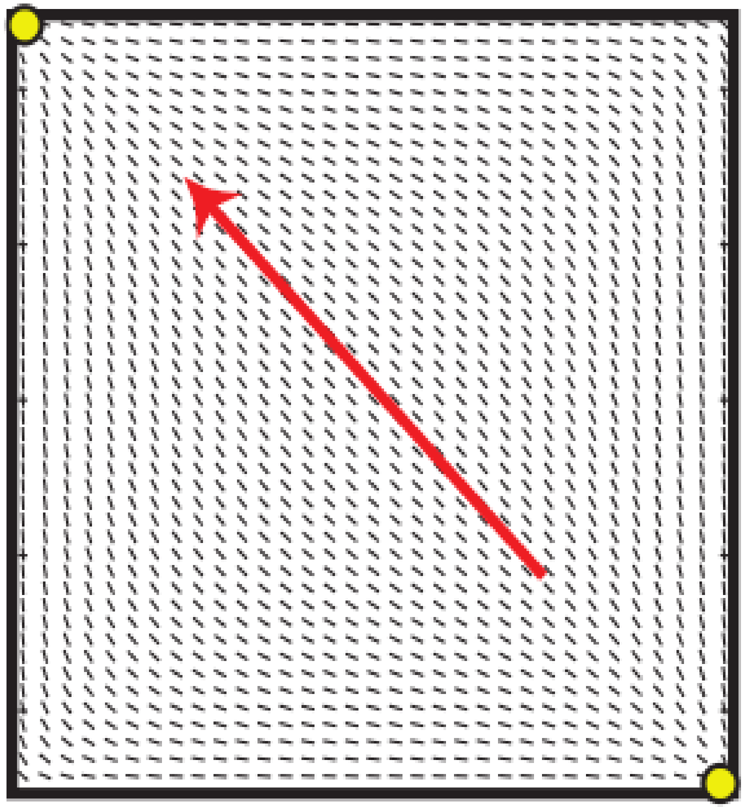
Tsakonas, Davidson, Brown, Mottram 2007

Chong Luo, Apala Majumdar and Radek Erban, 2012 **"Multistability in planar liquid crystal wells",** Physical Review E, Volume 85, Number 6, 061702
Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Bistability: two experimentally observed states

Diagonal state: liquid crystal alignment along one of the diagonals.

Defects pinned along diagonally opposite vertices.

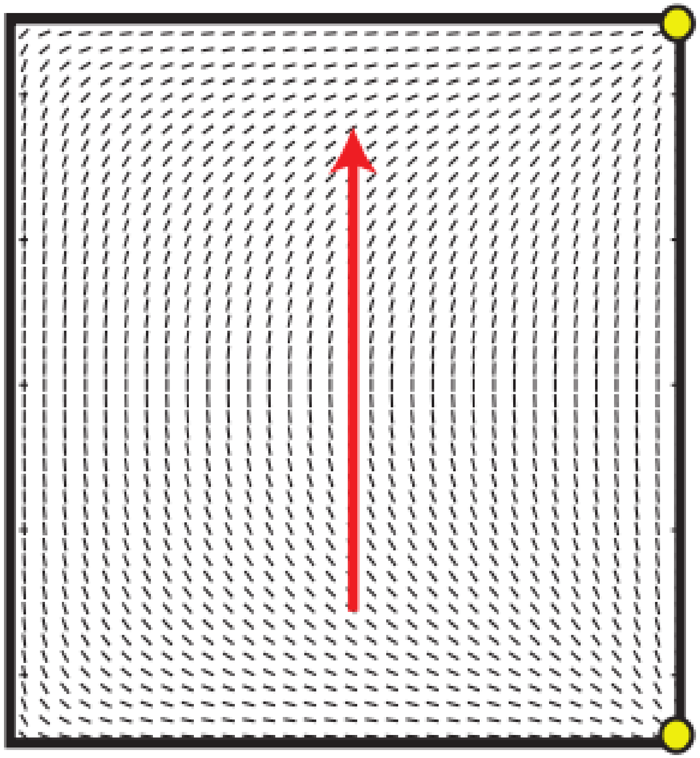


Tsakonas, Davidson, Brown, Mottram 2007

Also see
Lewis, A., Garlea, I., Alvarado, J., Dammone, O., Howell, P., Majumdar, A., Mulder, B., Lettinga, M. P., Koenderink, G. and Aarts, D., 2014. Colloidal liquid crystals in rectangular confinement : Theory and experiment. *Soft Matter*, 39, pp. 7865-7873.

Rotated state: vertical liquid crystal alignment in the interior.

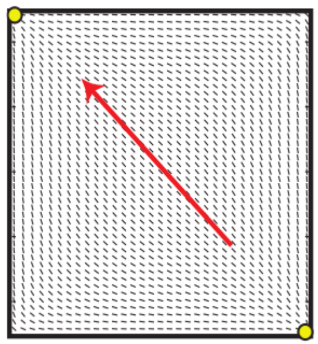
Defects pinned at two vertices along an edge.

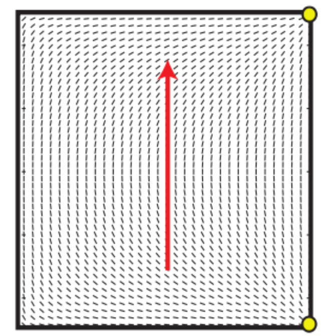


Tsakonas, Davidson, Brown, Mottram 2007

Optical contrast?

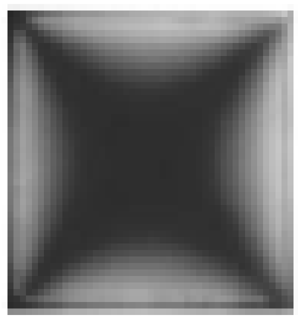
Theoretical and experimental optical textures:

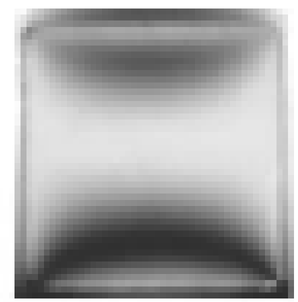




Tsakonas, Davidson, Brown, Mottram 2007

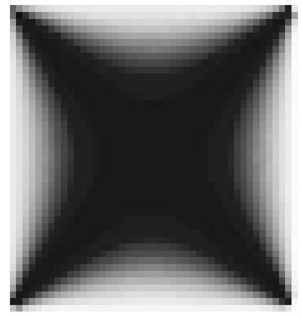
Theory:

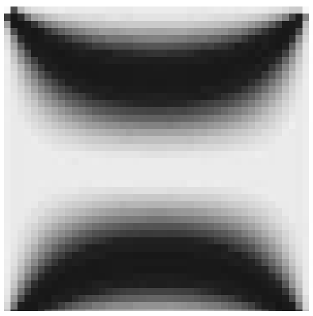




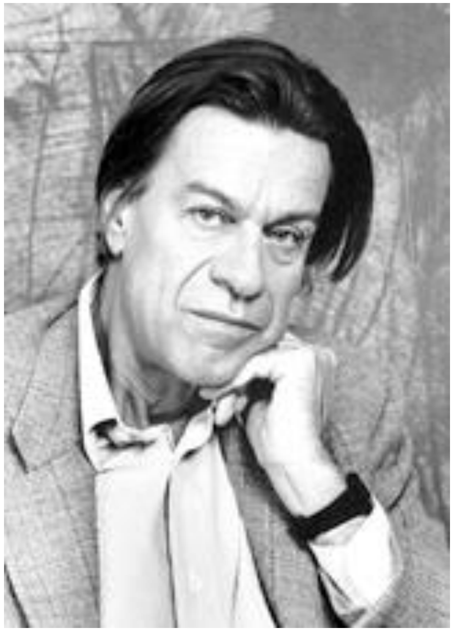
Role of aspect ratios in optical properties? Joint work with Alex Lewis, Peter Howell.

Experiment:





The Landau-de Gennes Theory



The Nobel Prize in Physics in 1991 was awarded to Pierre-Gilles de Gennes for "for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers“.

The Landau-De Gennes Theory

• General continuum theory that can account for all nematic phases and physically observable singularities.

•Define macroscopic order parameter that distinguishes nematic liquid crystals from conventional liquids, in terms of anisotropic macroscopic quantities such as the magnetic susceptibility and dielectric anisotropy.

• The **Q** – tensor order parameter is a symmetric, traceless 3×3 matrix.

$$Q = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{12} & Q_{22} & Q_{23} \\ Q_{13} & Q_{23} & -Q_{11} - Q_{22} \end{pmatrix}$$

- De Gennes' 1991 Nobel prize in Physics

  "for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers"

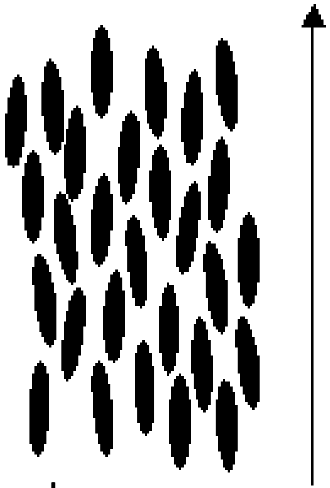
Five degrees of freedom.

The Q-tensor order parameter continued....

- From the spectral decomposition theorem, we can express a symmetric, traceless 3×3 matrix in terms of its eigenvectors and eigenvalues as shown below :

$$Q = \lambda_1 n \otimes n + \lambda_2 m \otimes m + \lambda_3 p \otimes p \qquad \sum_i \lambda_i = 0$$

- The eigenvectors contain information about the locally preferred directions of molecular alignment. The eigenvalues measure the degree of orientational ordering about these preferred directions.



- Classification according to eigenvalue structure of Q-tensor.

- isotropic – triad of zero eigenvalues

$$\lambda_1 = \lambda_2 = \lambda_3 = 0 \qquad \Rightarrow \qquad Q = 0$$

- uniaxial – a pair of equal non-zero eigenvalues; Q has three degrees of freedom

$$\lambda_1 = \lambda_2 = \lambda; \ \lambda_3 = -2\lambda \qquad \Rightarrow \qquad Q = -3\lambda\left(n \otimes n - \frac{1}{3} I\right)$$

- biaxial – three distinct eigenvalues and two locally preferred directions of molecular alignment. The Q-tensor order parameter has five degrees of freedom.

The Landau-de Gennes Energy

The physically observable configurations correspond to minimizers of the Landau-de Gennes liquid crystal energy functional subject to the imposed boundary conditions.

$$I[Q] = \int \frac{f_B(Q)}{L} + w(Q, \nabla Q)\, dV$$

The thermotropic potential : -

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

$$A(T) = \alpha \left(T - T^* \right) \qquad \alpha, b, c, T^* > 0$$

- non-convex , non-negative potential with multiple critical points
- dictates preferred phase of liquid crystal – isotropic/ uniaxial/ biaxial?

The elastic energy density : -

$$w(Q, \nabla Q) = L\, |\nabla Q|^2 = L \sum_{i,j,k=1}^{3} \left(Q_{ij,k} \right)^2$$

- L is a material-dependent elastic constant.

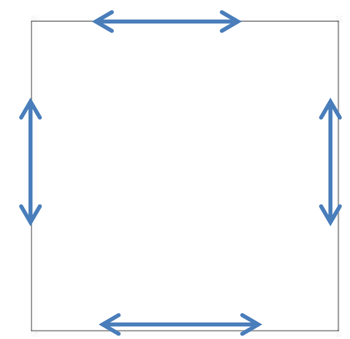
Modelling details

- We look for a particular kind of solution of the form

$$\mathbf{Q} = (q_3+q_1)\vec{e}_x\otimes\vec{e}_x+(q_3-q_1)\vec{e}_y\otimes\vec{e}_y+q_2(\vec{e}_x\otimes\vec{e}_y+\vec{e}_y\otimes\vec{e}_x)-2q_3\vec{e}_z\otimes\vec{e}_z,$$

- planar degenerate boundary conditions on top and bottom surfaces

- planar strong anchoring on lateral surfaces in xz- and yz-planes

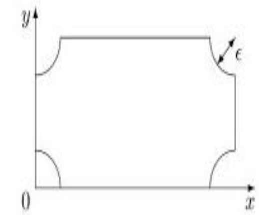


λ

$$\mathbf{Q}_s(0,y,z) = \mathbf{Q}_s(R,y,z) = \frac{S_{eq}}{3}\left(-\vec{e}_x\otimes\vec{e}_x + 2\vec{e}_y\otimes\vec{e}_y - \vec{e}_z\otimes\vec{e}_z\right)$$

$$\mathbf{Q}_s(x,0,z) = \mathbf{Q}_s(x,R,z) = \frac{S_{eq}}{3}\left(2\vec{e}_x\otimes\vec{e}_x - \vec{e}_y\otimes\vec{e}_y - \vec{e}_z\otimes\vec{e}_z\right).$$

$$S_{eq} = \frac{b+\sqrt{b^2-4ac}}{4c}$$



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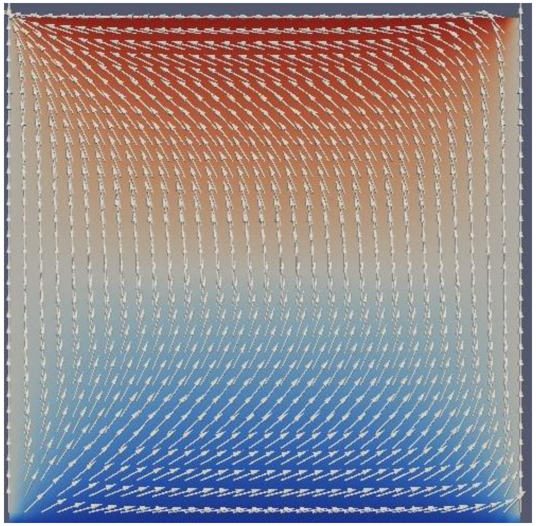
Large micron-sized wells

- Minimize the Landau-de Gennes energy with a surface potential to account for the planar boundary conditions.
- Recover six different stable states – two of the diagonal type and four of the rotated type.
- Stable states are effectively uniaxial everywhere away from the vertical edges, or the vertices of the bottom cross-section.



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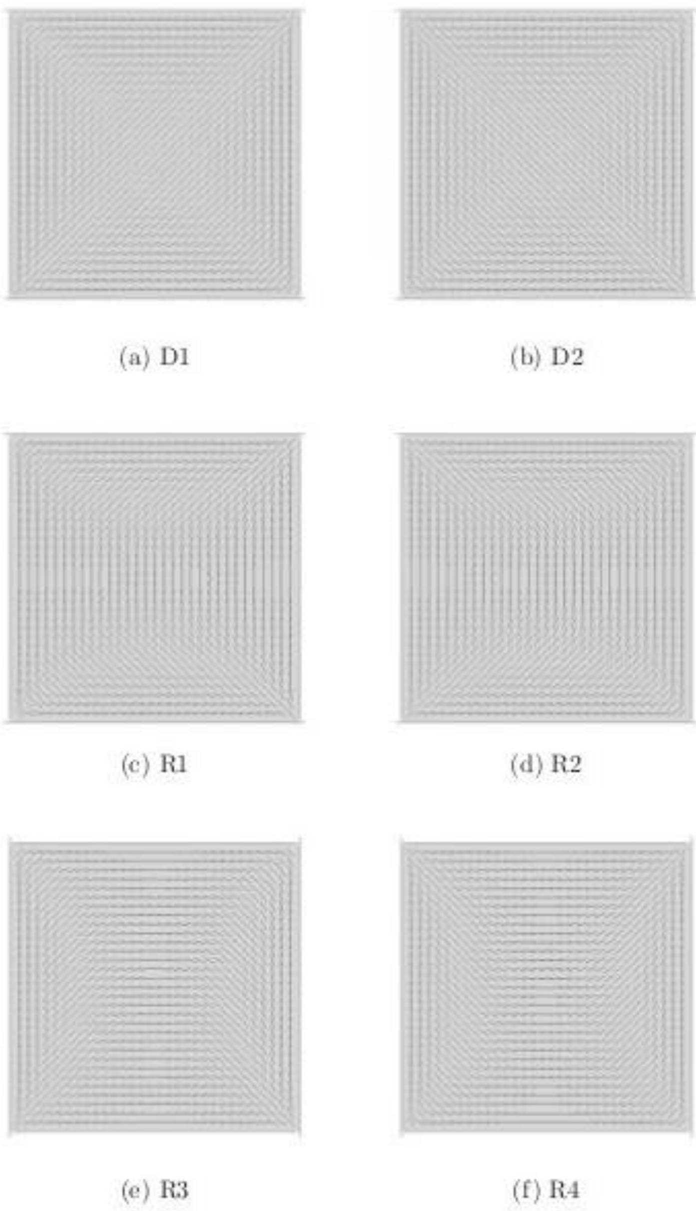
Dirichlet conditions on Lateral Surfaces

We find six different solutions : two diagonal and four rotated solutions.



(a) D1 (b) D2

(c) R1 (d) R2

(e) R3 (f) R4

Chong Luo, Apala Majumdar and Radek Erban, **"Multistability in planar liquid crystal wells",** *Physical Review E,* Volume 85, Number 6, 061702, 15 pages (2012)

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Structural Uniaxial-Biaxial Transitions

- Competition between two length scales: domain cross-sectional length `R' and bare biaxial correlation length, which is typically on the nano-meter scale

$$\xi_b^{(0)} = 2\sqrt{LC}/B$$

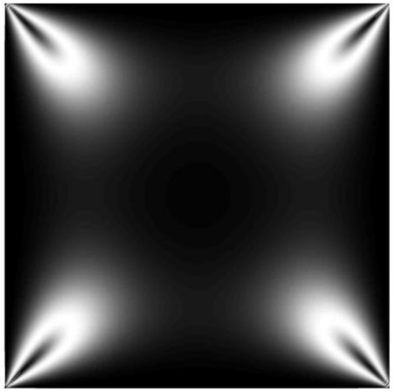
- Introduce ratio

$$\eta = R/\xi_b = \sqrt{\tau}R/\xi_b^{(0)}.$$

- τ : measure of temperature

$$\tau = 1 + \sqrt{(1-t)} \quad t = \frac{T - T_*}{T - T_{**}}$$

- Large η : predominantly uniaxial textures with biaxial rims around square vertices; recover diagonal and rotated solutions



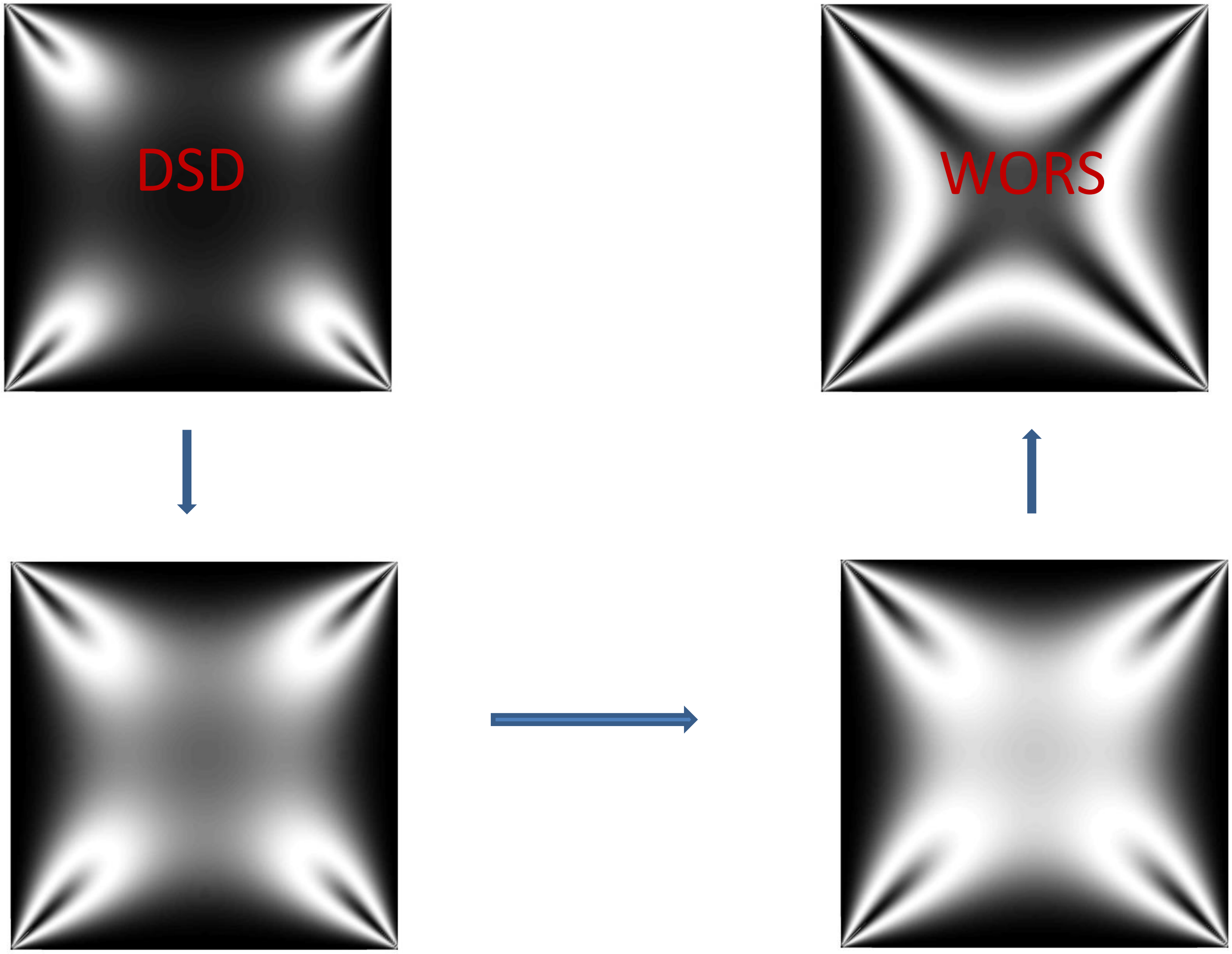
$$\beta^2 = 1 - 6\frac{\left(trQ^3\right)^2}{\left(trQ^2\right)^3}$$

$$0 \le \beta^2 \le 1$$

$$\beta^2 = 0 \Rightarrow uniaxial$$

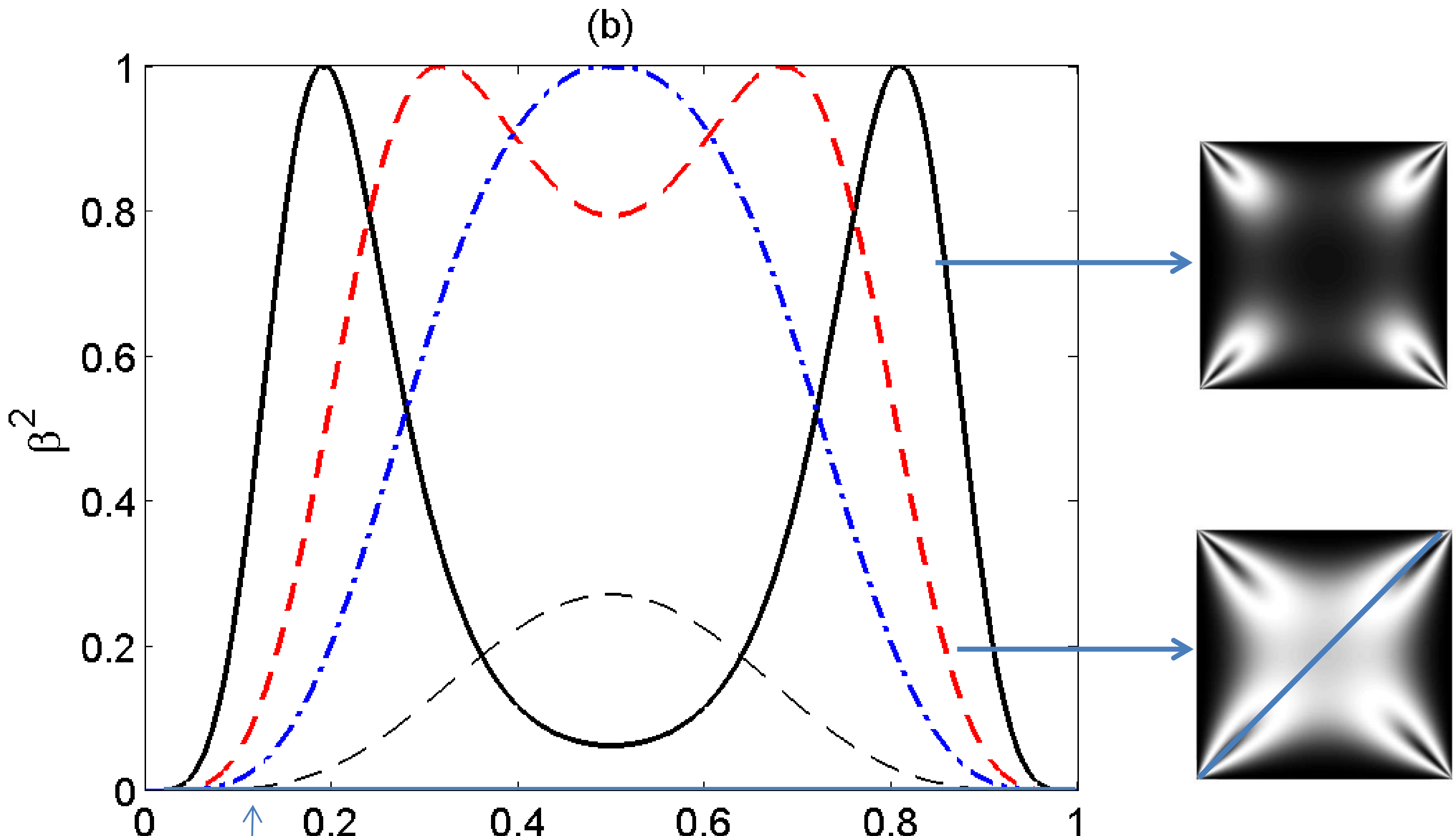
Decrease the ratio η: new structures for sub micron-sized wells

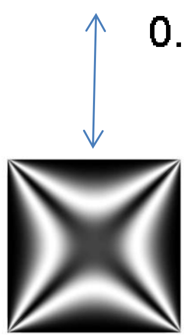
- Well Order Reconstruction Structure (WORS) at critical $\eta \sim 7$



Decrease the ratio η: track biaxiality along square diagonal

- Global order reconstruction phenomenon at critical $\eta \sim 7$





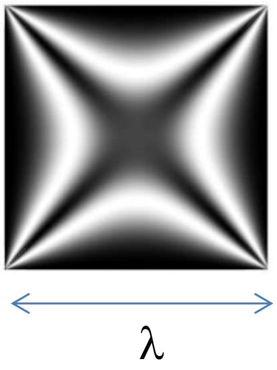
: zero β^2 along square diagonal

Analysis of OR solutions

- Want to construct a smooth critical point of

$$I[Q] = \int \frac{f_B(Q)}{L} + |\nabla Q|^2 \, dV$$

$$f_B(Q) = \frac{A}{2} \mathrm{tr}\, Q^2 - \frac{B}{3} \mathrm{tr}\, Q^3 + \frac{C}{4} \left(\mathrm{tr}\, Q^2 \right)^2 \qquad A < 0$$



- on a square / rectangular domain with tangent conditions on edges

- with constant eigenframe

- uniaxial cross connecting diagonals

$\Rightarrow$ mimic the OR solution!

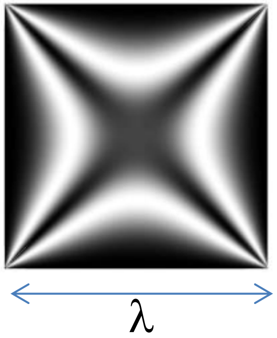
In discussion with Giacomo Canevari, Amy Spicer and Paul Milewski.

Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Analysis of OR solutions

- Look for particular kind of critical points of the Landau de Gennes energy

$$\mathbf{Q} = q_1\left(\hat{\mathbf{x}}_i\hat{\mathbf{x}}_i - \hat{\mathbf{y}}_i\hat{\mathbf{y}}_j\right) + q_2\left(\hat{\mathbf{x}}_i\hat{\mathbf{y}}_j + \hat{\mathbf{y}}_i\hat{\mathbf{x}}_j\right) + q_3\left(2\hat{\mathbf{z}}_i\hat{\mathbf{z}}_j - \hat{\mathbf{x}}_i\hat{\mathbf{x}}_j - \hat{\mathbf{y}}_i\hat{\mathbf{y}}_j\right)$$



- prove existence from variational arguments

$$\frac{L}{\lambda^2}\Delta q_1 = Aq_1 + 2Bq_1q_3 + C\left(2q_1^2 + 2q_2^2 + 6q_3^2\right)q_1$$
$$\frac{L}{\lambda^2}\Delta q_2 = Aq_2 + 2Bq_2q_3 + C\left(2q_1^2 + 2q_2^2 + 6q_3^2\right)q_2$$
$$\frac{L}{\lambda^2}\Delta q_3 = Aq_3 + B\left(\frac{1}{3}\left(q_1^2 + q_2^2\right) - q_3^2\right) + C\left(2q_1^2 + 2q_2^2 + 6q_3^2\right)q_3.$$

In discussion with Giacomo Canevari, Amy Spicer and Paul Milewski.

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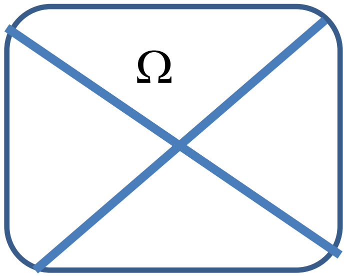
A Special Temperature

$$A = -\frac{B^2}{3C} < 0$$



- Existence of solution branch with

$$q_2 = 0; \quad q_3 = -\frac{B}{6C}$$

$$Q = q\left(e_x \otimes e_x - e_y \otimes e_y\right) - \frac{B}{6C}\left(2e_z \otimes e_z - e_x \otimes e_x - e_y \otimes e_y\right)$$

- The function q(x,y) is a critical point of

$$H[q]: \int_\Omega \frac{1}{\lambda^2}\left|\nabla q\right|^2 + \frac{1}{L}\left(Cq^4 - \frac{B^2}{2C}q^2\right)$$

$$\frac{1}{\lambda^2}\Delta q = \frac{1}{L}\left(2Cq^3 - \frac{B}{2C}q\right)$$

Multiple critical points as λ increases; how do we interpret the order reconstruction solution?

In discussion with Giacomo Canevari, Amy Spicer and Paul Milewski.

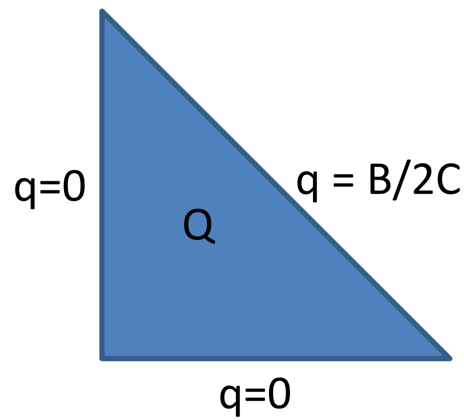
Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Saddle Solutions for the Bistable Diffusion Equation

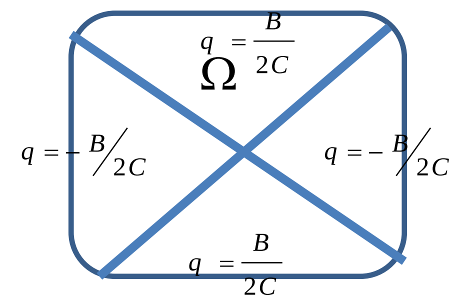
- Minimize the functional

$$q(x,y) \in W^{1,2}(Q)$$

$$H[q] := \int_Q \frac{1}{\lambda^2}|\nabla q|^2 + \frac{1}{L}\left(Cq^4 - \frac{B^2}{2C}q^2\right) dA$$



Need to round the corners and impose free boundary conditions on rounded edges around each corner.



- existence of minimizer , h(x,y), from direct methods in calculus of variations

- extend minimizer to a function on truncated square by odd reflection about the lines x=y and x=-y

- define function

$$q_s(x,y);\ (x,y) \in \Omega$$

$$q_s(x,x) = q_s(x,-x) = 0$$

In discussion with Giacomo Canevari, Amy Spicer and Paul Milewski.

Ha Dang, Paul C. Fife, L. A. Peletier, 1992 Zeitschrift für angewandte Mathematik und Physik ZAMP November 1992, Volume 43, Issue 6, pp 984-998

Saddle Solutions for the Bistable Diffusion Equation

- Minimizer on truncated quadrant

$$H[q\ ] := \int_Q \frac{1}{\lambda^2}|\nabla q|^2 + \frac{1}{L}\left(Cq^4 - \frac{B^2}{2C}q^2\right)$$

- Define

$$Q_{OR} = q_s(e_x \otimes e_x - e_y \otimes e_y) - \frac{B}{6C}(2e_z \otimes e_z - e_x \otimes e_x - e_y \otimes e_y)$$

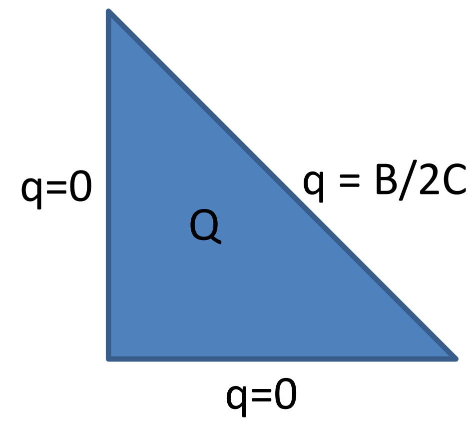
$$\frac{1}{\lambda^2}\Delta q_s = \frac{1}{L}\left(2Cq_s^3 - \frac{B}{2C}q_s\right)$$

- Defines critical point of Landau-de Gennes energy

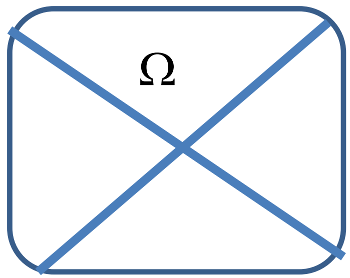
$$\mathrm{I}[\mathrm{Q}] = \int_\Omega \frac{\mathrm{f_B(Q)}}{\mathrm{L}} + |\nabla Q|^2\ \mathrm{dV}$$

at a special temperature $A = -\dfrac{B^2}{3C} < 0$

- Construction can be generalized to all A < 0.



Need to round the corners and impose free boundary conditions on rounded edges around each corner.



Uniaxial Cross

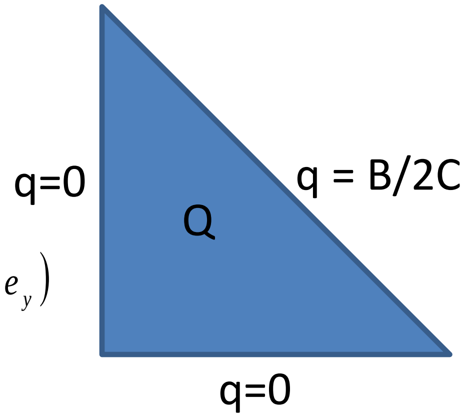
In discussion with Giacomo Canevari, Amy Spicer and Paul Milewski. Ha Dang, Paul C. Fife, L. A. Peletier, 1992 Zeitschrift für angewandte Mathematik und Physik ZAMP November 1992, Volume 43, Issue 6, pp 984-998

Stability of the OR solution

- Look at the scalar problem on truncated square

$$H[q] := \int_{\Omega} \frac{1}{\lambda^2} |\nabla q|^2 + \frac{1}{L}\left(Cq^4 - \frac{B^2}{2C} q^2 \right)$$

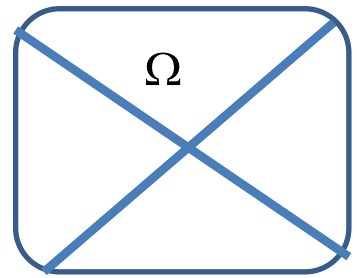
$$Q_{OR} = q_s(x,y)\left(e_x \otimes e_x - e_y \otimes e_y\right) - \frac{B}{6C}\left(2e_z \otimes e_z - e_x \otimes e_x - e_y \otimes e_y\right)$$



- The OR solution is the UNIQUE critical point for

$$\lambda^2 = O\left(\frac{CL}{B^2}\right)$$

Need to round the corners and impose free boundary conditions on rounded edges around each corner.



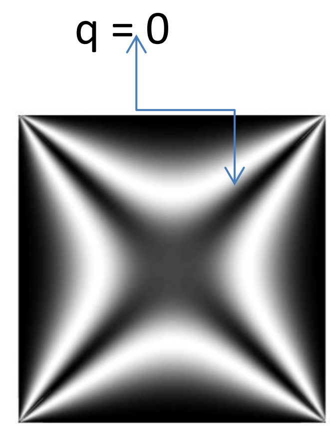
- The OR solution is an UNSTABLE critical point for sufficiently large λ.

⇒ Construct perturbation for which second variation is negative by using key idea from : M.Schatzman, Proceedings of the Royal Society of Edinburgh: Section A Mathematics / Volume 125 / Issue 06 / January 1995, pp 1241-1275

In discussion with Giacomo Canevari, Amy Spicer and Paul Milewski.
Also see Xavier Lamy, *Bifurcation analysis in a frustrated nematic cell*, J. Nonlinear Sci., 2014.

Stability for the scalar problem continued..

What are the qualitative properties of minimizers as $\lambda \to \infty$



$$H[q] := \int_{\Omega} \frac{1}{\lambda^2}|\nabla q|^2 + \frac{1}{L}\left(Cq^4 - \frac{B^2}{2C} q^2 \right)$$

THEOREM 2.7. *Let* $q_{\lambda_j} \in W^{1,2}\left(\tilde{\Omega}\right)$ *be a minimizer of*

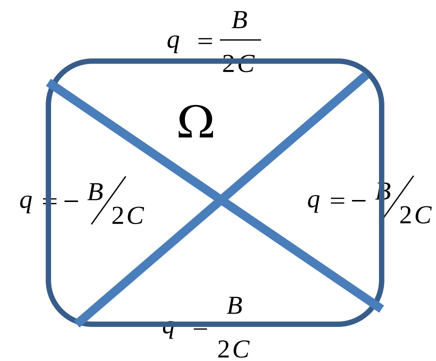
$$J_\lambda[q] := \begin{cases} \int_{\tilde{\Omega}} \frac{1}{\lambda}|\nabla q|^2 + \lambda\left(q^2 - \frac{B^2}{4C^2}\right)^2 d\tilde{x}d\tilde{y} \\ +\infty \ \text{otherwise.} \end{cases} \tag{2.19}$$

Define

$$J_0[h] := \begin{cases} \left(2\int_{-\frac{B}{2C}}^{\frac{B}{2C}} \left(\frac{B^2}{4C^2} - h^2\right) dh\right) Per_{\tilde{\Omega}}\left\{h = -\frac{B}{2C}\right\} \\ +\infty \ \text{otherwise.} \end{cases} \tag{2.20}$$

Suppose $q_{\lambda_j} \to q_0$ *in* $L^1\left(\tilde{\Omega}\right)$ *for some sequence* $\{\lambda_j\}$ *with* $\lambda_j \to \infty$ *as* $j \to \infty$. *Then* q_0 *is a solution of*

$$\inf_{q_0 \in BV\left(\tilde{\Omega}\right); q_0 = \pm\frac{B}{2C}} Per_{\tilde{\Omega}}\left\{q_0 = -\frac{B}{2C}\right\}. \tag{2.21}$$



P. Sternberg, 1988. The effect of a singular perturbation on nonconvex variational problems. ARMA 101, no. 3, 209 – 260.

Some Numerics…

$$0 = \nabla^2 q - \frac{\lambda^2}{L} q \left(q - \frac{B}{2C} \right) \left(q + \frac{B}{2C} \right),$$

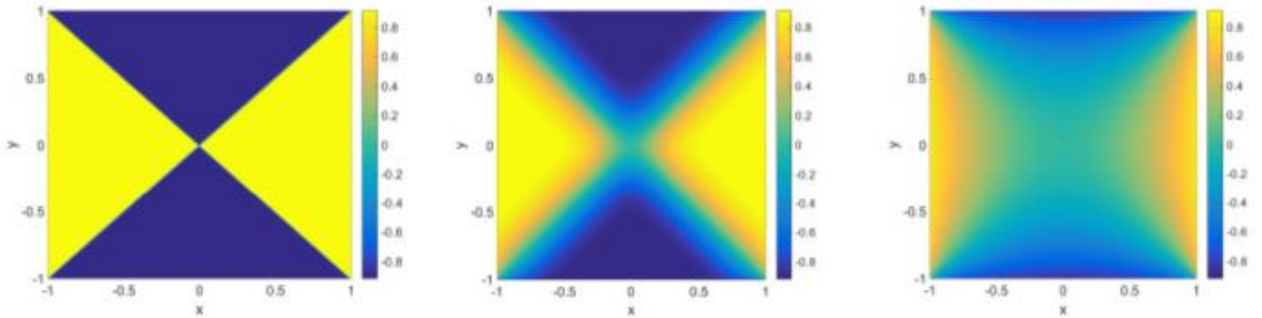
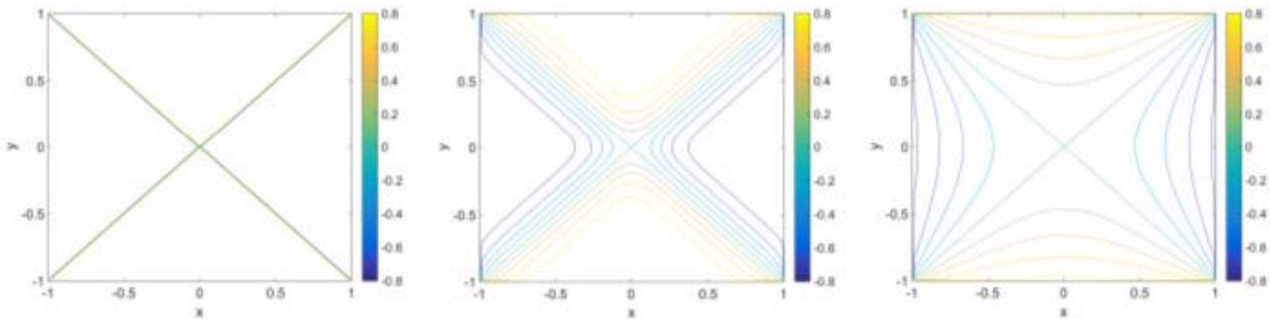


Figure 1: Plot of q for initial condition 1 for $\lambda^2/L = 0.05$ for $t = 0$, $t = 0.01$ and $t = 2$.

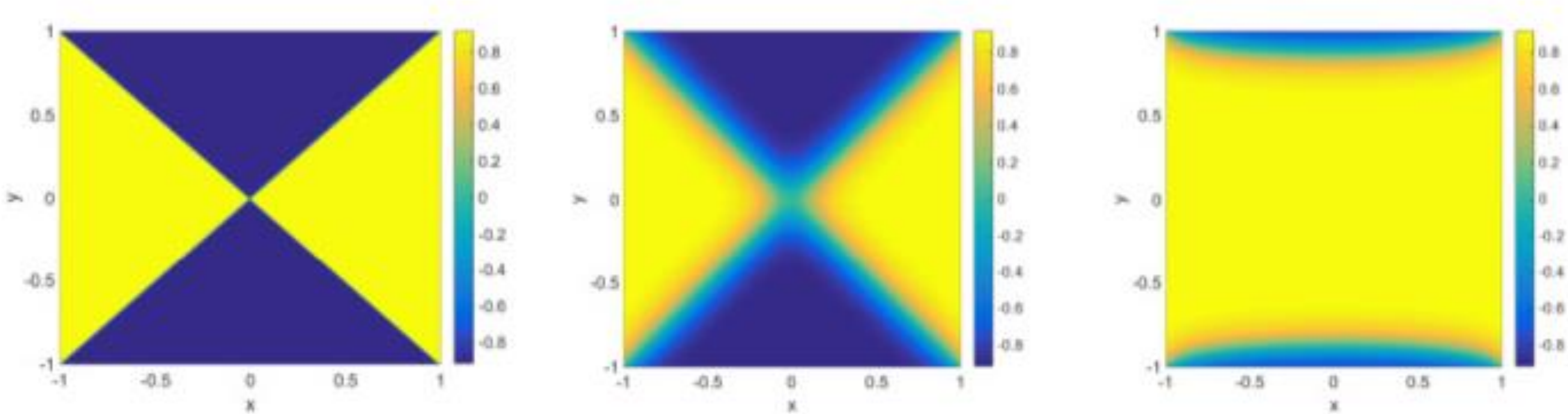


In discussion with Amy Spicer, Paul Milewski and Giacomo Canevari….

Some Numerics…

$$0 = \nabla^2 q - \frac{\lambda^2}{L} q \left(q - \frac{B}{2C}\right)\left(q + \frac{B}{2C}\right),$$

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

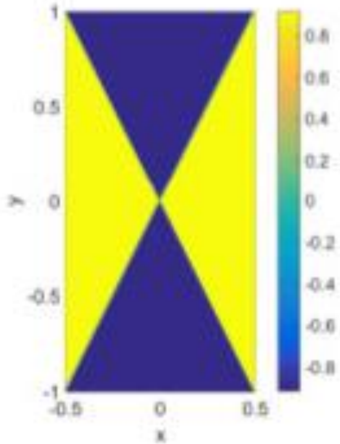


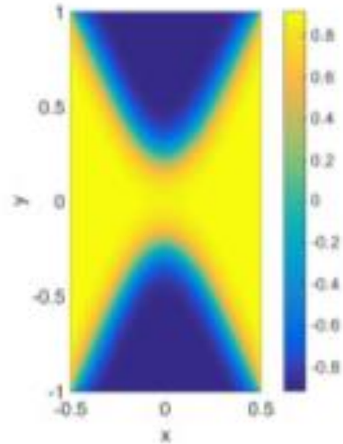
In discussion with Amy Spicer, Paul Milewski and Giacomo Canevari….

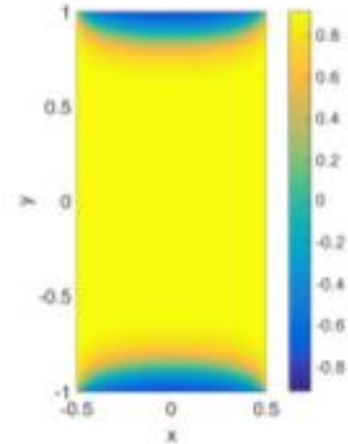
Some Numerics…

$$0 = \nabla^2 q - \frac{\lambda^2}{L} q \left(q - \frac{B}{2C} \right) \left(q + \frac{B}{2C} \right),$$

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





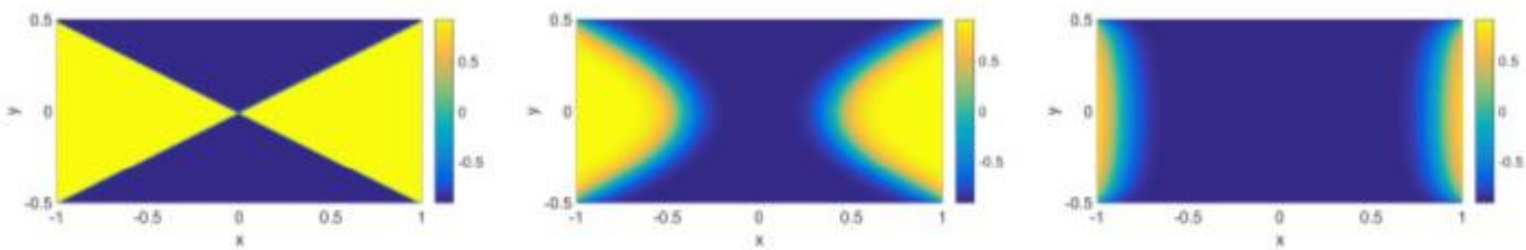


In discussion with Amy Spicer, Paul Milewski and Giacomo Canevari….

Some Numerics…

$$0 = \nabla^2 q - \frac{\lambda^2}{L} q \left(q - \frac{B}{2C}\right)\left(q + \frac{B}{2C}\right),$$

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

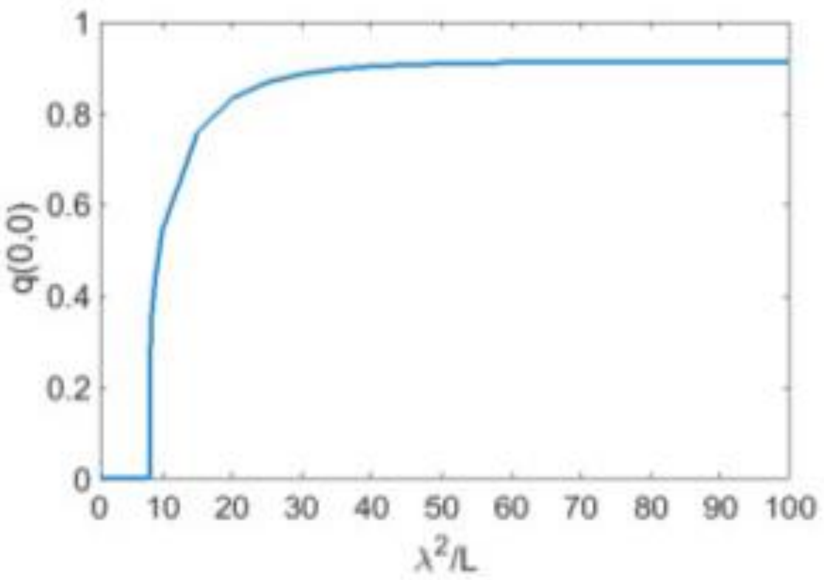


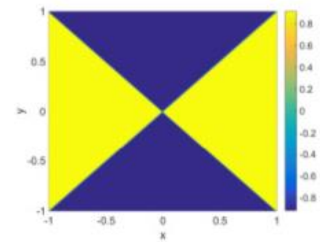
In discussion with Amy Spicer, Paul Milewski and Giacomo Canevari….

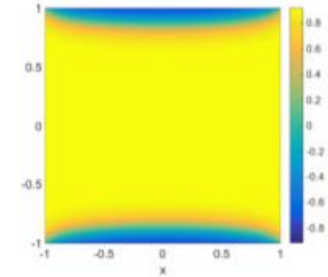
Some Numerics on a Square…

$$0 = \nabla^2 q - \frac{\lambda^2}{L} q \left(q - \frac{B}{2C} \right) \left(q + \frac{B}{2C} \right),$$

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







In discussion with Amy Spicer, Paul Milewski and Giacomo Canevari….

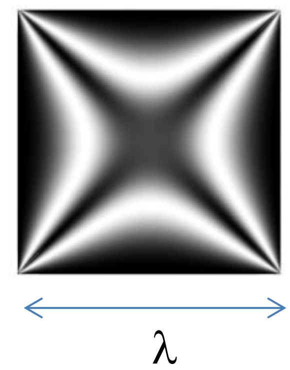
The Landau-de Gennes problem

- The OR solution is a critical point of

$$Q_{OR}(x,y) = q_s(x,y)\left(e_x \otimes e_x - e_y \otimes e_y\right) - \frac{B}{6C}\left(2e_z \otimes e_z - e_x \otimes e_x - e_y \otimes e_y\right)$$

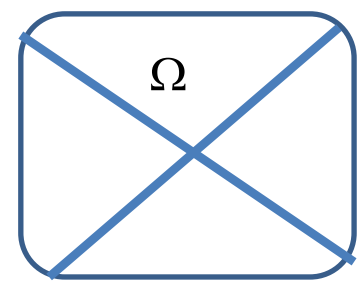
$$\mathrm{I}[\mathrm{Q}] = \int_\Omega \lambda^2 \frac{\mathrm{f_B}(\mathrm{Q})}{\mathrm{L}} + \left|\nabla Q\right|^2 \mathrm{dV}$$

$$\mathrm{f_B}(\mathrm{Q}) = \frac{\mathrm{A}}{2}\mathrm{tr\,Q}^2 - \frac{\mathrm{B}}{3}\mathrm{tr\,Q}^3 + \frac{\mathrm{C}}{4}\left(\mathrm{tr\,Q}^2\right)^2 \qquad A = -\frac{B^2}{3C}$$



- unique critical point for

$$\lambda^2 = O\left(\frac{CL}{B^2}\right)$$



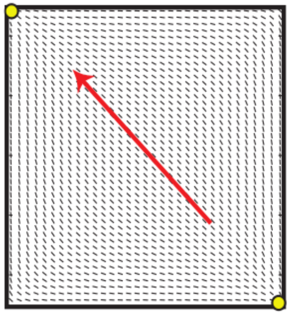
- unstable for large λ: find an explicit perturbation for which the second variation of the LdG energy is negative

$$\delta^2 I[\mathbf{V}] := \int_\Omega \frac{L}{2\lambda^2}\left|\nabla \mathbf{V}\right|^2 + \frac{-B^2}{6C}|\mathbf{V}|^2 + C\left(\mathbf{Q}\cdot\mathbf{V}\right)^2 + \frac{C}{2}|\mathbf{Q}|^2|\mathbf{V}|^2 - B\mathbf{Q}_{ij}\mathbf{V}_{jp}\mathbf{V}_{pi}\, dA.$$

The Landau-de Gennes problem

- Qualitative properties of minimizers of

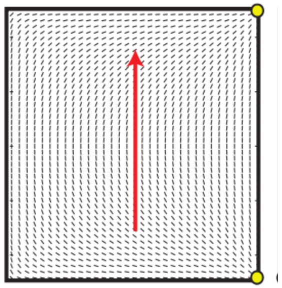
$$I[Q] = \int_\Omega \lambda^2 \frac{f_B(Q)}{L} + |\nabla Q|^2 \, dV$$



$$f_B(Q) = \frac{A}{2}\mathrm{tr}\,Q^2 - \frac{B}{3}\mathrm{tr}\,Q^3 + \frac{C}{4}\left(\mathrm{tr}\,Q^2\right)^2 \qquad A = -\frac{B^2}{3C}$$

as $\lambda \to \infty$; use arguments from Majumdar & Zarnescu 2010 to show that leading order approximation is

$$Q^* = \frac{B}{C}\left(n \otimes n - \frac{I}{3}\right) \qquad n \in W^{1,2}\left(\Omega; S^2\right)$$

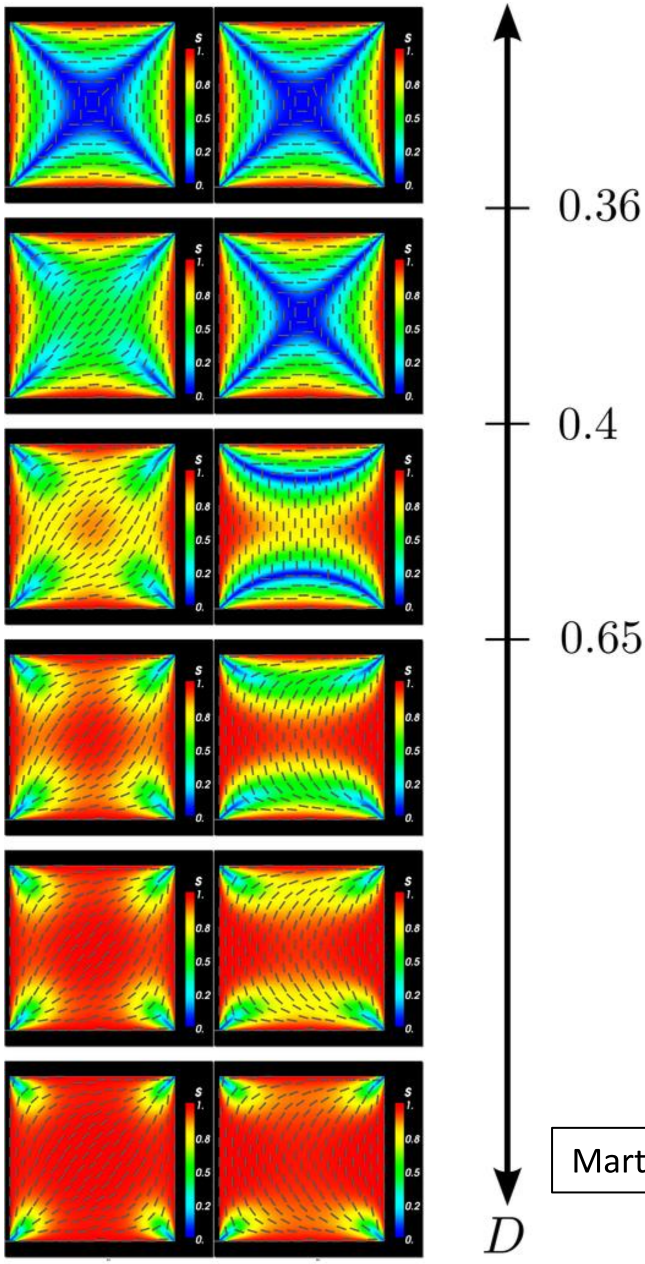


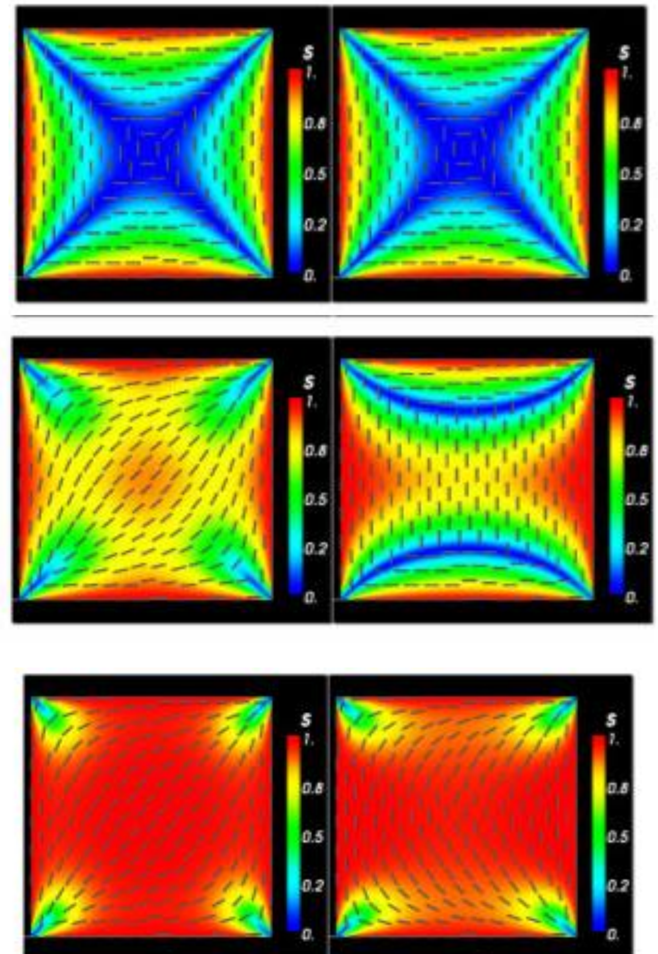
Remark: Leading order approximation is inconsistent with critical points of the form

$$Q = q\left(e_x \otimes e_x - e_y \otimes e_y\right) + q_3\left(2e_z \otimes e_z - e_x \otimes e_x - e_y \otimes e_y\right)$$

unless we have a one-dimensional director profile that does not match Dirichlet conditions.

Some More Numerics…



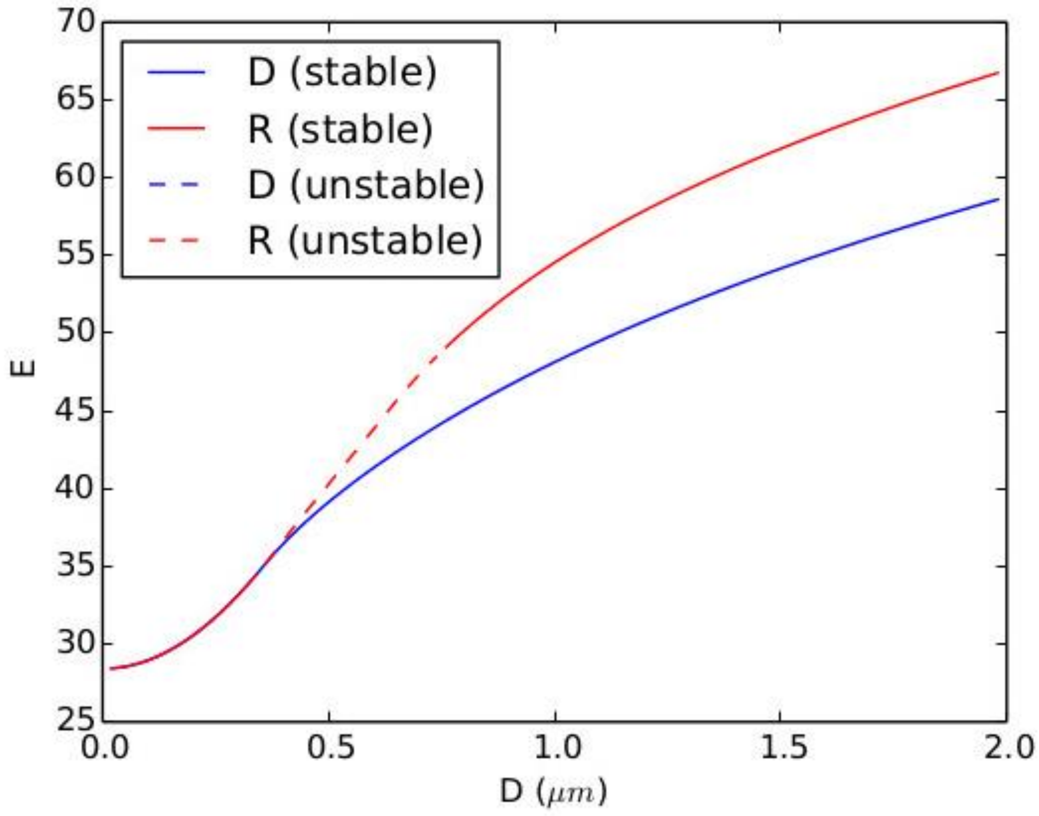


Uniqueness of solutions

R states lose stability

Martin Robinson, Chong Luo, Apala Majumdar, Radek Erban

What happens as we increase the cross-sectional dimension?



Co-authors: Martin Robinson, Chong Luo, Apala Majumdar & Radek Erban

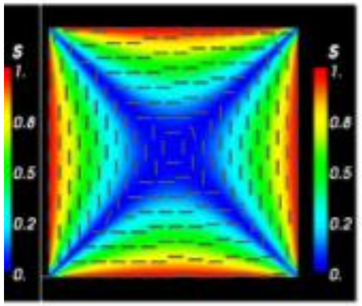
- Diagonal and Rotated solutions converge to unique solution for nano-scale wells $\Rightarrow$ new order reconstruction pattern!
- Rotated solutions only survive above a critical threshold

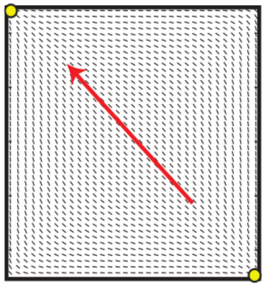
What next?

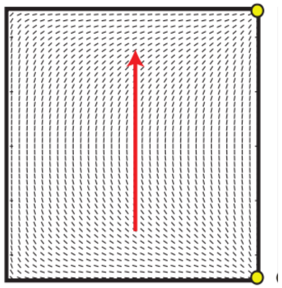
- New OR solution: interpret as a saddle-solution type critical point of the Landau-de Gennes energy

- Experimental/physical relevance?

- Interesting: offers possibility of very distinct optical properties from diagonal and rotated solutions with macroscopic biaxiality.







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