Multistability for Confined Nematic Systems: Analytical and Computational Approaches

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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

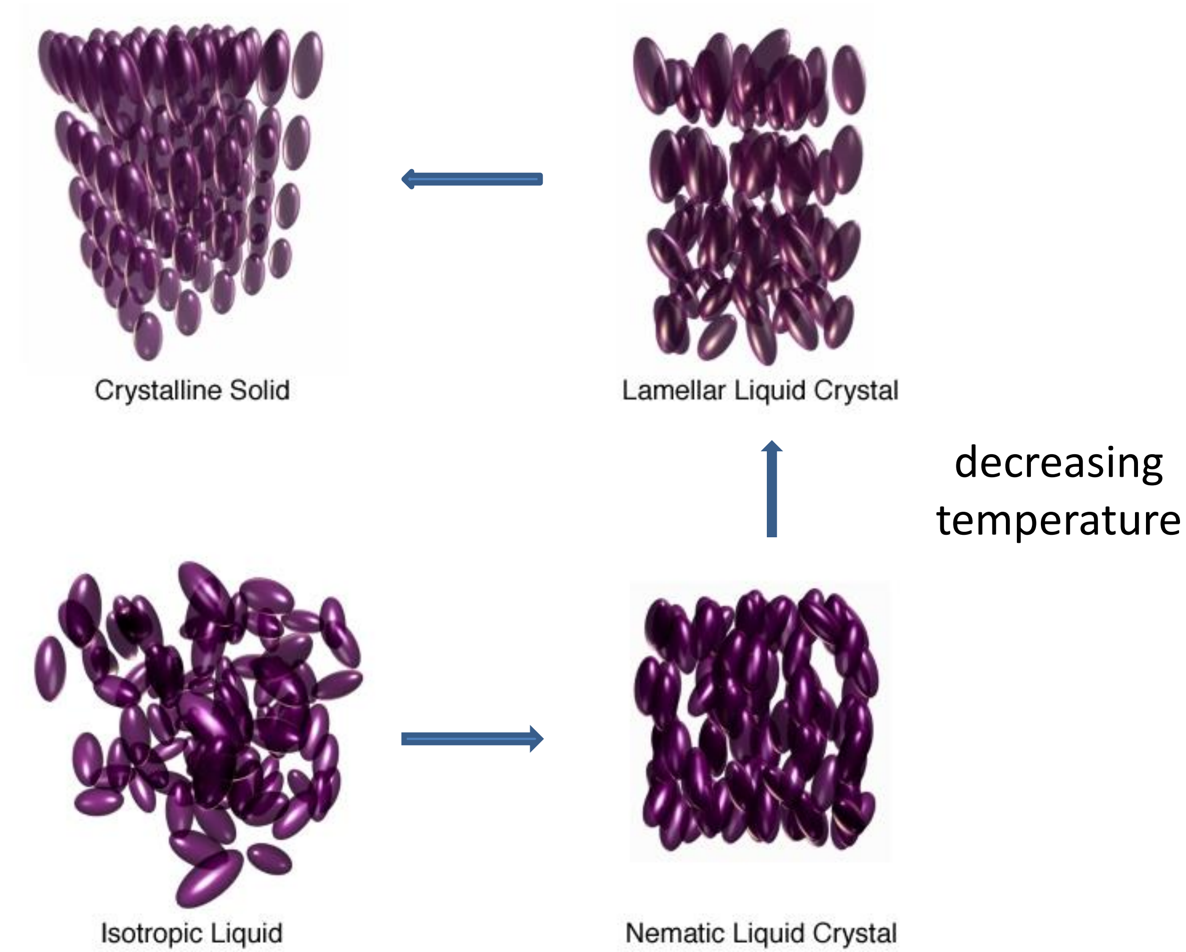
Keble College

- 2012 – 2013 : EPSRC Career Acceleration Fellow, University of Bath

- 2013 – present: Reader in Applied Mathematics, University of Bath

Liquid Crystals – what are they?

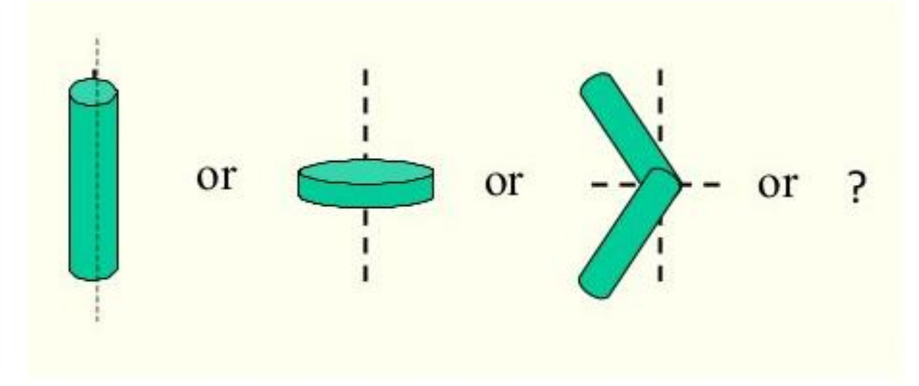
- Mesogenic phases of matter



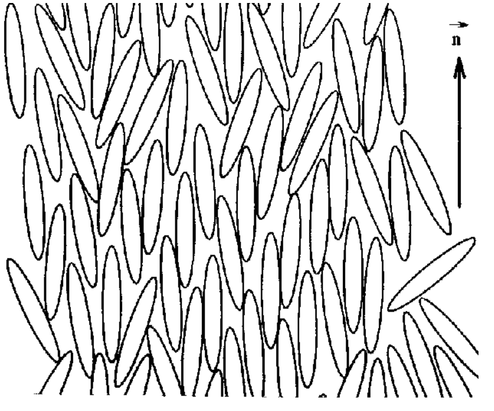
- Intermediate between solids and liquids

Nematic Liquid Crystals

- Anisotropic rod-like molecules with directional properties

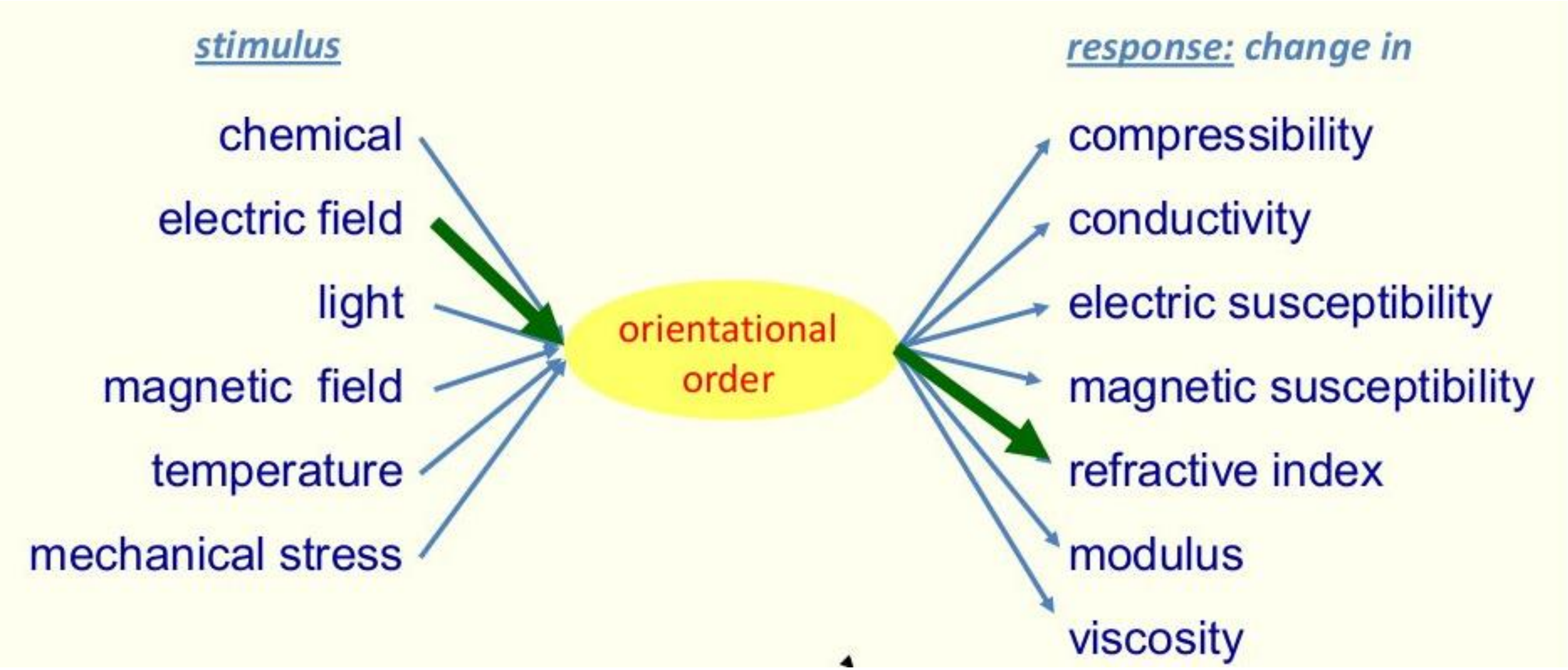


- Long-range orientational ordering: molecules line up with one another



Key word: anisotropy!!!

- Soft materials : responses to external stimuli

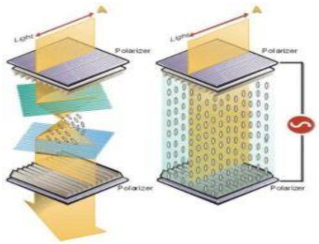


Courtesy: Images from Peter Palffy-Muhoray's lectures at Colorado - Boulder

Questions that interest me…

- The mathematics of

Orientational Order + Susceptibilities + Singularities



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- commonalities in mathematical theories for materials science: nematic liquid crystals, micromagnetics, superconductivity, nonlinear elasticity

↓

- predicting complex spatio-temporal patterns; role of symmetry, temperature and material properties

↓

- understanding the role of molecular-level details in macroscopic phenomena; role of microstructures

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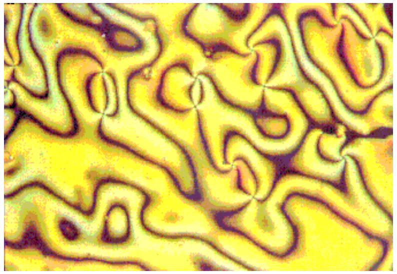
- Applications: multi-billion dollar liquid crystal display industry

Research themes

• Foundational aspects of continuum liquid crystal theories
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

Chen, G. Q., Majumdar, A., Wang, D. and Zhang, R., 2017. Global existence and regularity of solutions for active liquid crystals. *Journal of Differential Equations.* http://dx.doi.org/10.1016/j.jde.2017.02.035

Henao, D., Majumdar, A. & Pisante, A. Calc. Var. (2017) **Uniaxial versus biaxial character of nematic equilibria in three dimensions.** https://doi.org/10.1007/s00526-017-1142-8

G. Canevari, A. Majumdar and A. Spicer, Order Reconstruction for Nematics on Squares and Regular Polygons: A Landau-de Gennes Study, *SIAM J. Appl. Math.*, 77(1), 267–293.

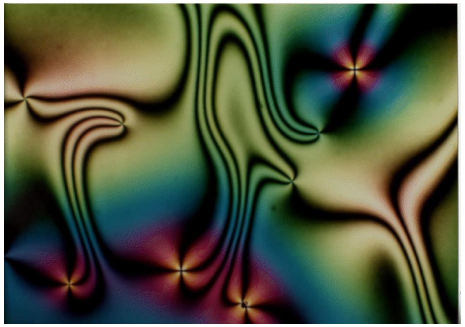
Majumdar, A., Milewski, P. A. and Spicer, A., 2016. Front Propagation at the Nematic-Isotropic Transition Temperature. *SIAM Journal on Applied Mathematics*, 76 (4), pp. 1296-1320.

Canevari, G., Ramaswamy, M. and Majumdar, A., 2016. Radial symmetry on three-dimensional shells in the Landau-de Gennes theory. *Physica D: Nonlinear Phenomena*, 314, pp. 18-34.

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.



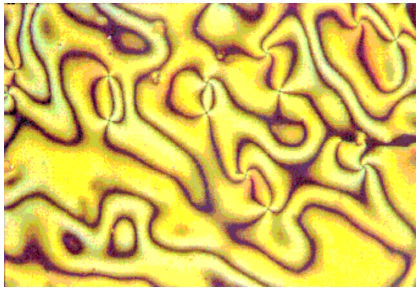
Point defects in liquid crystals.

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

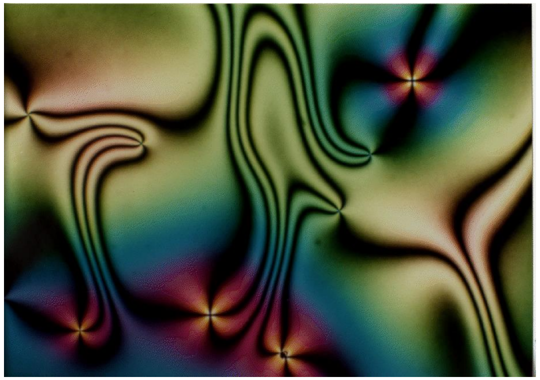
Research themes continued

• 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

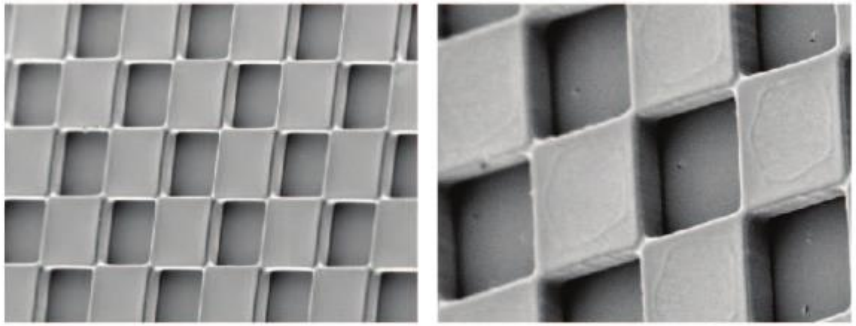
See the following paper for a mean-field to continuum analysis:
J.Ball & A.Majumdar, 2010 Nematic liquid crystals : from Maier-Saupe to a continuum theory. Molecular Crystals and Liquid Crystals, 525, 1—11.
Other relevant papers:
Robinson, M., Luo, C., Farrell, P. E., Erban, R. and Majumdar, A., 2017. From molecular to continuum modelling of bistable liquid crystal devices. *Liquid Crystals*
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 (Hewlett Packard)

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



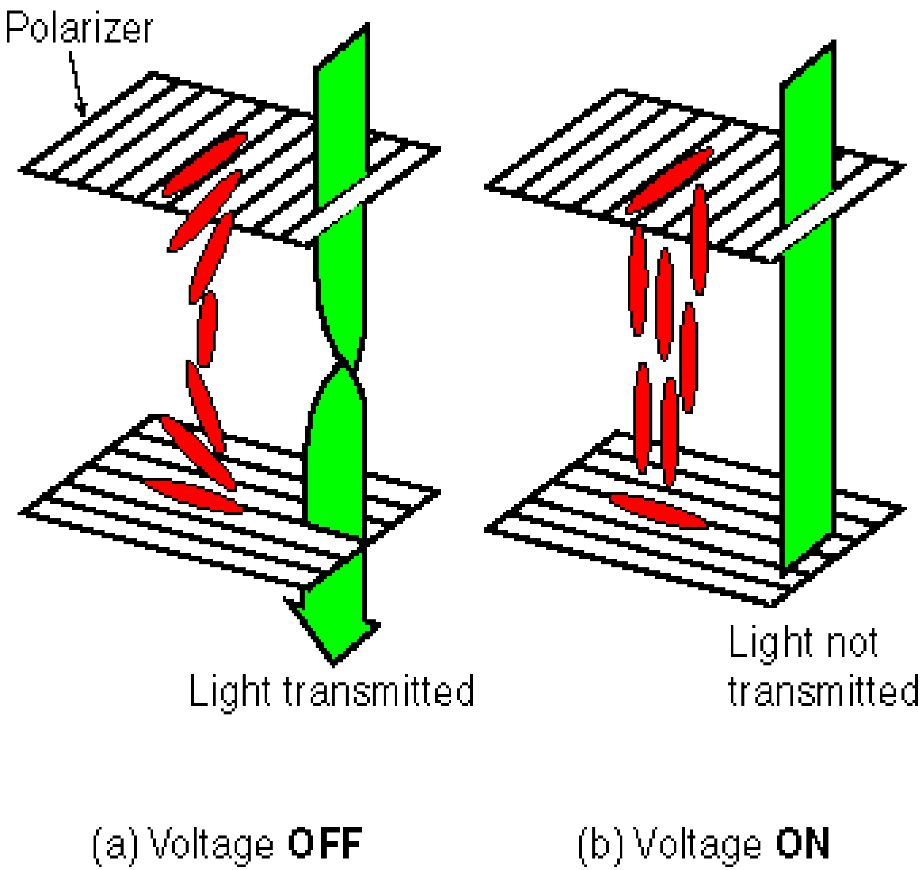
Tsakonas, Davidson, Brown, Mottram 2007

- A.Majumdar, C.Newton, J.Robbins, M.Zyskin 2007 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.
- **Solution landscapes in nematic microfluidics 2017** M. Crespo, A. Majumdar, A. Manuel Ramos & I.M. Griffiths. Physica D, Volumes 351–352, 1 August 2017, Pages 1-13
- Majumdar, A., Ockendon, J., Howell, P. and Surovyatkina, E., 2013. Transitions through critical temperatures in nematic liquid crystals. *Physical Review E*, 88 (2), 022501.

Display Applications

<u>Key properties:-</u>

- Anisotropic birefringent fluids – strong coupling to incident light
- Sensitive to external electric and magnetic fields .

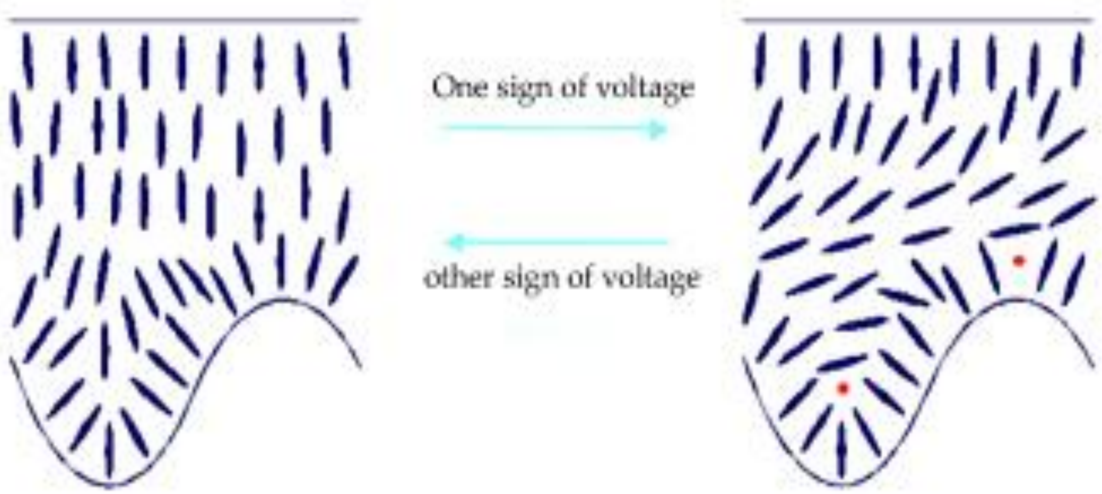


<u>Twisted Nematic Liquid Crystal Display</u> – a monostable liquid crystal display.

Bistable displays

Working principle:

- locally stable bright and dark states without an electric field
- power is needed to switch between distinct states but not to maintain them



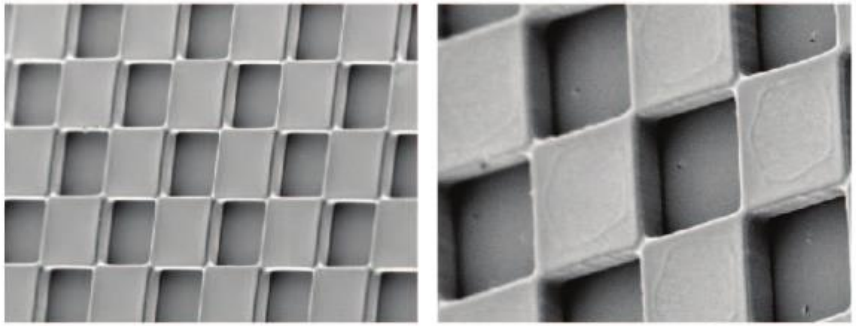
Zenithally Bistable Nematic Device

www.eng.ox.ac.uk

- larger, higher resolution displays with much reduced power consumption.

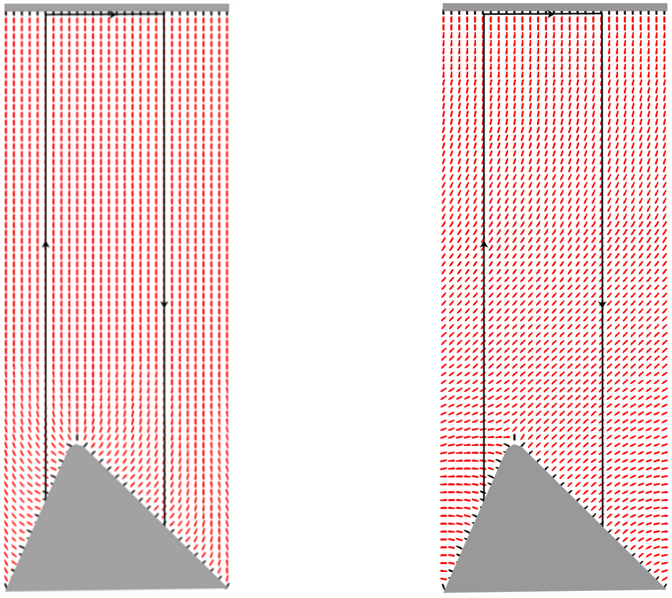
Examples of bistable displays:

• Planar bistable liquid crystal device



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

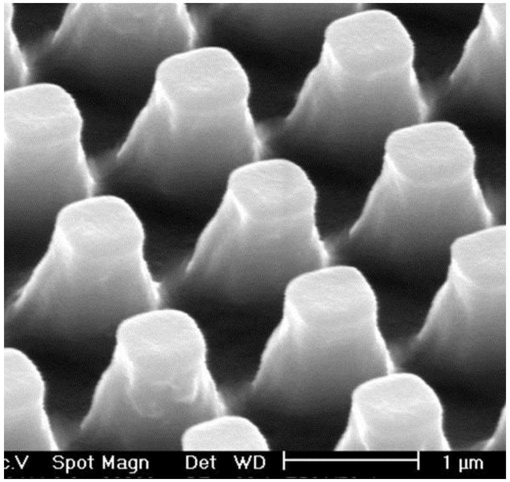
• Zenithally Bistable Nematic Device



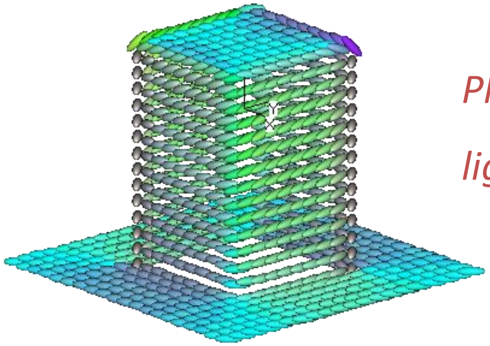
Numerical modelling by Chris Newton, HP

Examples of bistable displays continued:

• Post Aligned Bistable Nematic Device (Hewlett Packard Laboratories)



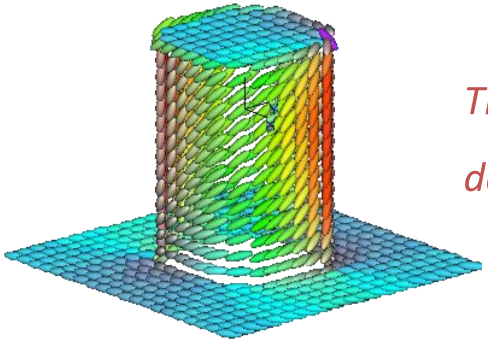
Kitson and Geisow, Applied Physics Letters, 80,2002.



Planar (P)

light

Numerical modelling by Chris Newton



Tilted (T)

dark

What can mathematics do for LC devices:

- **Stable states**

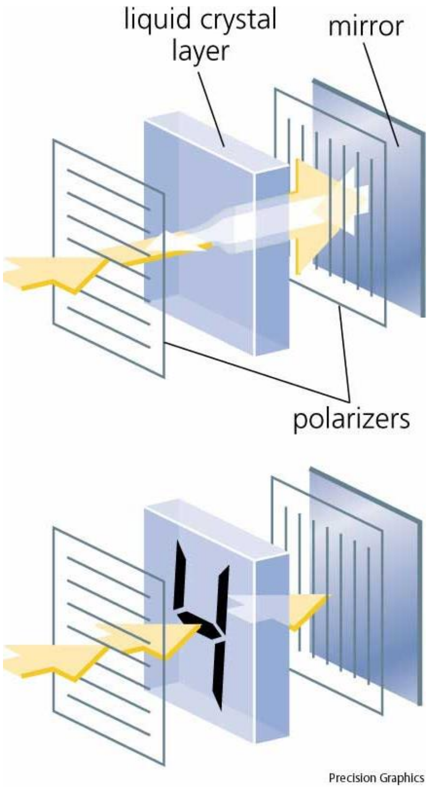
▪ structure
▪ multiplicity
▪ defects

- **Optical properties**?

Inverse problems

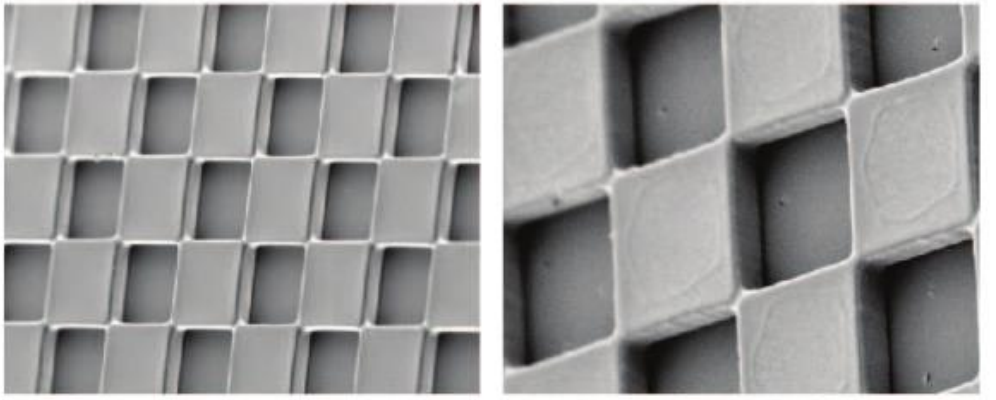
- **Switching mechanisms**

Estimates for switching times – relate to image control and refresh times?



See [1] A.Majumdar, C.J.P.Newton, J.M.Robbins and M.Zyskin, 2007 Topology and bistability in liquid crystal devices. Phys. Rev. E, 75, 051703--051714.
[2] 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.
[3] 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.

Another Example: The Planar Bistable LC Device



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

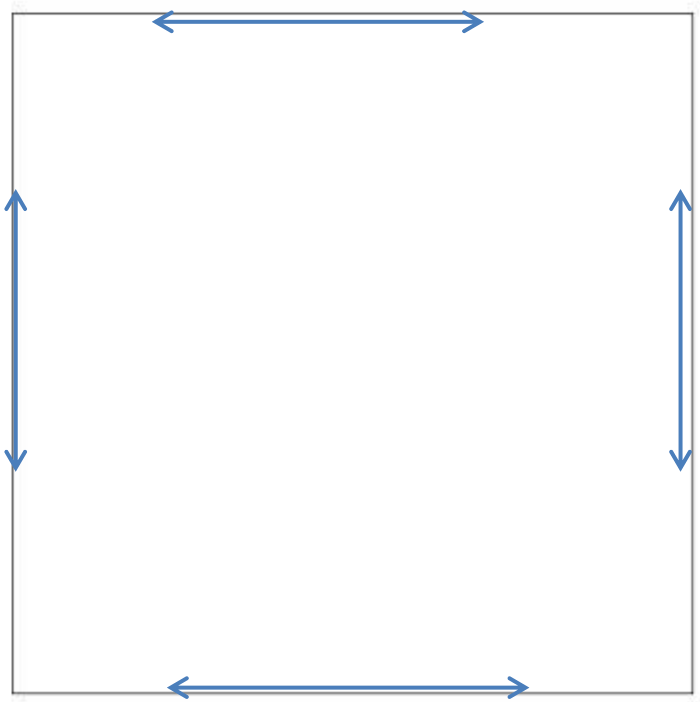
- Micro-confined liquid crystal system:

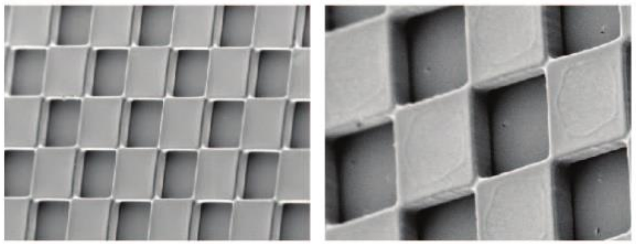
- Array of liquid crystal-filled square / rectangular wells with dimensions between 20×20×12 microns and 80×80×12 microns.

- 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

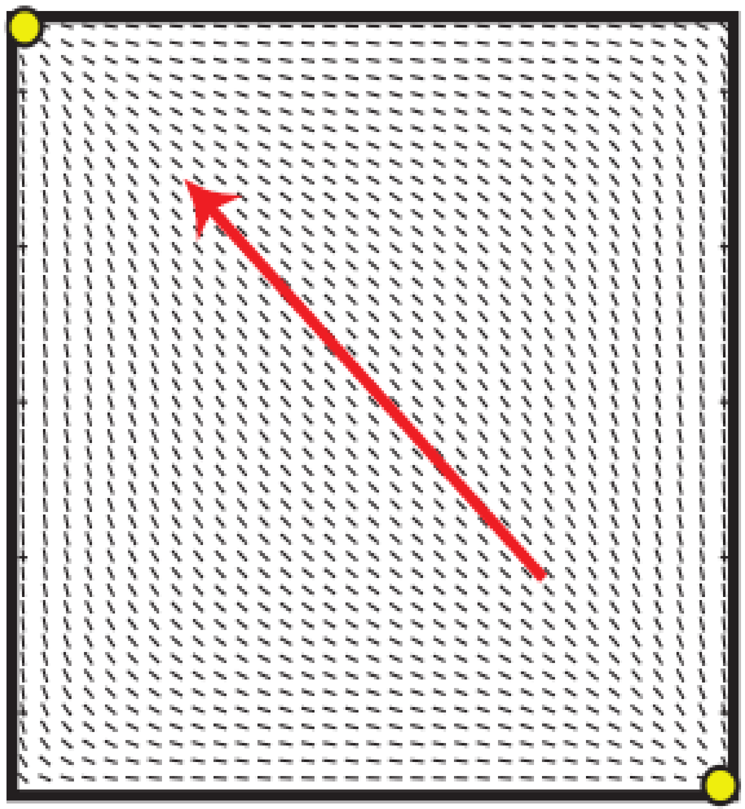
Chong Luo, Apala Majumdar and Radek Erban, 2012 **"Multistability in planar liquid crystal wells",** Physical Review E, Volume 85, Number 6, 061702

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.

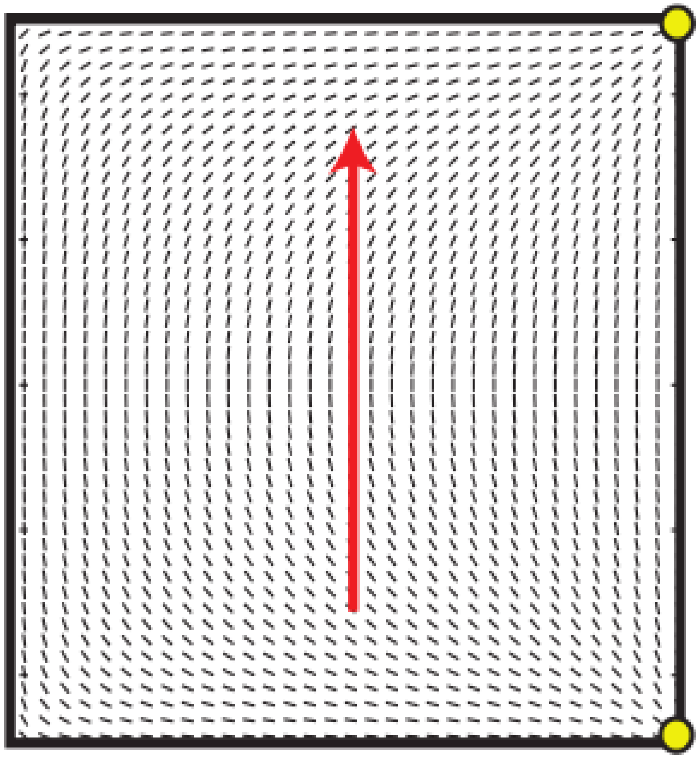


Tsakonas, Davidson, Brown, Mottram 2007

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.



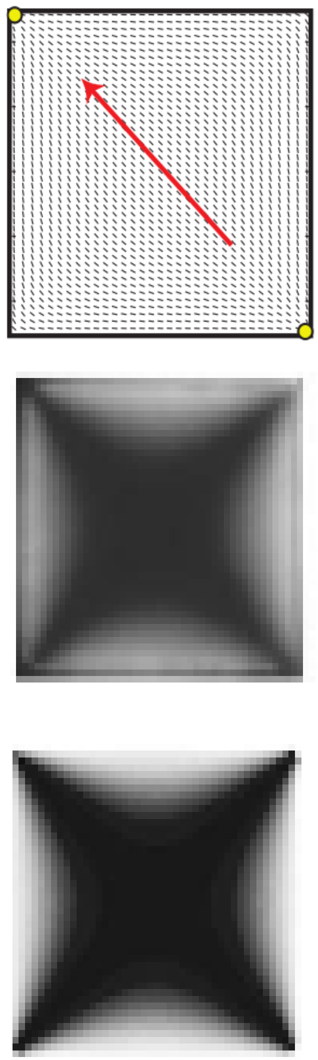
Tsakonas, Davidson, Brown, Mottram 2007

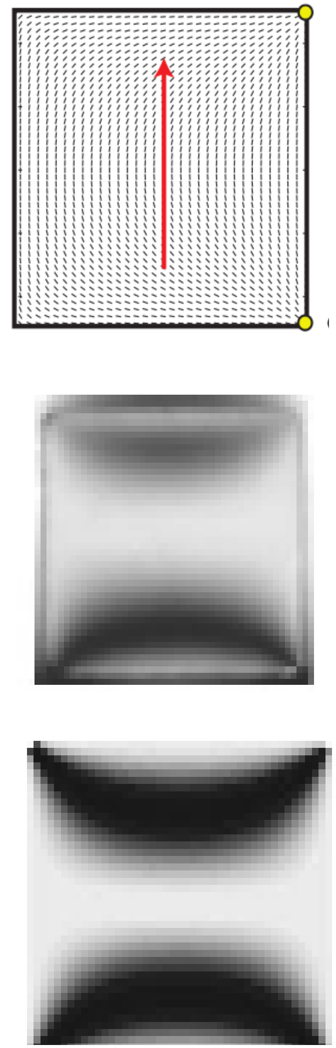
Optical contrast?

Theoretical and experimental optical textures:

Theory:

Experiment
:

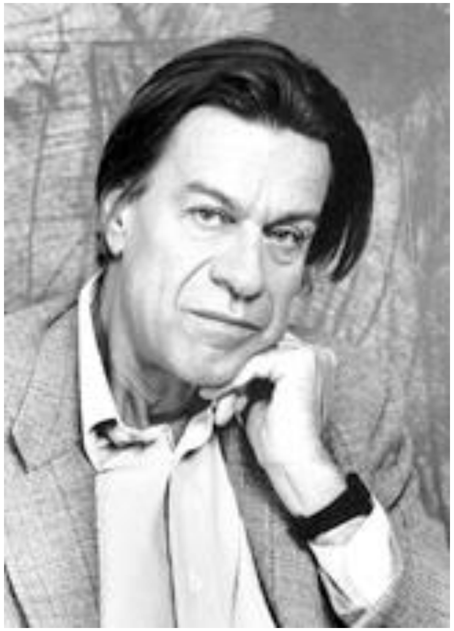




Tsakonas, Davidson, Brown, Mottram 2007

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

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

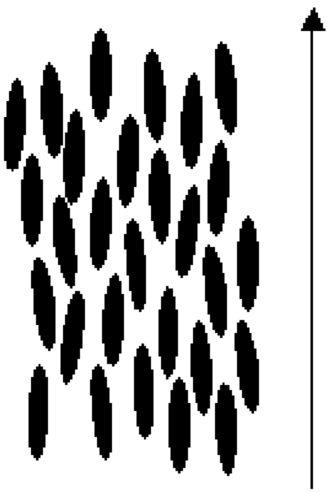
  "for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers"

Five degrees of freedom.

Eigenvalues of the Q-tensor and LC Phases

$$Q = \lambda_1 n \otimes n + \lambda_2 m \otimes m + \lambda_3 p \otimes p$$

$$\sum_{i=1}^{3} \lambda_i = 0$$



- 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; OF theory is a special uniaxial case with constant eigenvalues

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

- biaxial – three distinct eigenvalues and two locally preferred directions of molecular alignment.

The Landau-de Gennes Energy

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

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

The thermotropic potential : -

$$f_B(Q) = \frac{a}{2} tr\, Q^2 - \frac{b}{3} tr\, Q^3 + \frac{c}{4}\left(tr\, Q^2\right)^2 + C(a,b,c)$$

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

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

The elastic energy density : -

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

$$w(Q,\nabla Q) = L_1|\nabla Q|^2 + L_2 Q_{ij,j} Q_{ik,k}$$

The Landau-de Gennes Euler Lagrange Equations

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

The Euler-Lagrange equations :

$$\Delta Q_{ij} = \frac{1}{L}\left(a\, Q_{ij} - b\left(Q_{ip}\, Q_{pj} - \frac{1}{3}\left(tr\, Q^2\right)\delta_{ij} \right) + c\left(tr\, Q^2\right) Q_{ij} \right) \quad i,\ j = 1,2,3$$

- Energy minimizers are classical solutions of the Euler-Lagrange equations
- Smooth and analytic (standard results in elliptic regularity)
- How do we mathematically locate the defect structures?

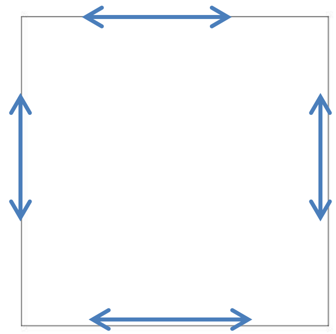
Modelling details

- 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



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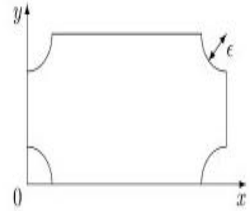
$$\mathbf{Q}_s(0,y,z) = \mathbf{Q}_s(R,y,z) = \frac{S_{eq}}{3}(-\vec{e}_x\otimes\vec{e}_x+2\vec{e}_y\otimes\vec{e}_y-\vec{e}_z\otimes\vec{e}_z)$$

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

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



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

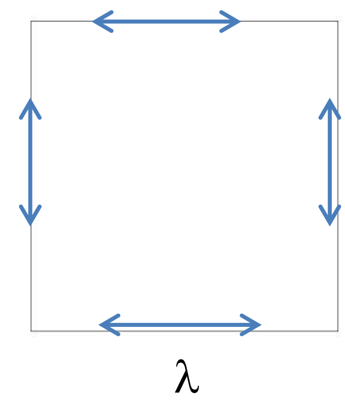
Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Model Reduction

- How good is the ansatz?

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

- Can rigorously prove using Gamma-convergence techniques (see below) that for thin geometries, with particular surface energies on top and bottom that allow for planar anchoring and Dirichlet uniaxial conditions on lateral sides, LdG energy minimizers will have this structure in the "thin film" limit.



- Benefit: study problem in terms of a 2D LdG approach at least to describe behaviour in the plane,

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

$$\Delta Q_{ij} = \frac{1}{L}\left(a\,Q_{ij} - c\left(tr\,Q^2\right)Q_{ij}\right) \quad i,\, j = 1,2$$

Golovaty, D., Montero, J.A. & Sternberg, P. J Nonlinear Sci (2015) 25: 1431. https://doi.org/10.1007/s00332-015-9264-7

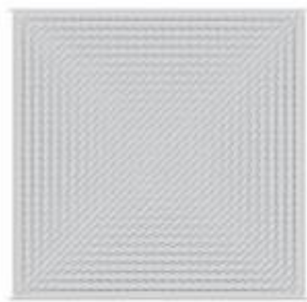
Large micron-sized wells

- 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.

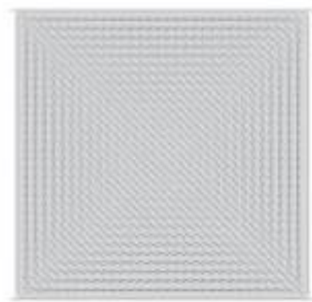
Chong Luo, Apala Majumdar and Radek Erban, 2012 **"Multistability in planar liquid crystal wells",** Physical Review E, Volume 85, Number 6, 061702
Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical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

Dirichlet conditions on Lateral Surfaces

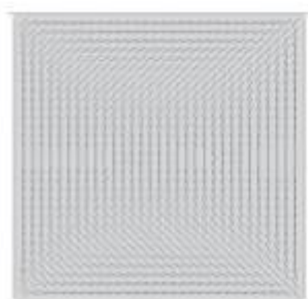
We find six different solutions : two diagonal and four rotated solutions.



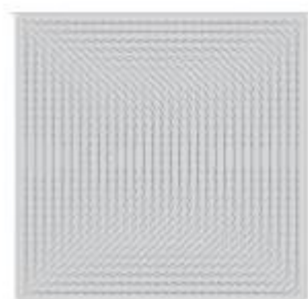
(a) D1



(b) D2

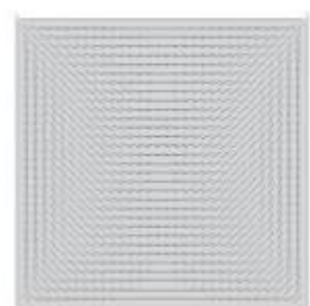


(c) R1



(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)

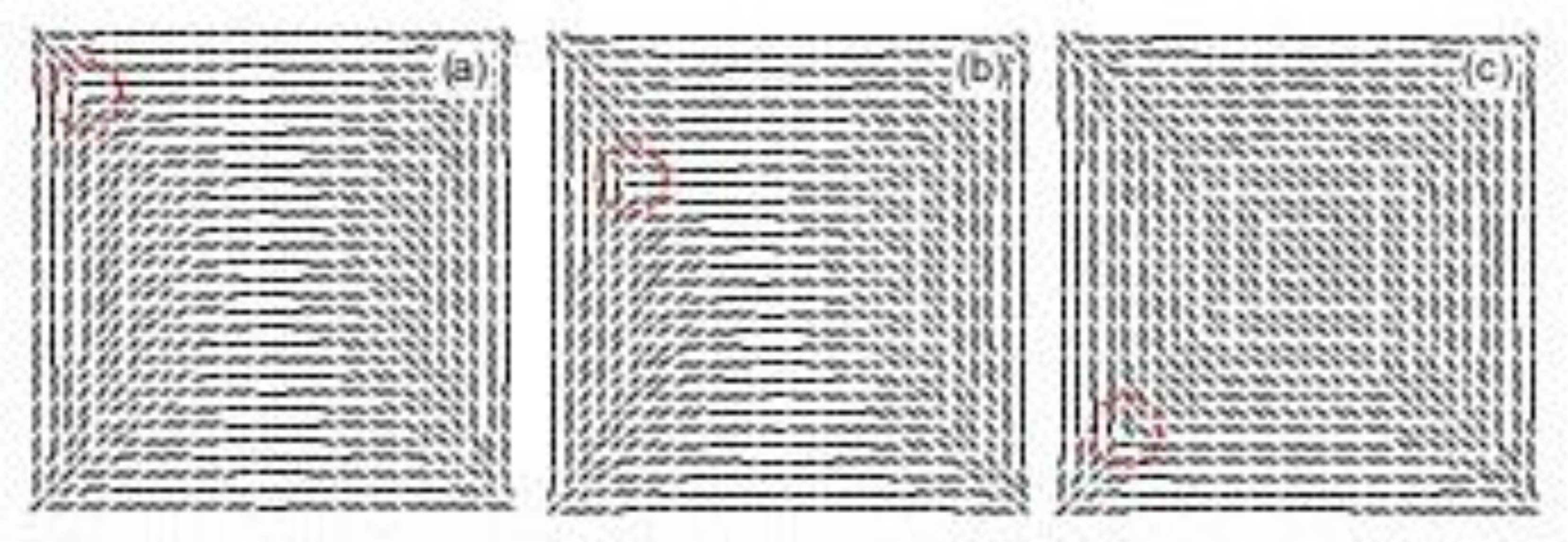
Kusumaatmaja, H. and Majumdar, A., 2015. Free energy pathways of a multistable liquid crystal device. *Soft Matter*, 11 (24), pp. 4809-4817.

Find explicit energy estimates (in the Oseen-Frank framework) in the paper 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.

Exploring the energy landscape

Switching between rotated and diagonal states: thermal excitations, anchoring conditions, boundary perturbations or external fields.

Transition pathways between diagonal and rotated states via saddle points of the Landau-de Gennes energy, that cannot be recovered via standard energy minimization procedures.

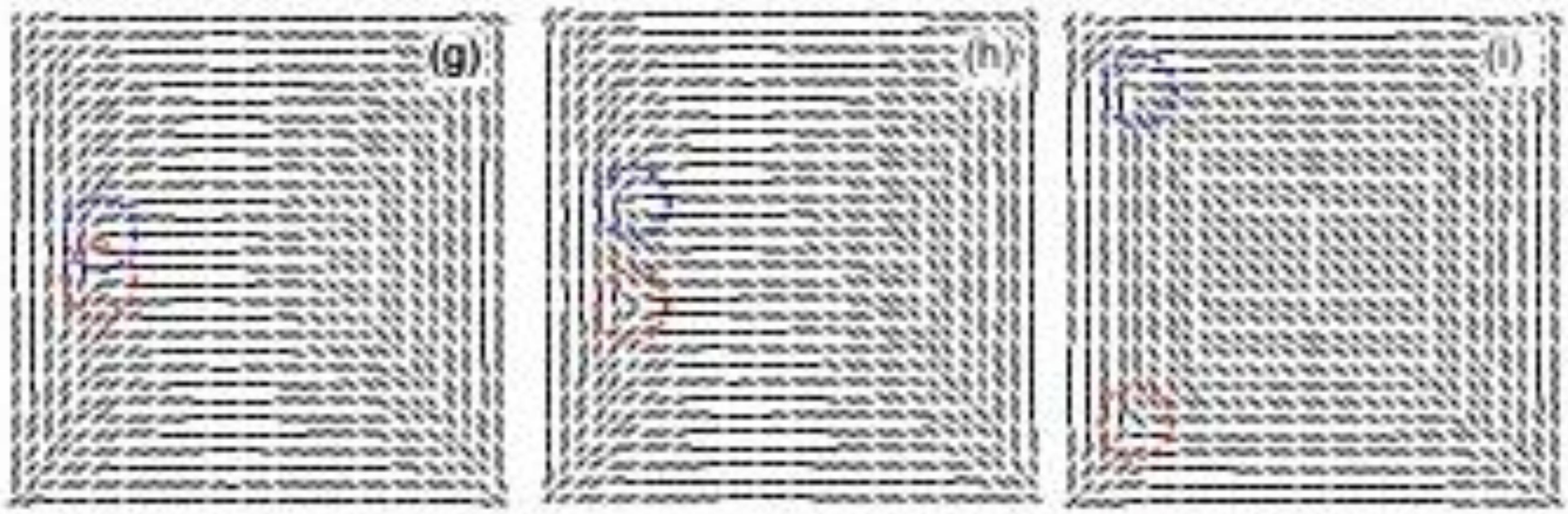


Rotated to Diagonal transition via the migration of a defect along an edge;

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

Exploring the energy landscape

Multiple transition pathways between diagonal and rotated states mediated by multiple defects along edges; see below



Rotated to Diagonal transition via creation and motion of two defects along an edge;

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

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

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

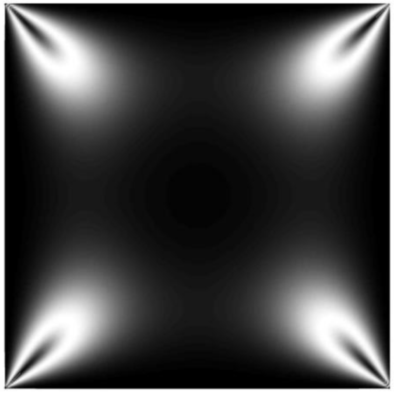
- Introduce ratio

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

- τ : measure of temperature

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

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



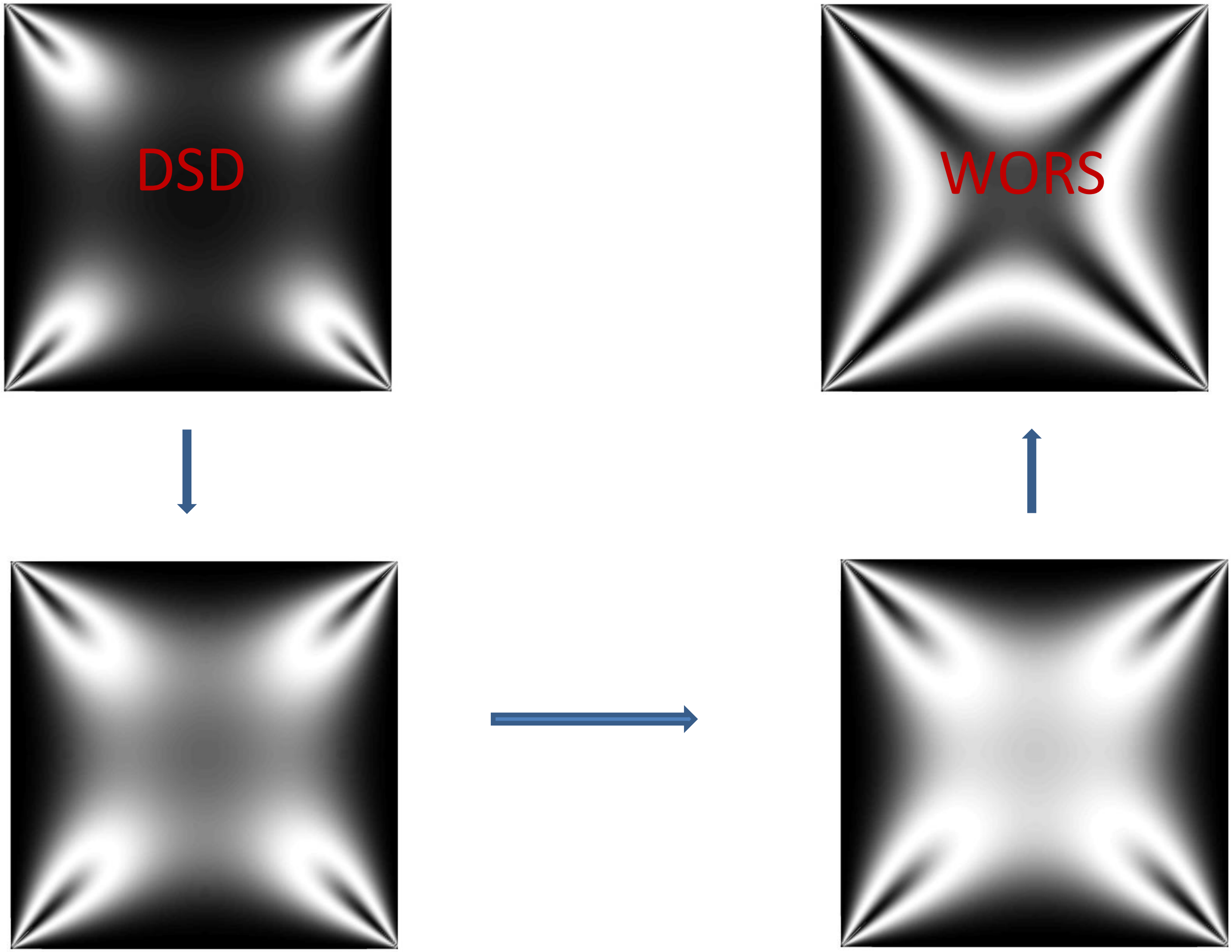
$$\beta^2 = 1 - 6\frac{\left(trQ^3\right)^2}{\left(trQ^2\right)^3}$$

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

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

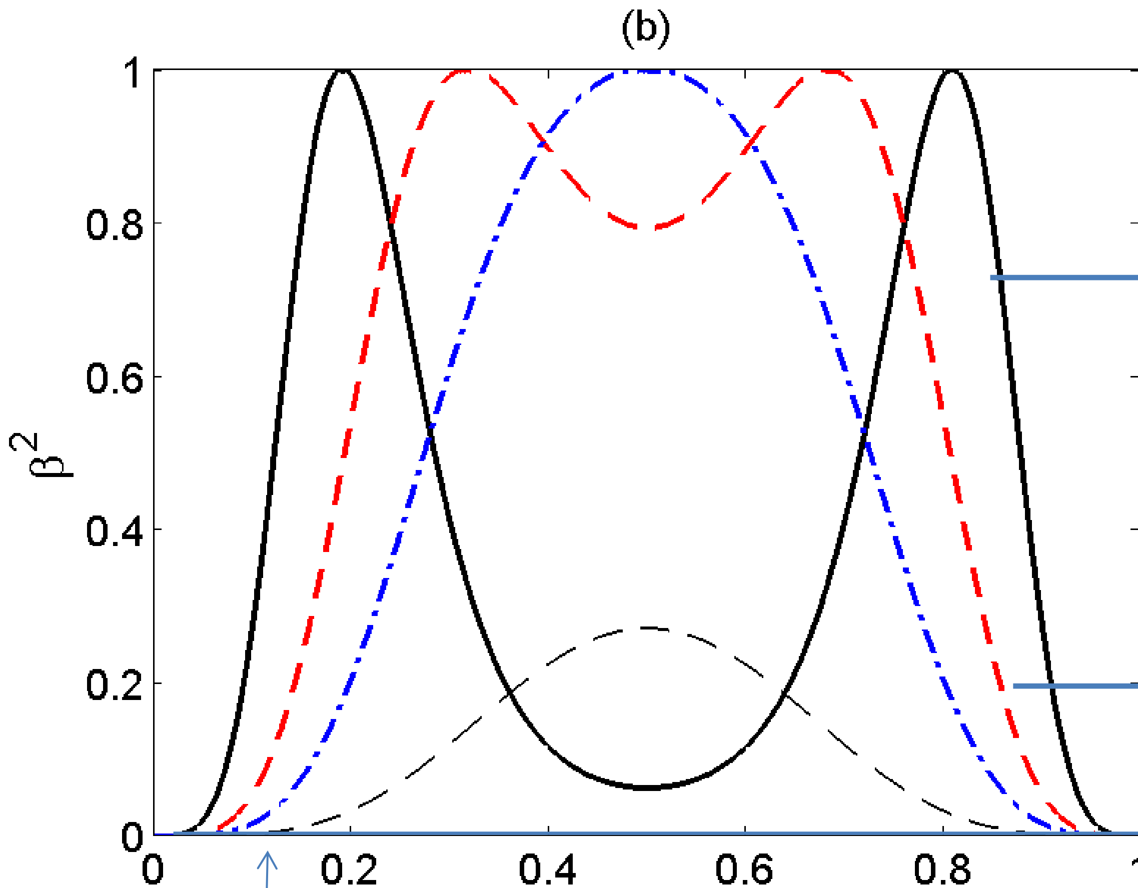
Decrease the ratio η: new structures for sub micron-sized wells

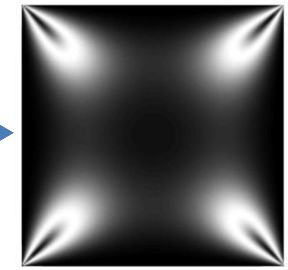
- Well Order Reconstruction Structure (WORS) at critical $\eta \sim 7$

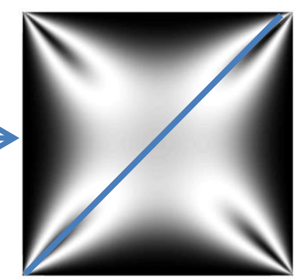


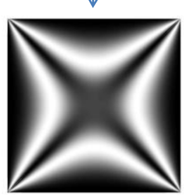
Decrease the ratio η: track biaxiality along square diagonal

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



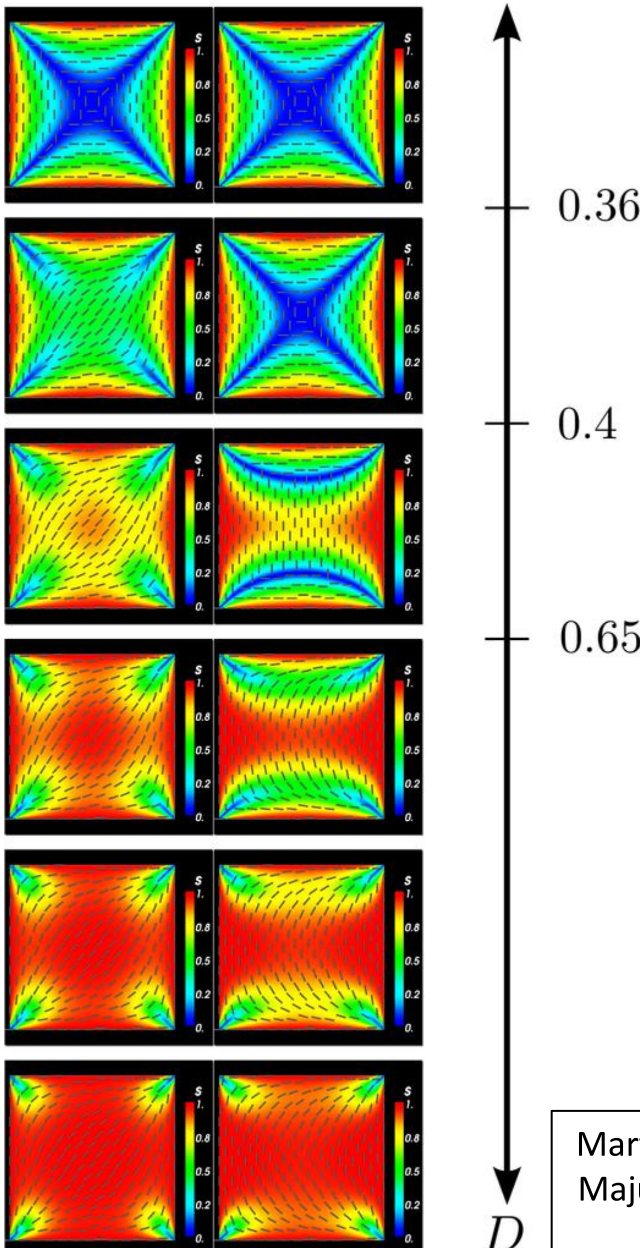


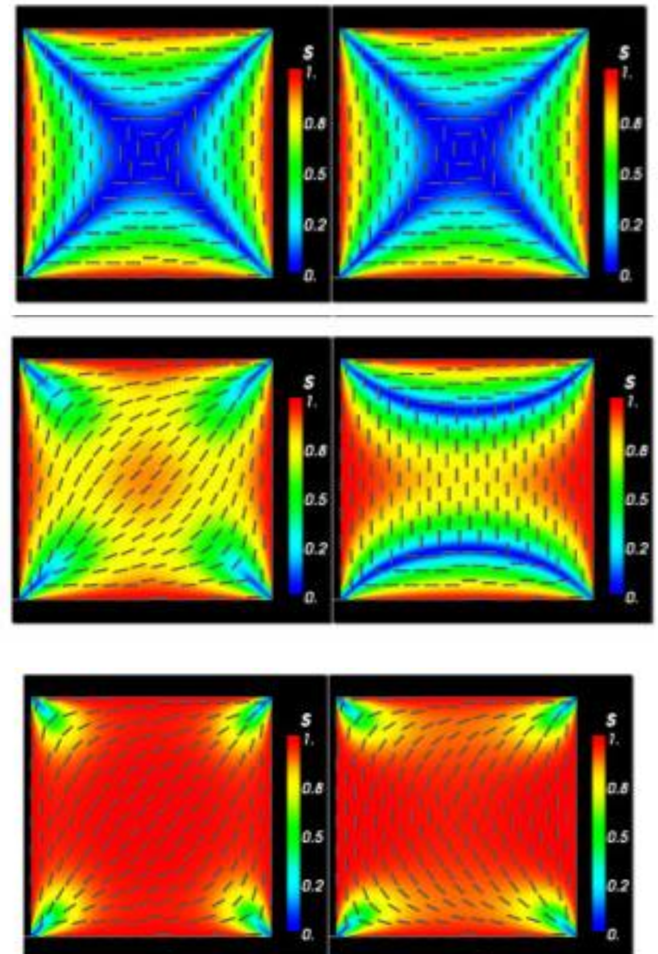




: zero β^2 along square diagonal

Some More Numerics…



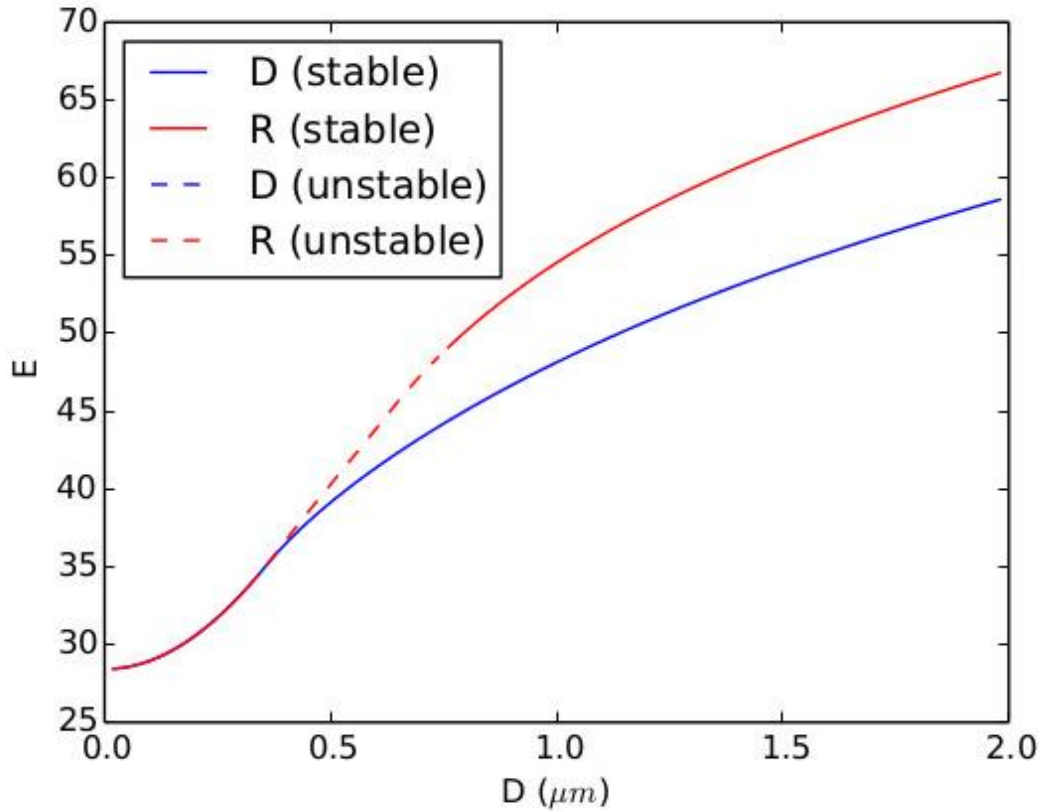


Uniqueness of solutions

R states lose stability

Martin Robinson, Chong Luo, Patrick Farrell, Radek Erban, and Apala Majumdar 2017 From molecular to continuum modelling of bistable liquid crystal devices. Liquid Crystals.

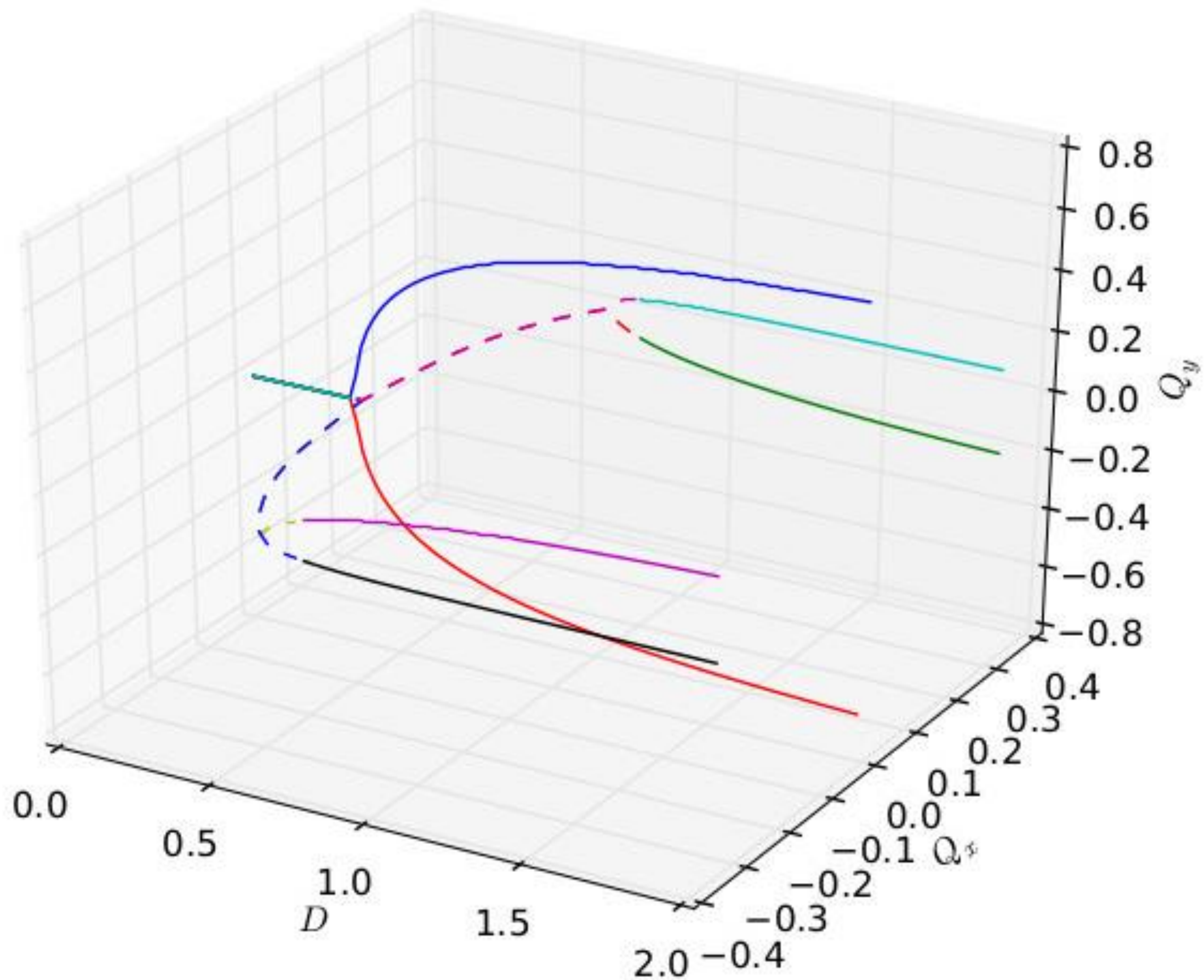
What happens as we increase the cross-sectional dimension?



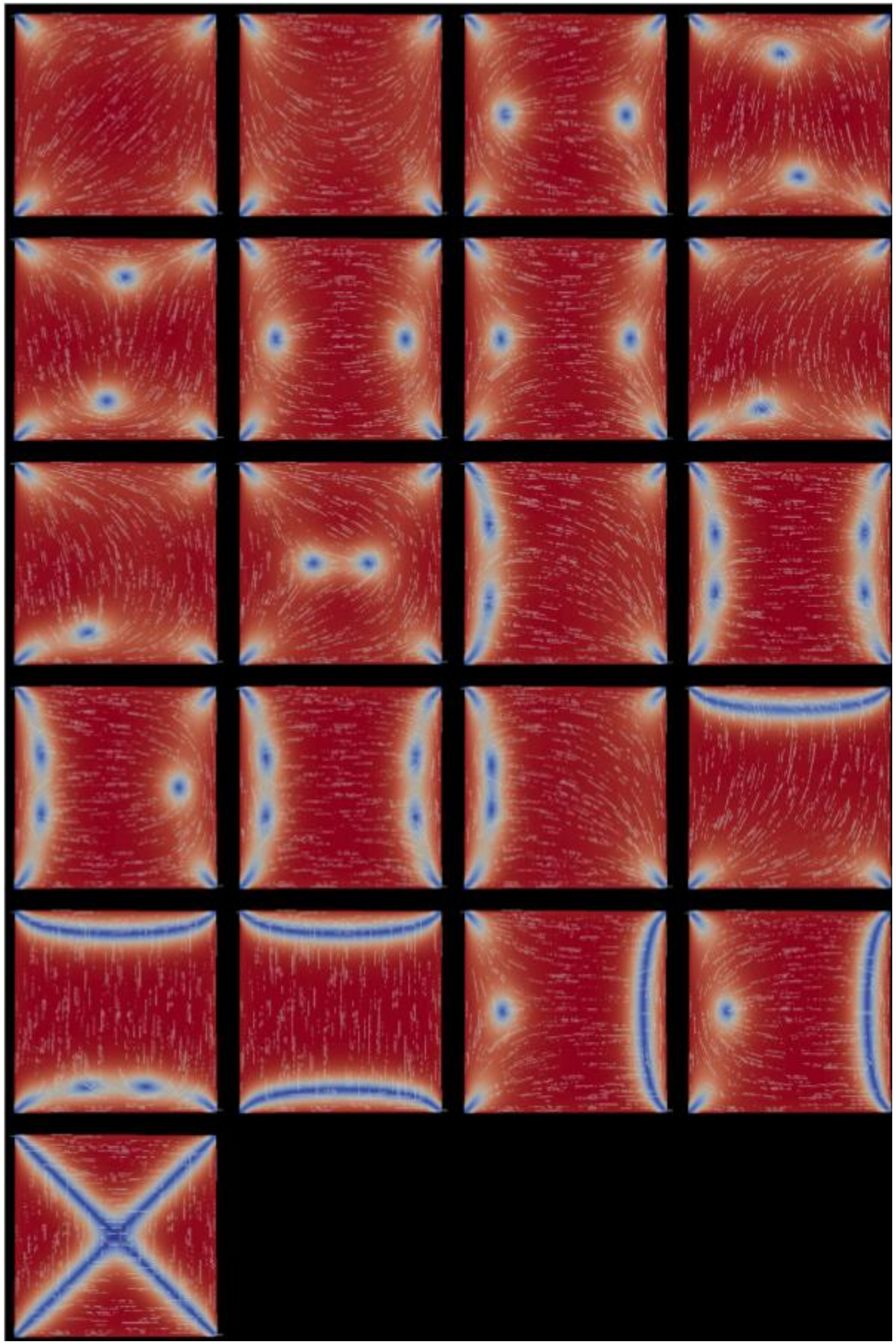
Co-authors: Martin Robinson, Chong Luo, Patrick Farrell, Apala Majumdar & Radek Erban

- 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

A detailed bifurcation plot



Martin Robinson, Chong Luo, Patrick Farrell, Radek Erban, and Apala Majumdar 2017 From molecular to continuum modelling of bistable liquid crystal devices. Liquid Crystals.



21 critical points….

From molecular to continuum modelling of bistable liquid crystal devices
Martin Robinson, Chong Luo, Patrick E. Farrell, Radek Erban & Apala Majumdar
http://www.tandfonline.com/doi/abs/10.1080/02678292.2017.1290284

For a rigorous three-dimensional analysis of the well order reconstruction solution,
see G. Canevari, A. Majumdar and A. Spicer, Order Reconstruction for Nematics on Squares and Regular Polygons: A Landau-de Gennes Study, *SIAM J. Appl. Math.*, 77(1), 267–293.

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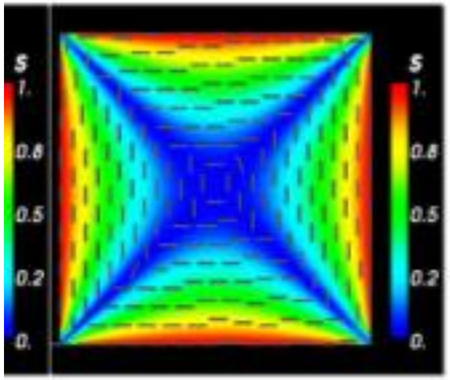
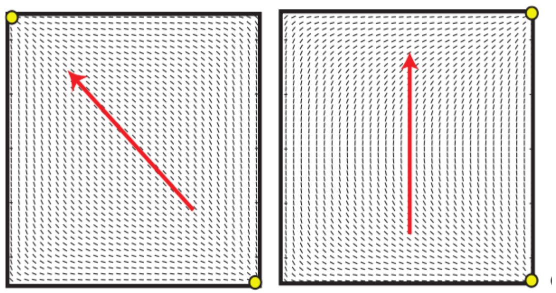




The Well Order Reconstruction Solution with Central Isotropic Inclusion

$$\Delta Q_{ij} = \bar{\lambda}^2 \left(A Q_{ij} - B \left(Q_{ip} Q_{pj} - \frac{1}{3} \left(tr\, Q^2 \right) \delta_{ij} \right) + C \left(tr\, Q^2 \right) Q_{ij} \right) \quad i, j = 1,2,3$$

$$\begin{aligned} Q(x,y) &= q_1(x,y)(e_x \otimes e_x - e_y \otimes e_y) + q_2(x,y)(e_x \otimes e_y + e_y \otimes e_x) \\ &+ q_3(x,y)(2e_z \otimes e_z - e_x \otimes e_x - e_y \otimes e_y) \\ &+ q_4(x,y)(e_x \otimes e_z + e_z \otimes e_x) + q_5(x,y)(e_y \otimes e_z + e_z \otimes e_y) \end{aligned}$$

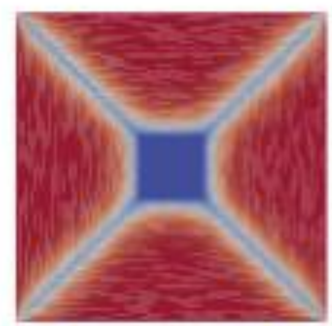
$$\Delta q_1 = \bar{\lambda}^2 (\tfrac{A}{2C} q_1 + \tfrac{B}{2C}(2q_1 q_3 - \tfrac{1}{2}(q_4^2 - q_5^2)) + (q_1^2 + q_2^2 + 3q_3^2 + q_4^2 + q_5^2) q_1)$$

$$\Delta q_2 = \bar{\lambda}^2 (\tfrac{A}{2C} q_2 + \tfrac{B}{2C}(2q_2 q_3 - q_4 q_5) + (q_1^2 + q_2^2 + 3q_3^2 + q_4^2 + q_5^2) q_2)$$

$$\Delta q_3 = \bar{\lambda}^2 (\tfrac{A}{2C} q_3 + \tfrac{B}{2C}(\tfrac{1}{3}(q_1^2 + q_2^2) - q_3^2 - \tfrac{1}{6}(q_4^2 + q_5^2)) + (q_1^2 + q_2^2 + 3q_3^2 + q_4^2 + q_5^2$$

$$\Delta q_4 = \bar{\lambda}^2 (\tfrac{A}{2C} q_4 - \tfrac{B}{2C}(q_3 q_4 + q_1 q_4 + q_2 q_5) + (q_1^2 + q_2^2 + 3q_3^2 + q_4^2 + q_5^2) q_4)$$

$$\Delta q_5 = \bar{\lambda}^2 (\tfrac{A}{2C} q_3 - \tfrac{B}{2C}(q_3 q_5 - q_1 q_5 + q_2 q_4) + (q_1^2 + q_2^2 + 3q_3^2 + q_4^2 + q_5^2) q_5)$$



Critical points with $q_4 = q_5 = 0$

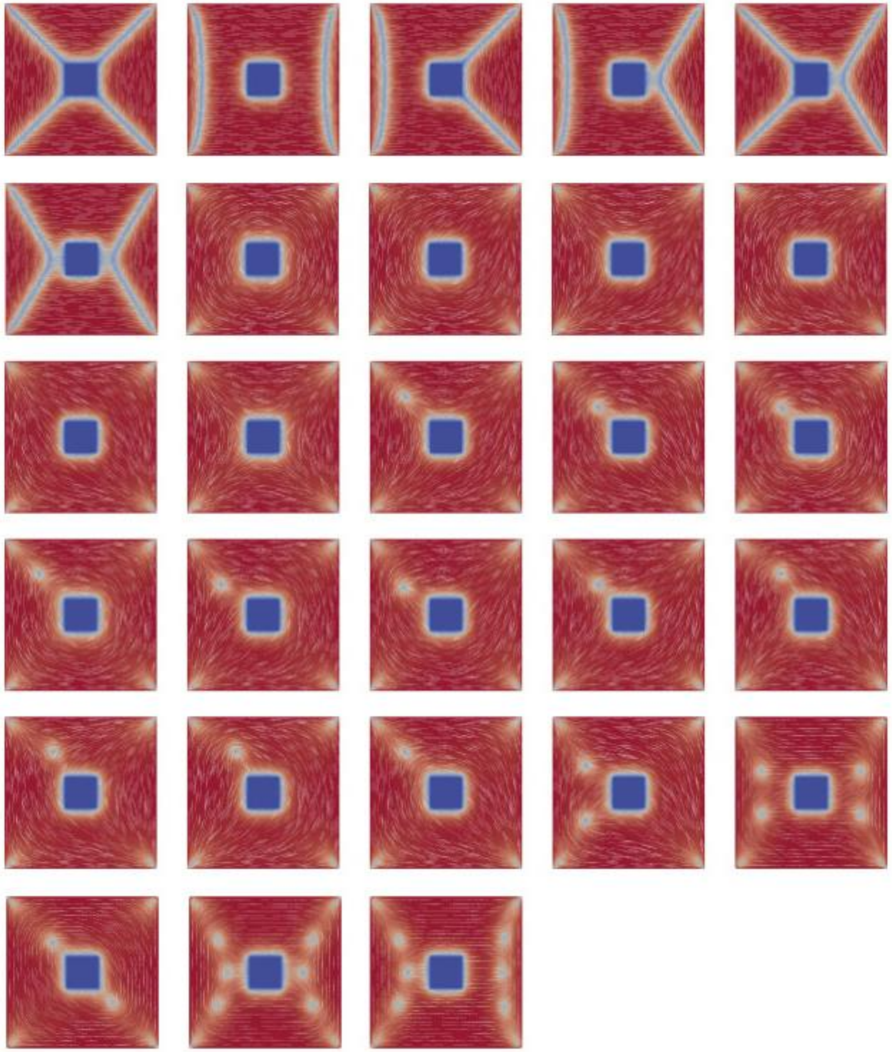
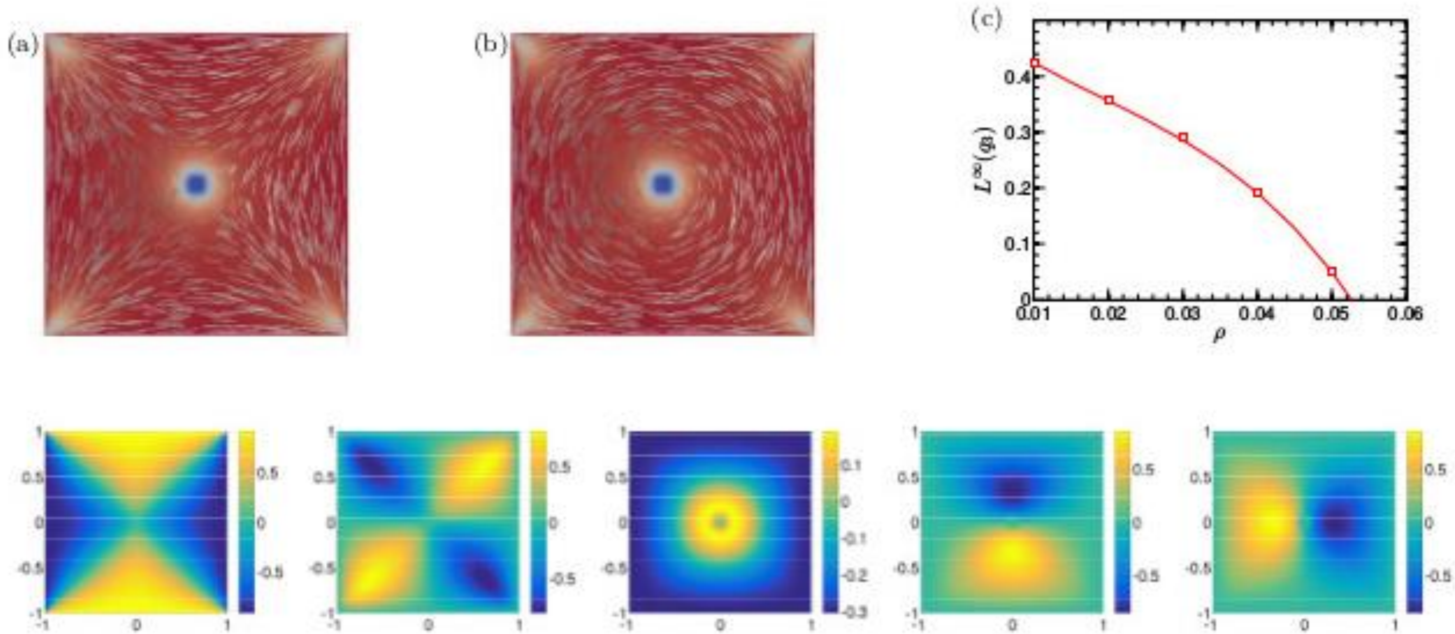


Figure 4.9: Critical Points found by deflation techniques for $\rho = 0.2$ ($\bar{\lambda}^2 = 200$), which are shown coloured by the order parameter s (blue at $s = 0$, increasing to red) and transparent white lines indicate the director direction n.

- Fix eigenvector in the z-direction
- Numerical deflation techniques
- Joint work with Yiwei Wang and Giacomo Canevari

Critical points with $q_4 \neq q_5 \neq 0$



(d) The profile of q_i in configuration(a)

- Allow for escape into third dimension by positivity of the third component
- Numerical deflation techniques
- Yiwei Wang, Giacomo Canevari, Apala Majumdar 2018 **Order Reconstruction for Nematics on Squares with Isotropic Inclusions: A Landau-de Gennes Study** https://arxiv.org/abs/1803.02597

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