Finite-Element Modelling of Liquid Crystal Equilibria

Scott MacLachlan
Department of Mathematics and Statistics
Memorial University of Newfoundland
smaclachlan@mun.ca

September 9, 2021

Acknowledgements

Core collaborators:

- James Adler (Tufts Math)
- Timothy Atherton (Tufts Physics)
- Patrick Farrell (Oxford Math)
- James Jackaman (NTNU Math)

Much of this work has been the focus of four PhD theses:

- David Emerson (Tufts, nematic liquid crystal models)
- Thomas Benson (Tufts, linear solvers)
- Jingmin Xia (Oxford, smectic liquid crystal models)
- Abdalaziz Hamdan (Memorial, smectic liquid crystal models)

Sponsors

- Tufts Collaborates! seed grant (JA/TA)
- National Science Foundation DMS-1216972 (JA/SM)
- NSERC Discovery Grants (SM)
- EPSRC fellowship EP/K030930/1 (PF)
- EPSRC Grants EP/R029423/1 and EP/V001493/1 (PF)
- National University of Defense Technology (JX)
- EPSRC Centre for Doctoral Training in Partial Differential Equations EP/L015811/1 (JX)
- NSF Grants DMR-1654283 and OAC-2003820 (TA)

Numerical Simulation

The point of numerical simulation is to use computers to answer science and engineering questions

Numerical Simulation

The point of numerical simulation is to use computers to answer science and engineering questions

The Question

↓

Mathematical Model

↓

Discrete Model

↓

Numerical Simulation

↓

Data/Answer

Mathematical Models

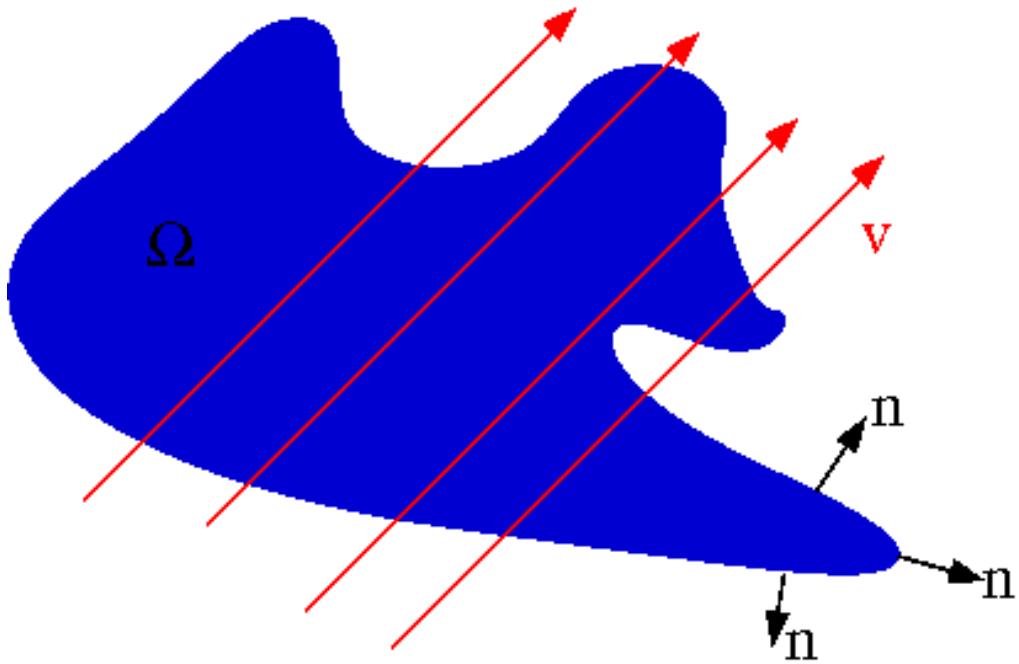
Often use PDE models, based on conservation principles

Mathematical Models

Often use PDE models, based on conservation principles

Consider a fluid moving with velocity $\boldsymbol{v}$

- Let L be the density of a conserved quantity
- Let Ω be an arbitrary control volume within the flow



Mathematical Models

Often use PDE models, based on conservation principles

Write conservation of L as

$$\frac{d}{dt}\int_\Omega L d\Omega = -\int_{\partial\Omega} L\boldsymbol{v}\cdot\boldsymbol{n} ds + \int_\Omega Q d\Omega$$

where

- $\boldsymbol{n}$ is the outward unit normal, and
- Q represents internal sources and sinks of L

Mathematical Models

Often use PDE models, based on conservation principles

Apply Leibnitz rule and Divergence theorem to get

$$\int_\Omega \frac{\partial}{\partial t} L d\Omega = -\int_\Omega \nabla \cdot (L\boldsymbol{v}) d\Omega + \int_\Omega Q d\Omega$$

or

$$\int_\Omega \left(\frac{\partial L}{\partial t} + \nabla \cdot (L\boldsymbol{v}) - Q \right) d\Omega = 0$$

This holds for an arbitrary control volume, Ω, so need

$$\frac{\partial L}{\partial t} + \nabla \cdot (L\boldsymbol{v}) = Q$$

Euler Equations

Applying conservation to mass, momentum, and energy gives:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0$$

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v} \cdot \nabla \boldsymbol{v} + \nabla p = \rho \boldsymbol{g}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)\boldsymbol{v}) = 0$$

- Need equation of state to close system

Navier-Stokes Equations

Applying conservation to mass and momentum, adding assumptions that the fluid is

- Incompressible: ρ is constant
- Newtonian: viscous stress is linear in local strain rate

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} - \frac{1}{Re} \nabla^2 \boldsymbol{v} + \nabla p = \boldsymbol{f}$$

$$\nabla \cdot \boldsymbol{v} = 0$$

PDE-based Simulation

Lots of effort invested in developing simulation tools for PDE-based mathematical models

Spatial discretization tools:

- Finite Differences
- Finite Elements
- Finite Volumes
- Spectral Methods

Temporal integration tools:

- Runge-Kutta methods
- Multistep (BDF, Adams) methods, predictor-corrector
- Space-Time discretizations

These are our "go-to" tools for many problems

PDE-based Simulation Failures

Difficulties arise in this framework when PDEs under consideration don't have unique solutions

PDE-based Simulation Failures

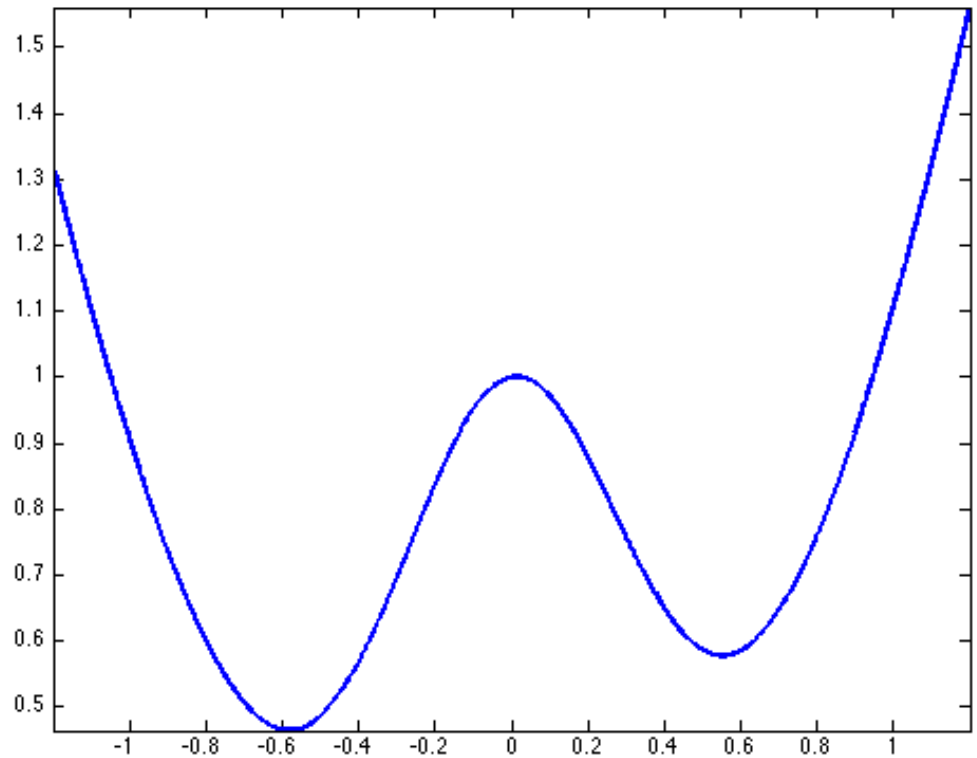
Difficulties arise in this framework when PDEs under consideration don't have unique solutions

Difficulties in **Mathematical Modeling**

- PDE models can also come from equilibrium conditions
- These are sufficient conditions to be a physical solution
- Need to distinguish between multiple solutions

PDE-based Simulation Failures

Difficulties arise in this framework when PDEs under consideration don't have unique solutions



PDE-based Simulation Failures

Difficulties arise in this framework when PDEs under consideration don't have unique solutions

Difficulties in **Mathematical Modeling**

- PDE models can also come from equilibrium conditions
- These are sufficient conditions to be a physical solution
- Need to distinguish between multiple solutions

Need underlying energy model to identify meaningful solutions

- Mathematical/numerical treatment of constraints, mathematical reformulations can change picture of energy landscape

Nematic liquid crystals

- Substances which possess liquid and crystalline properties.
- Nematic liquid crystals: rod shaped molecules with a preferred local average direction.
- The director, $\boldsymbol{n}(x, y, z) \in \mathbb{R}^3$, is *unit length*.

Local average direction, $\boldsymbol{n}$.

J. P. Lagerwall and G. Scalia, 2012.

Nematic liquid crystals

Free-energy minimization of Lagrangian:

$$\mathcal{L}(\boldsymbol{n}, \boldsymbol{E}, \lambda) = \int_\Omega w_F(\boldsymbol{n}) - \frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E} - \boldsymbol{P}\cdot\boldsymbol{E} + \lambda(\boldsymbol{n}\cdot\boldsymbol{n} - 1)dV.$$

where

$$w_F(\boldsymbol{n}) = \frac{1}{2}K_1\left(\nabla\cdot\boldsymbol{n}\right)^2 + \frac{1}{2}K_2\left(\boldsymbol{n}\cdot\nabla\times\boldsymbol{n}\right)^2 + \frac{1}{2}K_3\left|\boldsymbol{n}\times\nabla\times\boldsymbol{n}\right|^2$$

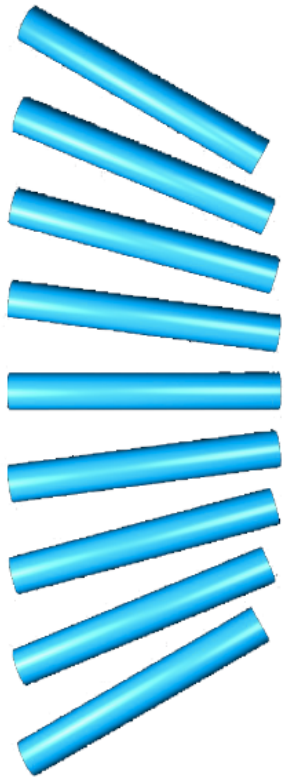
$$\boldsymbol{D} = \epsilon_0\epsilon_\perp\boldsymbol{E} + \epsilon_0\epsilon_a(\boldsymbol{n}\cdot\boldsymbol{E})\boldsymbol{n}$$

$$\boldsymbol{P} = e_s\left(\nabla\cdot\boldsymbol{n}\right)\boldsymbol{n} + e_b\boldsymbol{n}\times\nabla\times\boldsymbol{n}$$

Considering the case where constants are anisotropic

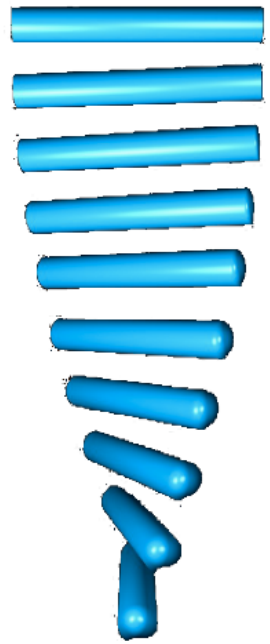
- K_1, K_2, K_3 not all the same
- $\epsilon_a \neq 0$

Elastic Free Energy Density



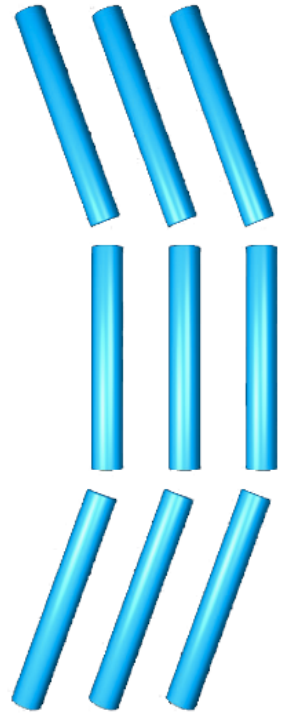
Splay

$K_1(\boldsymbol{\nabla} \cdot \boldsymbol{n})^2$



Twist

$K_2(\boldsymbol{n} \cdot \boldsymbol{\nabla} \times \boldsymbol{n})^2$



Bend

$K_3|\boldsymbol{n} \times \boldsymbol{\nabla} \times \boldsymbol{n}|^2$

K_1, K_2, and K_3 depend on temperature and liquid crystal type.

Frank-Oseen Elastic Free Energy Density

$$w_F(\boldsymbol{n}) = \frac{1}{2}K_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + \frac{1}{2}K_2(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})^2 + \frac{1}{2}K_3|\boldsymbol{n}\times\boldsymbol{\nabla}\times\boldsymbol{n}|^2.$$

A common analytical technique relies on the "one-constant approximation"

$$K_1 = K_2 = K_3 \;\Rightarrow\; w_F(\boldsymbol{n}) = \frac{1}{2}K_1|\nabla\boldsymbol{n}|^2.$$

A. Ramage and E. Gartland, SISC 2013

H. Wu, X. Xu, and C. Liu, Arch. Rational Mech. Anal. 2013.

Frank-Oseen Elastic Free Energy Density

$$w_F(\boldsymbol{n}) = \frac{1}{2}K_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + \frac{1}{2}K_2(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})^2 + \frac{1}{2}K_3|\boldsymbol{n}\times\boldsymbol{\nabla}\times\boldsymbol{n}|^2.$$

A common analytical technique relies on the "one-constant approximation"

$$K_1 = K_2 = K_3 \;\Rightarrow\; w_F(\boldsymbol{n}) = \frac{1}{2}K_1|\nabla\boldsymbol{n}|^2.$$

In contrast, we'll take

$$\boldsymbol{Z} = \kappa\boldsymbol{n}\otimes\boldsymbol{n} + (\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n}) = \boldsymbol{I} - (1-\kappa)\boldsymbol{n}\otimes\boldsymbol{n},$$

where $\kappa = K_2/K_3$ with $K_2, K_3 > 0$ and write

$$w_F(\boldsymbol{n}) = \frac{1}{2}K_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + \frac{1}{2}K_3\,(\boldsymbol{Z}\boldsymbol{\nabla}\times\boldsymbol{n})\cdot(\boldsymbol{\nabla}\times\boldsymbol{n})$$

A. Ramage and E. Gartland, SISC 2013

H. Wu, X. Xu, and C. Liu, Arch. Rational Mech. Anal. 2013.

Electric Effects

External **static** electric fields affect energy and orientation

Augment elastic free energy by

$$-\frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E} = -\frac{1}{2}\left(\epsilon_0\epsilon_\perp\boldsymbol{E} + \epsilon_0\epsilon_a(\boldsymbol{n}\cdot\boldsymbol{E})\boldsymbol{n}\right)\cdot\boldsymbol{E}$$

where

ϵ_0 = permittivity of free space,

$\epsilon_\perp$ = perpendicular permittivity of the dielectric,

$\epsilon_\parallel$ = parallel permittivity of the dielectric,

$\epsilon_a = \epsilon_\parallel - \epsilon_\perp$.

Also need to ensure $\boldsymbol{\nabla}\cdot\boldsymbol{D} = 0$, $\boldsymbol{\nabla}\times\boldsymbol{E} = 0$

Electric Potential

Write $\boldsymbol{E} = \nabla\phi$

- Ensures Faraday's Law satisfied

Static electric field augmentation becomes

$$-\frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E} = -\frac{1}{2}\left(\epsilon_0\epsilon_\perp\nabla\phi\cdot\nabla\phi + \epsilon_0\epsilon_a(\boldsymbol{n}\cdot\nabla\phi)\cdot(\boldsymbol{n}\cdot\nabla\phi)\right)$$

where

ϵ_0 = permittivity of free space,

$\epsilon_\perp$ = perpendicular permittivity of the dielectric,

$\epsilon_\parallel$ = parallel permittivity of the dielectric,

$\epsilon_a = \epsilon_\parallel - \epsilon_\perp$.

Still need to ensure $\nabla\cdot\boldsymbol{D} = 0$

Flexoelectric Effects

Polarization induced by curvature

- Several causes:
  - shape asymmetry
  - quadrupolar molecules
  - effects of splay and bend on association between molecules
- important in conversion of mechanical to electrical energy

Gives total electric displacement as

$$\boldsymbol{D}_{total} = \boldsymbol{D} + \boldsymbol{P} = \epsilon_0 \epsilon_\perp \boldsymbol{E} + \epsilon_0 \epsilon_a (\boldsymbol{n} \cdot \boldsymbol{E}) \boldsymbol{n} + \boldsymbol{P}$$
$$\boldsymbol{P} = e_s \left(\nabla \cdot \boldsymbol{n}\right) \boldsymbol{n} + e_b \boldsymbol{n} \times \nabla \times \boldsymbol{n}$$

Augment energy density by

$$-\boldsymbol{P} \cdot \boldsymbol{E} = -\left(e_s \left(\nabla \cdot \boldsymbol{n}\right) \boldsymbol{n} + e_b \boldsymbol{n} \times \nabla \times \boldsymbol{n}\right) \cdot \nabla \phi$$

Need $\nabla \cdot \boldsymbol{D}_{total} = 0$

Unit Length Constraint

Need to ensure director field is unit length pointwise:

$$\boldsymbol{n} \cdot \boldsymbol{n} = 1$$

Impose this using Lagrange multiplier, λ.

- Augment physical energy density by $\lambda\left(\boldsymbol{n} \cdot \boldsymbol{n} - 1\right)$
- When satisfied, contributes no energy
- Could also use penalty approach
  - Avoids adding extra variable
  - Leads to less accurate solutions
  - Linearized systems are harder to solve

Adler, Emerson, MacLachlan, Manteuffel, SISC 2016

Complete Lagrangian

Free-energy minimization of Lagrangian:

$$\mathcal{L}(\boldsymbol{n}, \phi, \lambda) = \int_\Omega w_F(\boldsymbol{n}) - \frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E} - \boldsymbol{P}\cdot\boldsymbol{E} + \lambda(\boldsymbol{n}\cdot\boldsymbol{n} - 1)dV.$$

where

$$w_F(\boldsymbol{n}) = \frac{1}{2}K_1\left(\nabla\cdot\boldsymbol{n}\right)^2 + \frac{1}{2}K_2\left(\boldsymbol{n}\cdot\nabla\times\boldsymbol{n}\right)^2 + \frac{1}{2}K_3\left|\boldsymbol{n}\times\nabla\times\boldsymbol{n}\right|^2$$

$$\boldsymbol{E} = \nabla\phi$$

$$\boldsymbol{D} = \epsilon_0\epsilon_\perp\boldsymbol{E} + \epsilon_0\epsilon_a(\boldsymbol{n}\cdot\boldsymbol{E})\boldsymbol{n}$$

$$\boldsymbol{P} = e_s\left(\nabla\cdot\boldsymbol{n}\right)\boldsymbol{n} + e_b\boldsymbol{n}\times\nabla\times\boldsymbol{n}$$

Additionally, need $\nabla\cdot(\boldsymbol{D}+\boldsymbol{P}) = 0$

First-Order Optimality Conditions

Minimize Lagrangian when first variations are zero:

$$\mathcal{L}_{\boldsymbol{n}}[\boldsymbol{v}] = \frac{\partial}{\partial \boldsymbol{n}}\mathcal{L}(\boldsymbol{n},\phi,\lambda)[\boldsymbol{v}] = 0, \qquad \forall \boldsymbol{v} \in \mathcal{H}_0^{DC}(\Omega),$$

$$\mathcal{L}_{\phi}[\psi] = \frac{\partial}{\partial \phi}\mathcal{L}(\boldsymbol{n},\phi,\lambda)[\boldsymbol{\psi}] = 0, \qquad \forall \psi \in H_0^1(\Omega),$$

$$\mathcal{L}_{\lambda}[\gamma] = \frac{\partial}{\partial \lambda}\mathcal{L}(\boldsymbol{n},\phi,\lambda)[\gamma] = 0, \qquad \forall \gamma \in L^2(\Omega).$$

Necessary function spaces:

$$L^2(\Omega) = \left\{\gamma : \int \gamma^2 < \infty\right\}$$

$$H^1(\Omega) = \{\psi \in L^2(\Omega) : \nabla\psi \in L^2(\Omega)\}$$

$$H_0^1(\Omega) = \{\psi \in H^1(\Omega) : \psi(\boldsymbol{x}) = 0 \ \forall \boldsymbol{x} \in \partial\Omega\}$$

First-Order Optimality Conditions

Minimize Lagrangian when first variations are zero:

$$\mathcal{L}_{\boldsymbol{n}}[\boldsymbol{v}] = \frac{\partial}{\partial \boldsymbol{n}}\mathcal{L}(\boldsymbol{n},\phi,\lambda)[\boldsymbol{v}] = 0, \qquad \forall \boldsymbol{v} \in \mathcal{H}_0^{DC}(\Omega),$$

$$\mathcal{L}_{\phi}[\psi] = \frac{\partial}{\partial \phi}\mathcal{L}(\boldsymbol{n},\phi,\lambda)[\boldsymbol{\psi}] = 0, \qquad \forall \psi \in H_0^1(\Omega),$$

$$\mathcal{L}_{\lambda}[\gamma] = \frac{\partial}{\partial \lambda}\mathcal{L}(\boldsymbol{n},\phi,\lambda)[\gamma] = 0, \qquad \forall \gamma \in L^2(\Omega).$$

Necessary function spaces:

$$H(\mathsf{curl},\Omega) = \{\boldsymbol{v} \in L^2(\Omega) : \nabla \times \boldsymbol{v} \in L^2(\Omega)\}$$

$$H(\mathsf{div},\Omega) = \{\boldsymbol{v} \in L^2(\Omega) : \nabla \cdot \boldsymbol{v} \in L^2(\Omega)\}$$

$$\mathcal{H}_0^{DC}(\Omega) = \{\boldsymbol{v} \in H(\mathsf{div},\Omega) \cap H(\mathsf{curl},\Omega) : B(\boldsymbol{v}) = \mathbf{0}\}$$

Nonlinearities

First-order optimality equations are nonlinear variational forms

- Weak form of Euler-Lagrange equations
- Could extract these as PDEs and continue in classical way
- Instead, ask for weak solution directly

Nonlinearities

First-order optimality equations are nonlinear variational forms

- Weak form of Euler-Lagrange equations
- Could extract these as PDEs and continue in classical way
- Instead, ask for weak solution directly

Use Newton's method to linearize variational system

$$\begin{bmatrix} \mathcal{L}_{\boldsymbol{nn}} & \mathcal{L}_{\boldsymbol{n}\phi} & \mathcal{L}_{\boldsymbol{n}\lambda} \\ \mathcal{L}_{\phi\boldsymbol{n}} & \mathcal{L}_{\phi\phi} & \mathbf{0} \\ \mathcal{L}_{\lambda\boldsymbol{n}} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta\boldsymbol{n} \\ \delta\phi \\ \delta\lambda \end{bmatrix} = - \begin{bmatrix} \mathcal{L}_{\boldsymbol{n}} \\ \mathcal{L}_{\phi} \\ \mathcal{L}_{\lambda} \end{bmatrix}.$$

for all $(\boldsymbol{v}, \psi, \gamma)$

$$\begin{aligned} \boldsymbol{n}_{k+1} &= \boldsymbol{n}_k + \omega\,\delta\boldsymbol{n} \\ \text{Then update } \phi_{k+1} &= \phi_k + \omega\,\delta\phi \\ \lambda_{k+1} &= \lambda_k + \omega\,\delta\lambda \end{aligned}$$

Discretization

Linearized variational system pairs naturally with finite-element discretization

Use standard uniform tensor-product meshes in 2D

- Represent three-dimensional "slab" geometry
- Functions vary smoothly over rectangular elements

Restrict all functions to finite-dimensional subspaces:

- $\boldsymbol{n}_k$, $\delta\boldsymbol{n}$, $\boldsymbol{v}$ as continuous piecewise biquadratic vector fields
- ϕ_k, $\delta\phi$, ψ as continuous piecewise biquadratic functions
- λ_k, $\delta\lambda$, γ as discontinuous piecewise constant functions

Well-Posedness

Relying on two key facts:

- Solution satisfies first-order optimality conditions
  - Ensure weak satisfaction of $\nabla \cdot (\boldsymbol{D} + \boldsymbol{P}) = 0$
- Newton's method will converge to a solution
  - Use nested-iteration or trust-region methods to ensure

Adler, Atherton, Emerson, MacLachlan, SINUM 2015

Adler, Atherton, Benson, Emerson, MacLachlan, SISC 2015

Well-Posedness

Relying on two key facts:

- Solution satisfies first-order optimality conditions
  - Ensure weak satisfaction of $\nabla \cdot (\boldsymbol{D} + \boldsymbol{P}) = 0$
- Newton's method will converge to a solution
  - Use nested-iteration or trust-region methods to ensure

Need to ensure each linearization step has unique solution

- Weak form has *saddle-point* structure
- Existence and uniqueness of solutions to update equations not immediately guaranteed
  - Make use of weak coercivity arguments at discrete level
  - Show discretized linear systems have unique solutions when "close enough" to a continuum solution
  - Also need weak(?) assumptions on physical parameters

Adler, Atherton, Emerson, MacLachlan, SINUM 2015

Adler, Atherton, Benson, Emerson, MacLachlan, SISC 2015

Sketch of Proof

Consider "elastic" problem (no ϕ), of saddle-point form:

$$\begin{aligned} a(\delta\boldsymbol{n}, \boldsymbol{v}) + b(\boldsymbol{v}, \delta\lambda) &= G(\boldsymbol{v}), \qquad && \forall \boldsymbol{v} \in \mathcal{H}_0^{DC}(\Omega), \\ b(\delta\boldsymbol{n}, \gamma) &= H(\gamma), && \forall \gamma \in L^2(\Omega). \end{aligned}$$

Under reasonable assumptions:

- $a(\boldsymbol{u}, \boldsymbol{v})$ and $b(\boldsymbol{v}, \gamma)$ are continuous
- If λ_k is pointwise non-negative, there exist ϵ_1, $\epsilon_2 > 0$ such that if $1 - \epsilon_2 < \kappa < 1 + \epsilon_1$, then $a(\boldsymbol{u}, \boldsymbol{v})$ is coercive on $\boldsymbol{V}_h$
- For properly chosen $\boldsymbol{V}_h$ and Q_h,

$$\sup_{\boldsymbol{v} \in \boldsymbol{V}_h} \frac{|b(\boldsymbol{v}, \gamma)|}{\|\boldsymbol{v}\|_{DC}} \geq Ch\|\gamma\|_0, \qquad \forall \gamma \in Q_h$$

- Finite-element pair is convergent but sub-optimal

Adler, Atherton, Emerson, MacLachlan, SINUM 2015

Adler, Atherton, Benson, Emerson, MacLachlan, SISC 2015

Sketch of Proof

Adding electric effects gives 3×3 block system

$$\begin{bmatrix} \mathcal{L}_{\boldsymbol{nn}} & \mathcal{L}_{\boldsymbol{n}\phi} & \mathcal{L}_{\boldsymbol{n}\lambda} \\ \mathcal{L}_{\phi\boldsymbol{n}} & \mathcal{L}_{\phi\phi} & \mathbf{0} \\ \mathcal{L}_{\lambda\boldsymbol{n}} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta\boldsymbol{n}_H \\ \delta\phi_H \\ \delta\lambda_H \end{bmatrix} = - \begin{bmatrix} \mathcal{L}_{\boldsymbol{n}} \\ \mathcal{L}_{\phi} \\ \mathcal{L}_{\lambda} \end{bmatrix}.$$

For invertibility, need

- Maintain coercivity of $a(\boldsymbol{u}, \boldsymbol{v})$
  - Natural if $\epsilon_a < 0$, or if $|\nabla\phi_k|$ is not too large
- Weak coercivity of $b(\boldsymbol{v}, \gamma)$
- Negative definiteness of $\mathcal{L}_{\phi\phi}$
  - Natural if $\epsilon_a \geq 0$, or if $|\boldsymbol{n}_k| \leq \beta < \epsilon_\perp / |\epsilon_a|$

Benzi, Golub, Liesen, Acta Numerica 2005

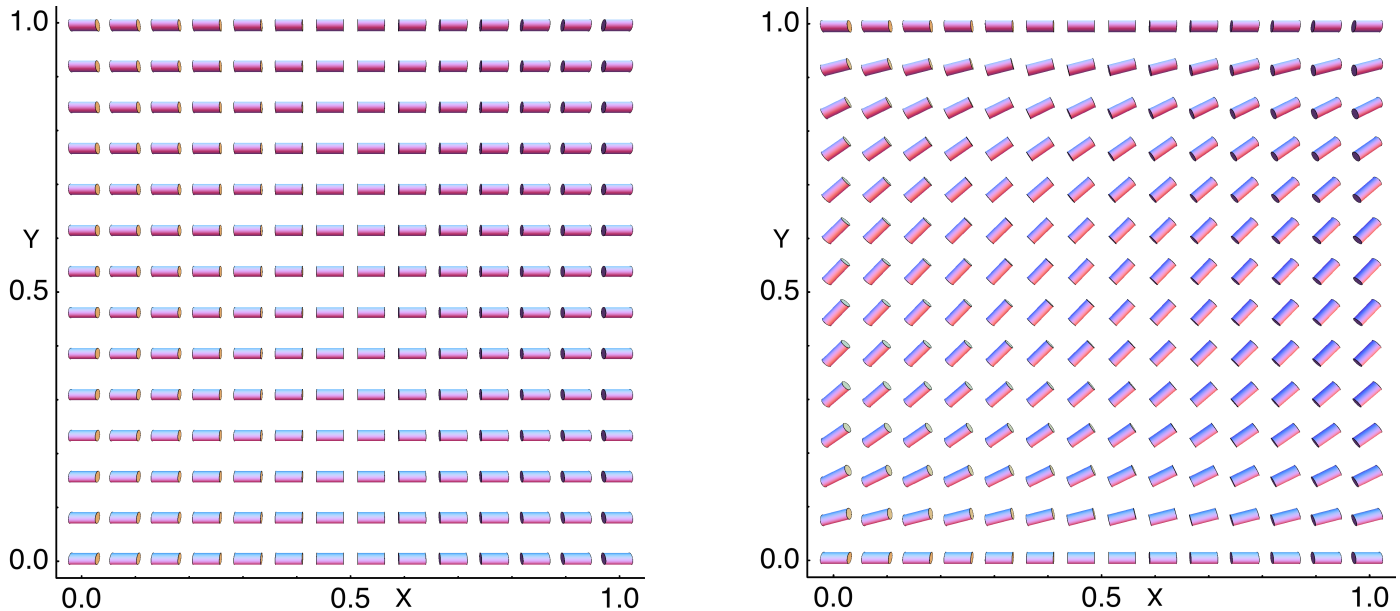
Adler, Atherton, Benson, Emerson, MacLachlan, SISC 2015

Simplest Test Problems

- Ω consists of parallel substrates distance 1 apart.
- Periodic boundary conditions along $x = 0$ and $x = 1$.
- Dirichlet boundary conditions on the y-boundaries.
- $\boldsymbol{n}$ may have a non-zero z component, but $\frac{\partial \boldsymbol{n}}{\partial z} = \mathbf{0}$.
  - 2-D domain: $\Omega = \{(x, y) \mid 0 \leq x, y \leq 1\}$.

Freedericksz Transition

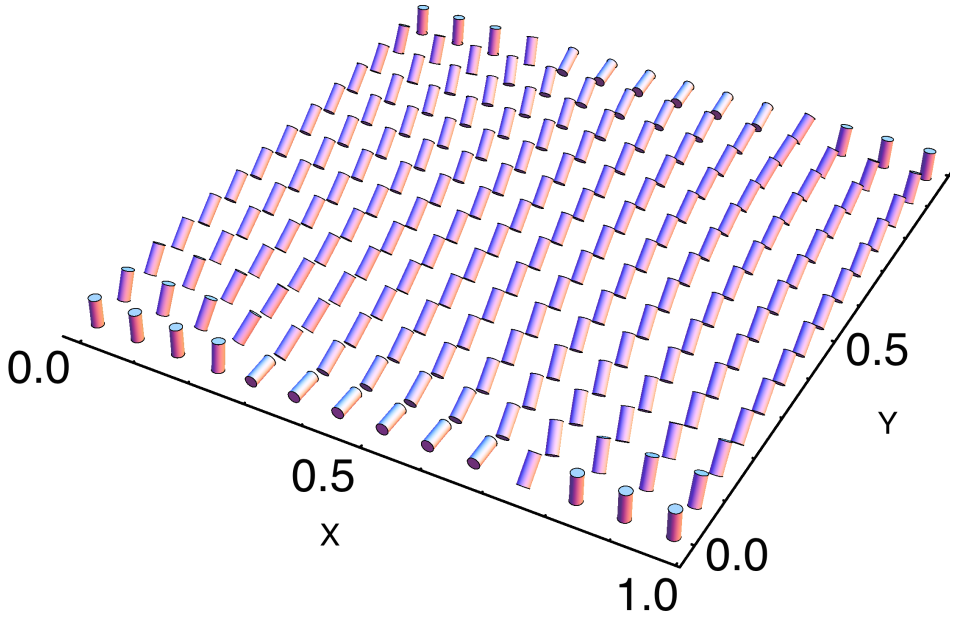
- $\boldsymbol{n}$ lies parallel to x-axis on boundaries.
- $\phi(y = 1) = 1$ and $\phi(y = 0) = 0$.
- $K_1 = 1$, $K_2 = 0.62903$, $K_3 = 1.32258$.
- $\epsilon_0 = 1.42809$, $\epsilon_{\parallel} = 18.5$, $\epsilon_{\perp} = 7$, $\epsilon_a = 11.5$.



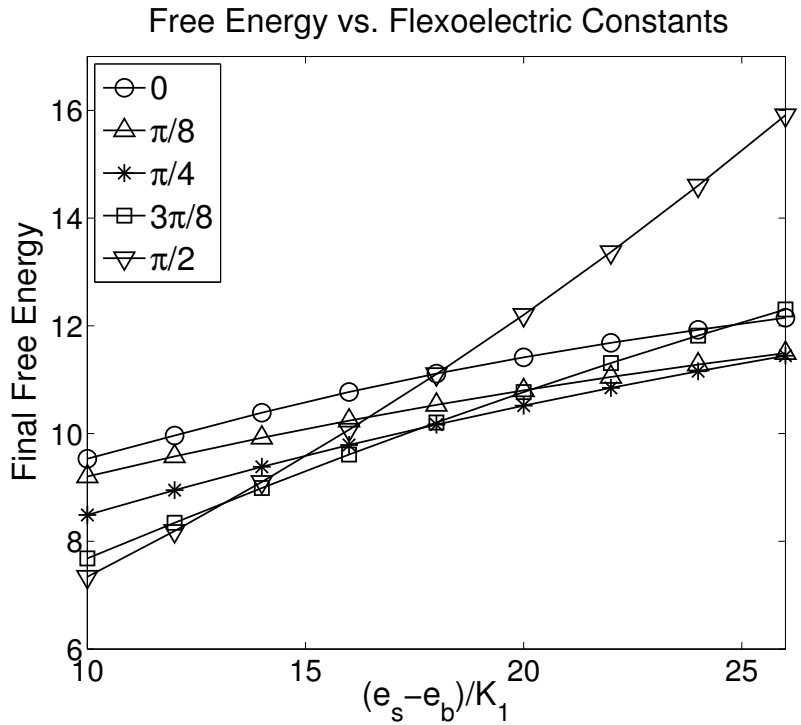
Left: Degenerate solution with free energy, -6.05.
Right: Energy-minimizing solution with free energy, -6.78.

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Bistability



Nano-patterned boundary conditions



Free Energy for different values of θ as a function of flexoelectric constants

Adler, Atherton, Benson, Emerson, MacLachlan, SISC 2015

Finding Multiple Solutions

Brute-force approaches to finding more solutions are natural

- Multistart methods
  - Aim for initial guesses to sample solution space
- Difficulty when solution space is high-dimensional

We use an approach that augments Newton functional

- Use Newton's method to find a solution, r, to $F(x) = 0$
- Construct new functional, $G(x)$, such that
  - For all $x \neq r$ such that $F(x) = 0$, $G(x) = 0$
  - $G(r) \neq 0$
- Now apply Newton's method to $G(x) = 0$

J. Larson, S. M. Wild, Optim Eng 2016

P. E. Farrell, Á. Birkisson, S. W. Funke, SISC 2015

Deflation

Let $F(x) : \mathbb{R}^m \to \mathbb{R}^n$ be a function and r be a known solution to the equation $F(x) = 0$. Let

$$M_{p,\alpha}(x; r) = \left(\frac{1}{\|x - r\|^p} + \alpha \right) \boldsymbol{I}, \quad G(x) = M_{p,\alpha}(x; r) F(x).$$

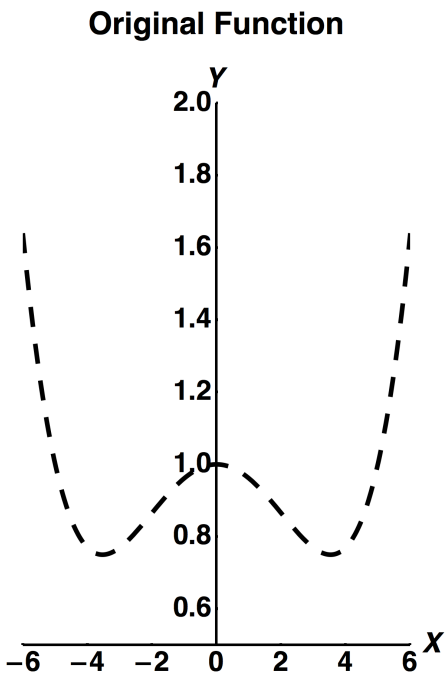
$\to G(x) = 0$ is the deflated problem.
$\to$ Apply Newton's method to solve this problem.

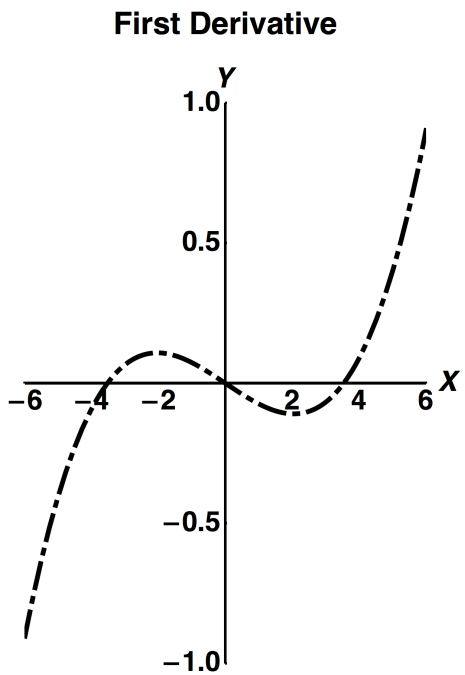
P. E. Farrell, Á. Birkisson, S. W. Funke, SISC 2015

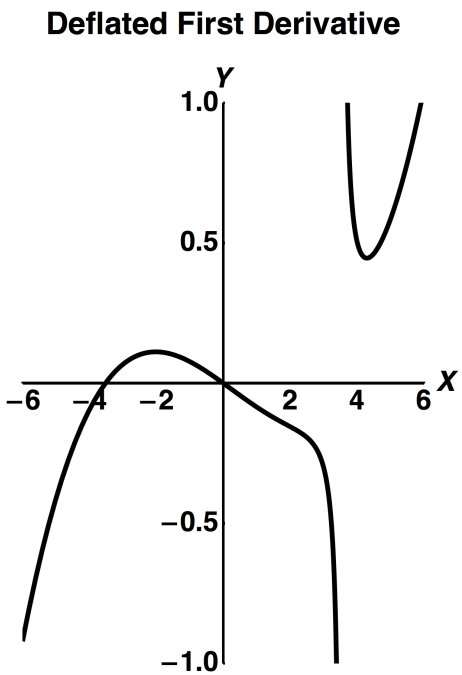
1D Minimization Example

Consider the function

$$f(x) = \frac{1}{5^4}x^4 - \frac{1}{5^2}x^2 + 1, \qquad f'(x) = \frac{4}{5^4}x^3 - \frac{2}{5^2}x.$$







Deflation for Functionals

Consider $\mathcal{F}(u) : U \to \mathbb{R}^n$

- U is some function space
- Solving $\mathcal{F}(u) = \mathbf{0}$, know $\mathcal{F}(r) = \mathbf{0}$

Define

$$M_{p,\alpha}(u; r) = \left(\frac{1}{\|u - r\|_U^p} + \alpha \right) \boldsymbol{I},$$

where $\boldsymbol{I}$ is the n-dimensional identity.

Deflation for Functionals

Consider $\mathcal{F}(u) : U \to \mathbb{R}^n$

- U is some function space
- Solving $\mathcal{F}(u) = \mathbf{0}$, know $\mathcal{F}(r) = \mathbf{0}$

Define

$$M_{p,\alpha}(u; r) = \left(\frac{1}{\|u - r\|_U^p} + \alpha \right) \boldsymbol{I},$$

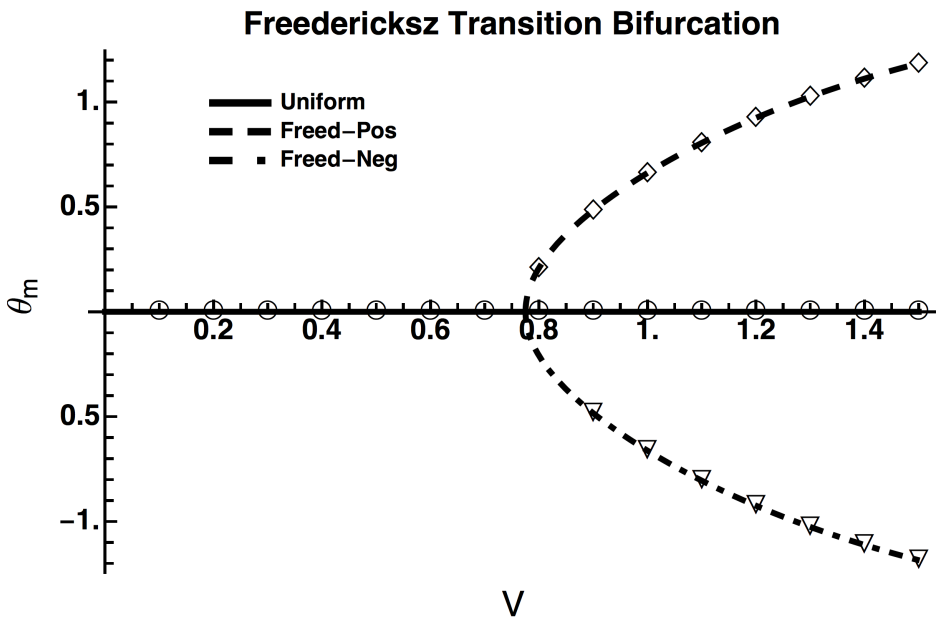
where $\boldsymbol{I}$ is the n-dimensional identity. Then, we solve

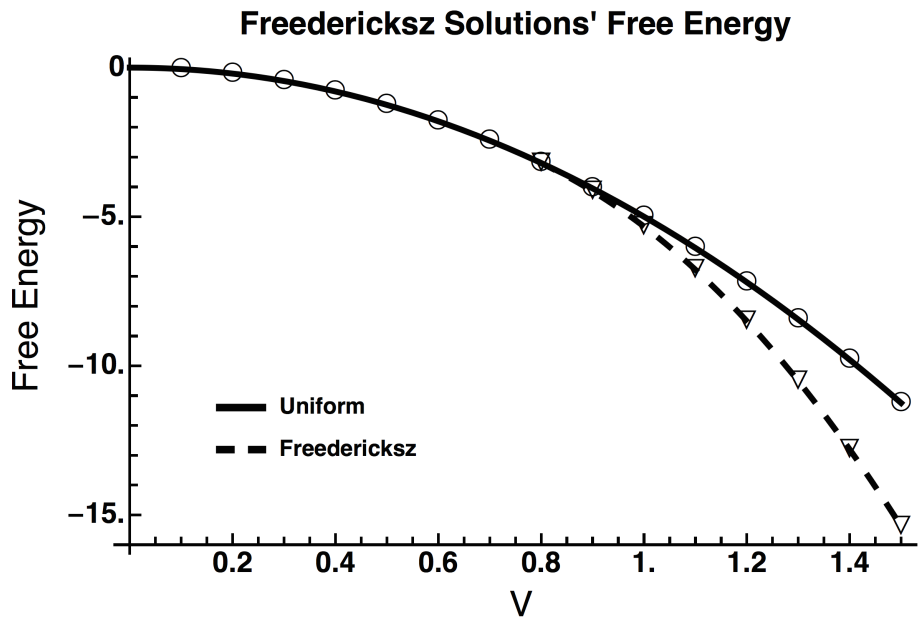
$$\mathcal{G}(u) = M_{p,\alpha}(u; r)\mathcal{F}(u) = \mathbf{0}.$$

Freedericksz Bifurcation

Bifurcation occurs with increasing applied voltage gap

- Alignment with electric field overpowers elastic effects



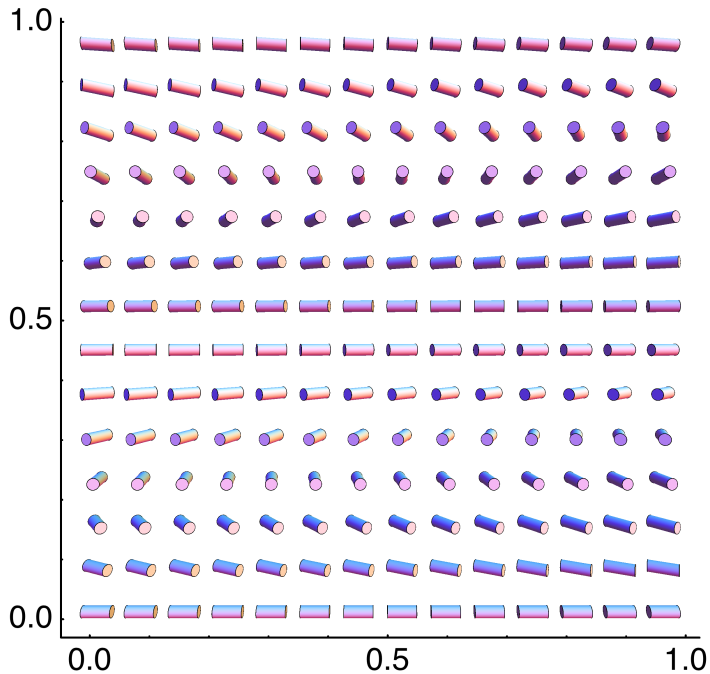


Maximum tilt angle (left), free energy (right), as a function of V

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Cholesteric Liquid Crystals

- Cholesteric LCs are similar to nematics
- Inherent chirality breaks some symmetry
  - Distinguishable configurations due to "handedness"
- For given parameter, preferred thickness to layers formed



Cholesteric Liquid Crystals

- Cholesteric LCs are similar to nematics
- Inherent chirality breaks some symmetry
  - Distinguishable configurations due to "handedness"
- For given parameter, preferred thickness to layers formed

$$\begin{aligned}\mathcal{C}(\boldsymbol{n}) &= \frac{K_1}{2}\|\boldsymbol{\nabla}\cdot\boldsymbol{n}\|_0^2 + \frac{K_2}{2}\|\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n} + t_0\|_0^2 + \frac{K_3}{2}\|\boldsymbol{n}\times\boldsymbol{\nabla}\times\boldsymbol{n}\|_0^2 \\ &= \mathcal{F}(\boldsymbol{n}) + K_2\langle t_0, \boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n}\rangle_0 + \frac{K_2}{2}\|t_0\|^2,\end{aligned}$$

where t_0 is a constant depending on liquid crystal type.

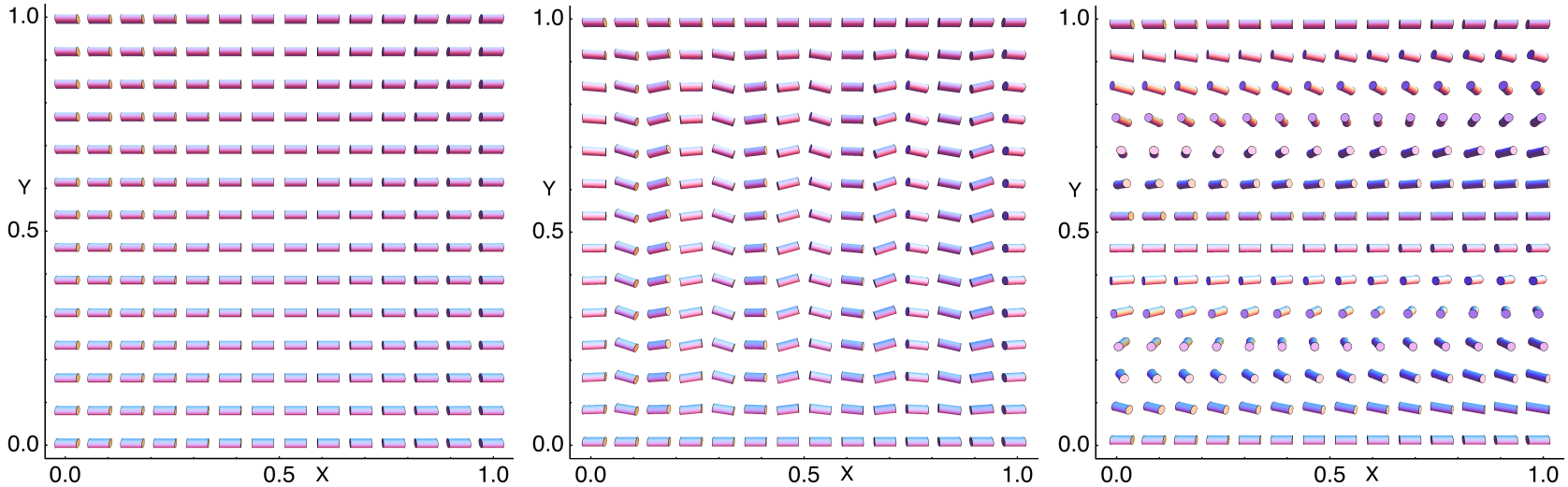
Simple Cholesteric

- Elastic-only model, no electric terms
- $K_1 = 1.0$, $K_2 = 3.0$, $K_3 = 1.2$
- Cholesteric parameter: $t_0 = -2\pi$ (left-handed)
- Deflation parameters: $p = 3.0$ and $\alpha = 1.0$

Start with 3 initial guesses, then run Newton + Deflation

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Simple Cholesteric

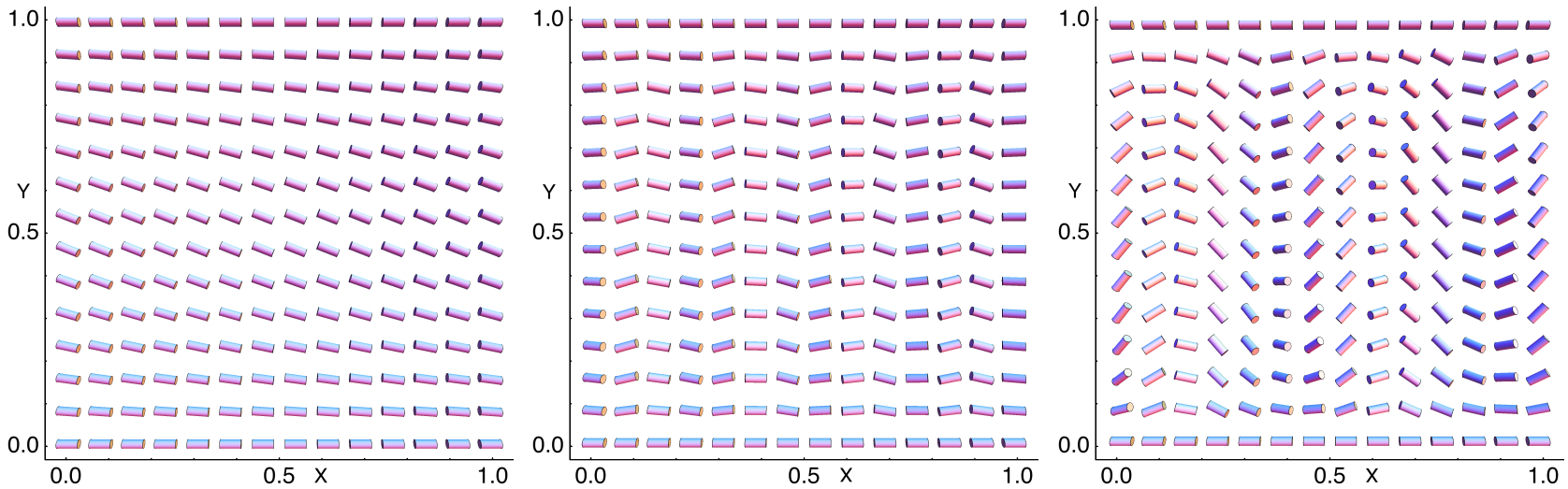


Computed solutions, found left-to-right order

- computed free energies are 59.218, 56.553, and 3×10^{-8}

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Simple Cholesteric

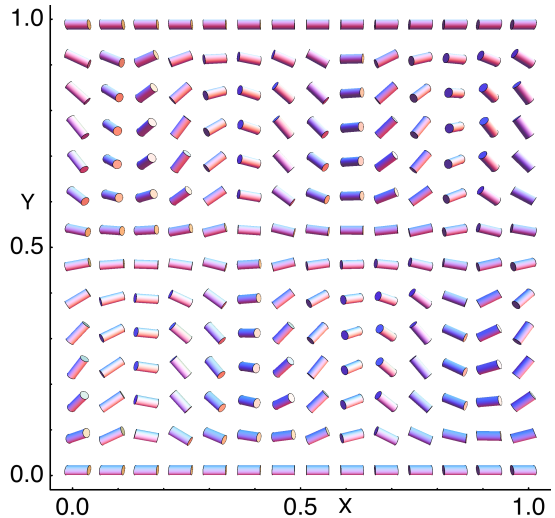


Computed solutions, found left-to-right order

- computed free energies are 59.378, 56.553, and 31.821

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Simple Cholesteric



Additional computed solution with $p = 2.0$ and $\alpha = 1.0$

- computed free energy is 41.480

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Simple Cholesteric

	Newton iteration counts						
Grid	(1)	(2)	(3)	(4)	(5)	(6)	Total Anon.
8×8	46	**56**	**50**	–	–	–	**100**
16×16	1	22	19	**87**	**55**	–	**100**
32×32	1	12	10	8	12	–	**228**
64×64	1	7	5	4	7	–	**233**
128×128	1	2	2	2	2	**63**	**200**
256×256	1	2	2	2	2	2	**253**

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Simple Cholesteric

	Average multigrid iteration counts					
Grid	(1)	(2)	(3)	(4)	(5)	(6)
8×8	46.2	**52.9**	**11.3**	–	–	–
16×16	66.0	54.3	9.0	**67.7**	**66.8**	–
32×32	65.0	33.2	8.0	53.9	34.1	–
64×64	61.0	28.4	8.0	35.8	26.9	–
128×128	62.0	33.0	9.0	52.5	32.5	**29.0**
256×256	78.0	30.5	9.5	46.0	30.0	18.5
Work Units	100.7	103.7	28.5	156.9	108.7	493.0

1 WU = equivalent MG V-cycles on finest grid (256×256)

Adler, Emerson, Farrell, MacLachlan, SISC 2017

Geometric Frustration

Interesting Physics happens with cholesteric LCs in elliptical domains

- In circular domains, cholesterics can form layers matching preferred pitch, just as in rectangular case
- As aspect-ratio varies, promote competition between this desire to form layers and shape of domain
- This frustration leads to potentially large numbers of solutions, particularly as cholesteric pitch increases

Geometric Frustration

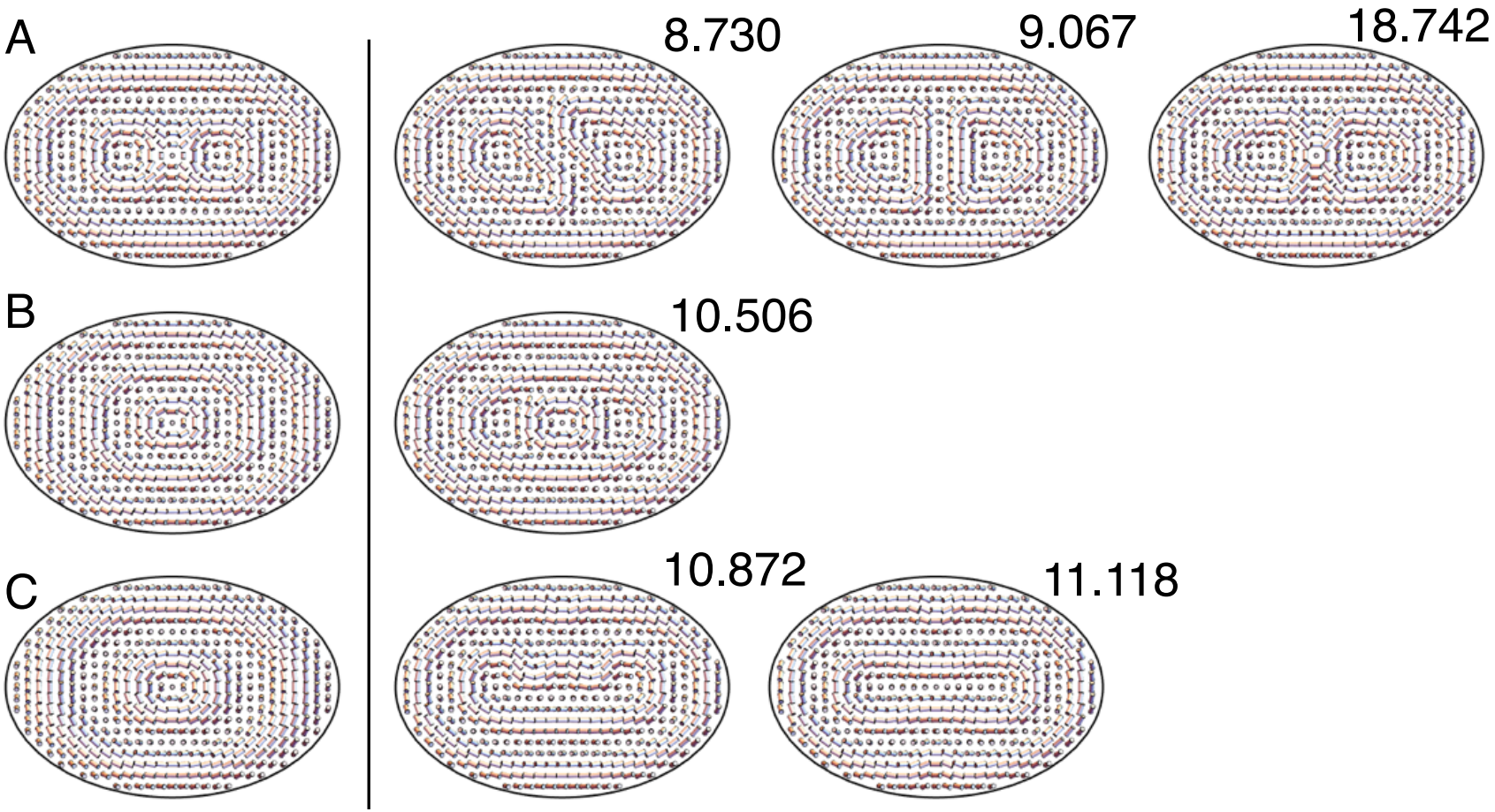
Interesting Physics happens with cholesteric LCs in elliptical domains

- In circular domains, cholesterics can form layers matching preferred pitch, just as in rectangular case
- As aspect-ratio varies, promote competition between this desire to form layers and shape of domain
- This frustration leads to potentially large numbers of solutions, particularly as cholesteric pitch increases

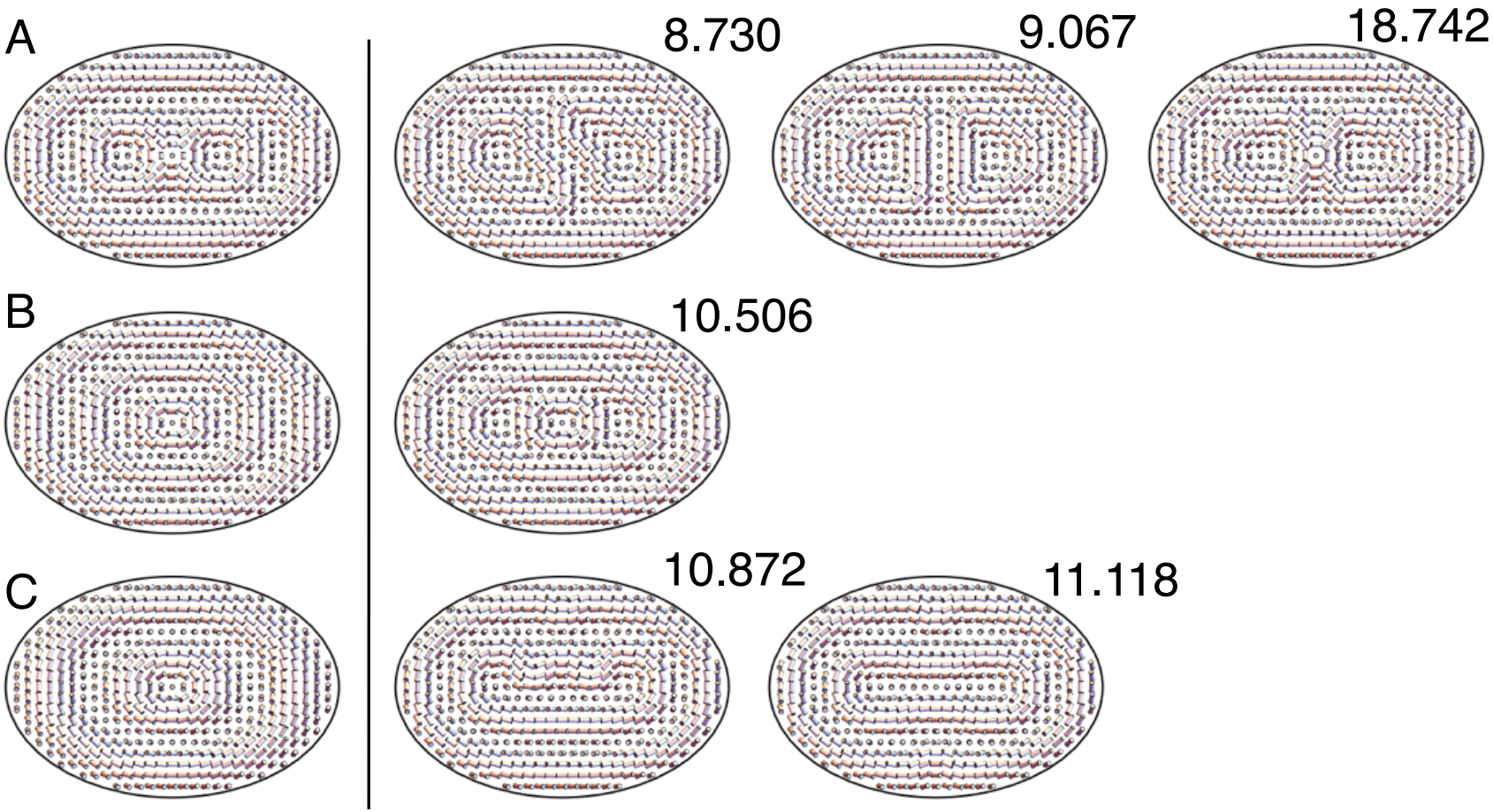
Consider ellipses of area $3\pi/2$

- $K_1 = 1.0$, $K_2 = 3.2$, $K_3 = 1.1$
- Vary aspect ratio, μ, and cholesteric pitch, q_0

First Example: $\mu = 1.5$, $q_0 = 8$



First Example: $\mu = 1.5$, $q_0 = 8$



None of these is a minimizer of the energy!

Ground State and Stability

Believe we should have unique *stable* "ground-state solution" to equilibrium equations

How do we compute stability?

Nocedal and Wright, Numerical Optimization (Springer Verlag, 2006).

Ground State and Stability

Believe we should have unique *stable* "ground-state solution" to equilibrium equations

How do we compute stability?

- Discretized system is of saddle-point form, given constrained free-energy density
- Solution is stable if Hessian projected onto nullspace of the linearized constraints is positive-definite
- Relate this to number of negative eigenvalues of saddle-point system, count these using LDL^T factorization

---

Nocedal and Wright, Numerical Optimization (Springer Verlag, 2006).

How Reliable Is Deflation + Nested Iteration?

Consider two-dimensional parameter space

- 7 values of μ: 1.0, 1.15, 1.35, 1.5, 1.65, 1.85, 2.0
- 8 values of q_0: 3, 4, 5, 6, 7, 8, 9, 10

Out of 56 trials, 10 yield lowest-energy solutions that are unstable

- Occur for both small and large μ, q_0

How Reliable Is Deflation + Nested Iteration?

Consider two-dimensional parameter space

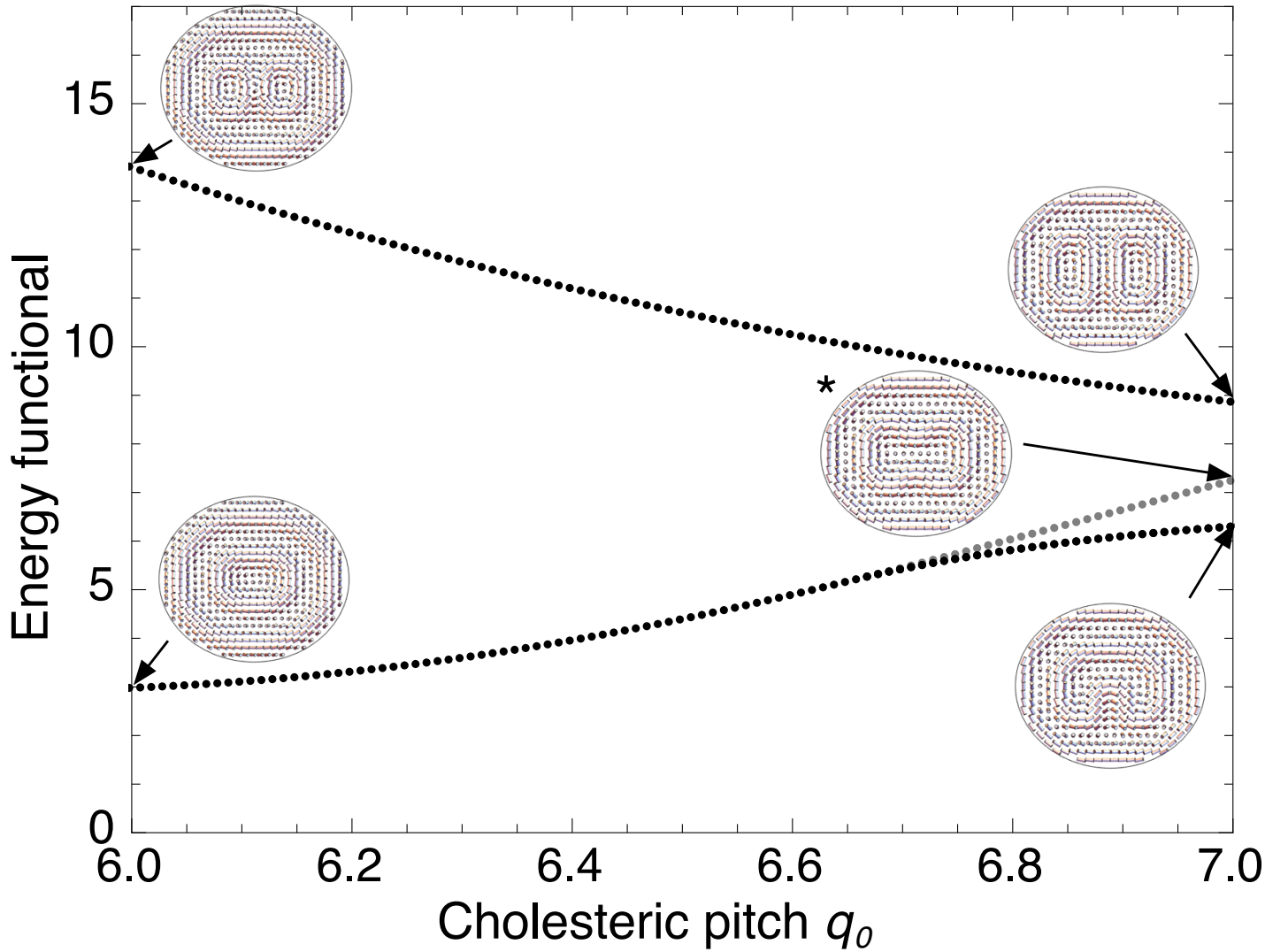
- 7 values of μ: 1.0, 1.15, 1.35, 1.5, 1.65, 1.85, 2.0
- 8 values of q_0: 3, 4, 5, 6, 7, 8, 9, 10

Out of 56 trials, 10 yield lowest-energy solutions that are unstable

- Occur for both small and large μ, q_0

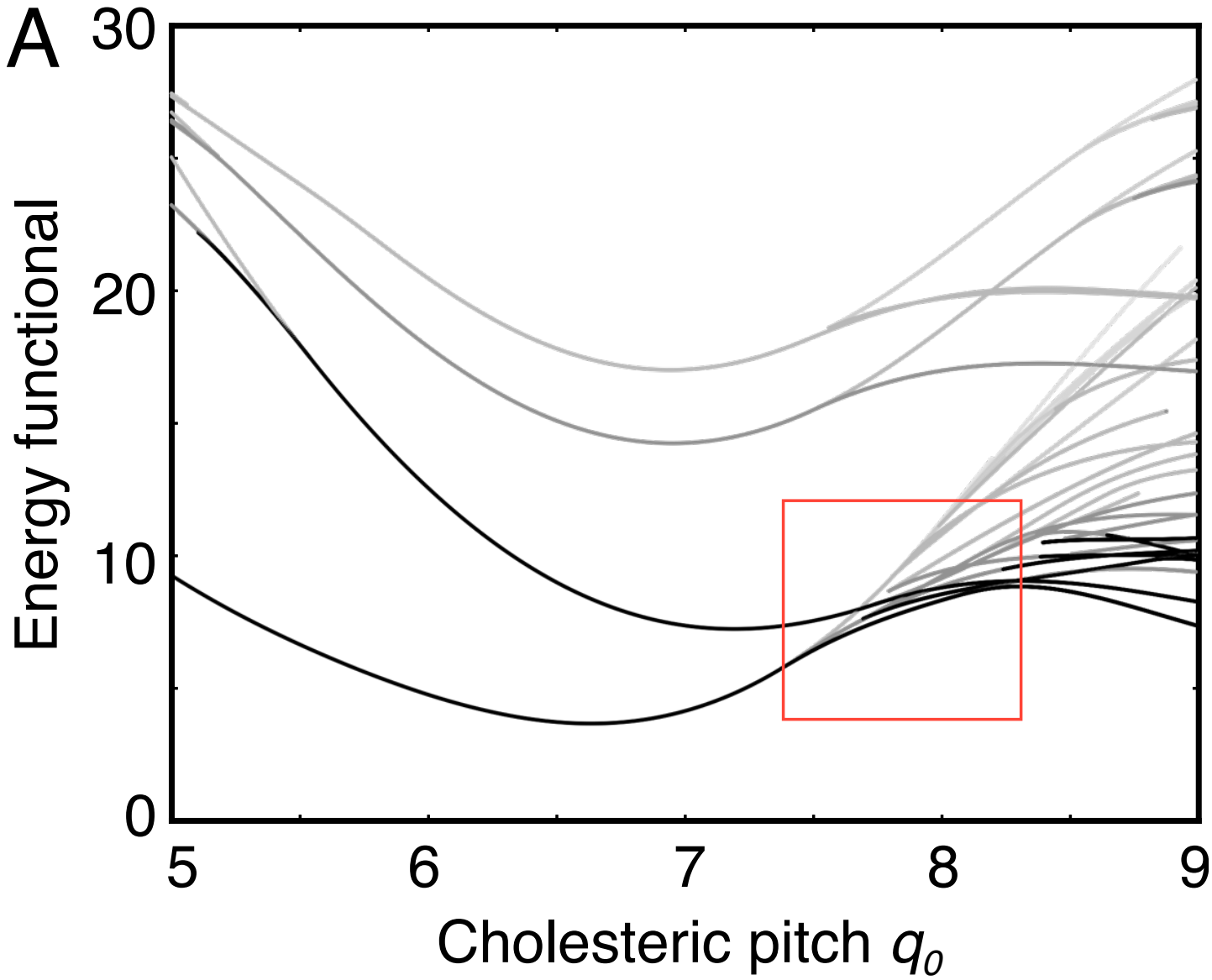
Use deflation + continuation to more reliably identify ground states

Bifurcation for $\mu = 1.15$



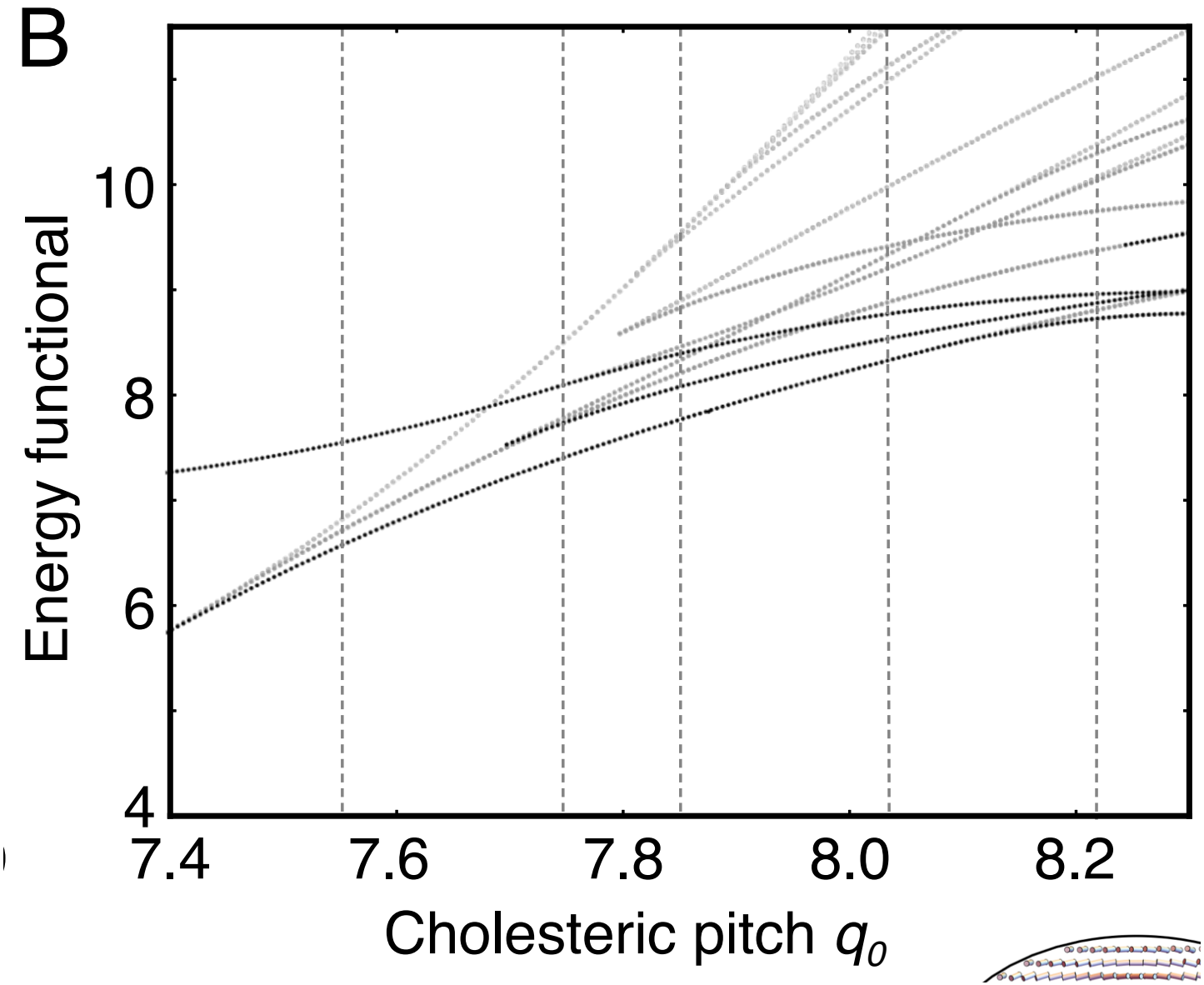
Emerson, Farrell, Adler, MacLachlan, Atherton, Liquid Crystals 2018

Bifurcation for $\mu = 1.5$



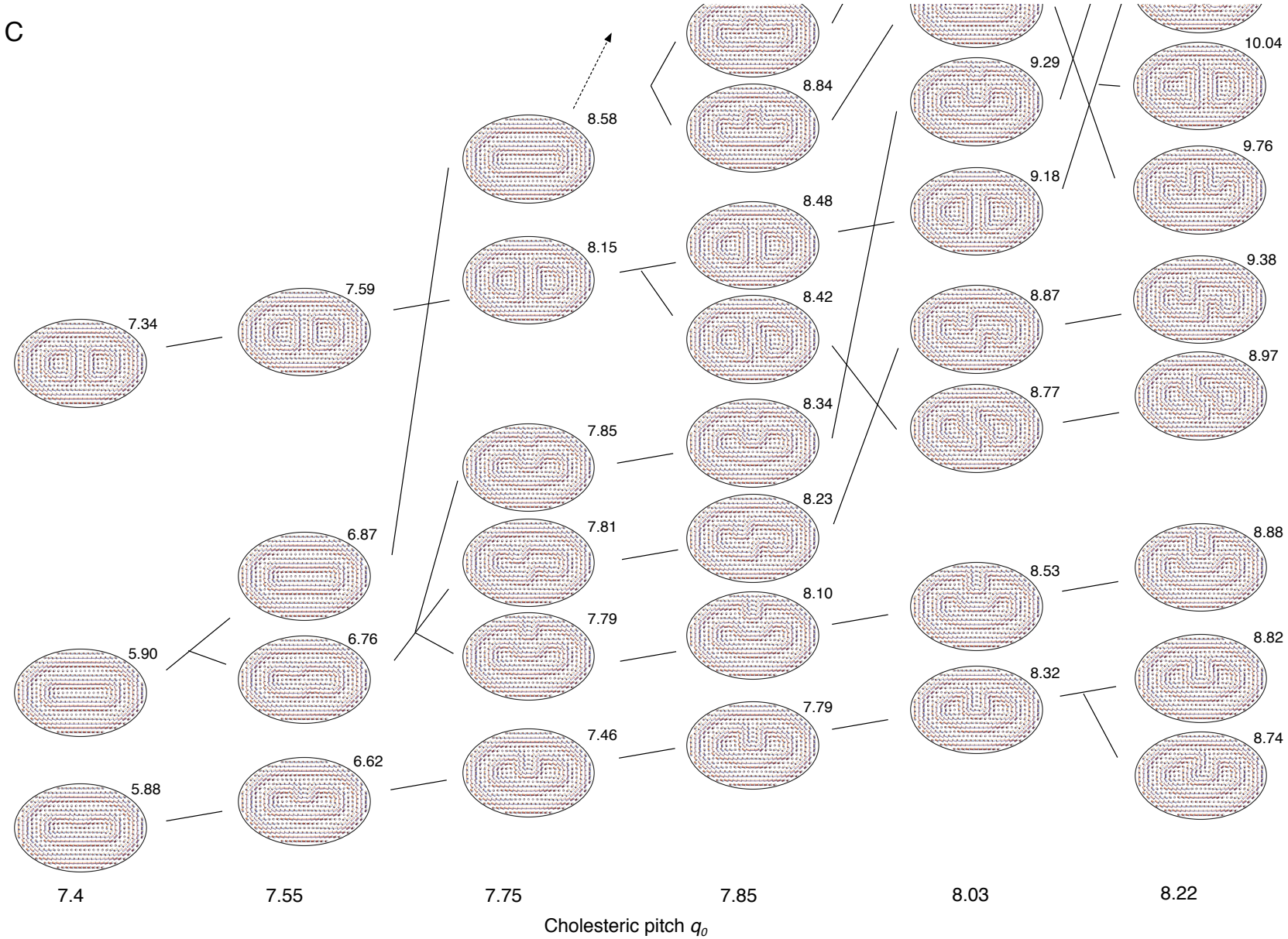
Emerson, Farrell, Adler, MacLachlan, Atherton, Liquid Crystals 2018

Bifurcation for $\mu = 1.5$



Emerson, Farrell, Adler, MacLachlan, Atherton, Liquid Crystals 2018

Bifurcation for $\mu = 1.5$



Emerson, Farrell, Adler, MacLachlan, Atherton, Liquid Crystals 2018

Effects of Temperature

Spectrum of behaviours of liquid crystals

- At sufficiently high temperatures, they act like liquids
- As temperature drops, enter nematic phase
- As temperature drops further, enter smectic phases
- At sufficiently low temperatures, they act like solids

In nematic phase, see no long-range ordering in alignment between crystals

Effects of Temperature

Spectrum of behaviours of liquid crystals

- At sufficiently high temperatures, they act like liquids
- As temperature drops, enter nematic phase
- As temperature drops further, enter smectic phases
- At sufficiently low temperatures, they act like solids

In nematic phase, see no long-range ordering in alignment between crystals

In smectic phases, we do see long-range ordering, as well as asymmetry in behaviour

Models for Smectic A LCs

Various models for Smectic A LCs - we use

$$F(\delta\rho, Q) = \int_\Omega \left[\frac{a}{2}(\delta\rho)^2 + \frac{b}{3}(\delta\rho)^3 + \frac{c}{4}(\delta\rho)^4 \right.$$
$$\left. + B\left| \mathcal{D}^2\delta\rho + q^2\left(Q + \frac{I_d}{d}\right)\delta\rho \right|^2 + \frac{K}{2}|\nabla Q|^2 + l f_n(Q) \right],$$

with

$$f_n(Q) = \begin{cases} -\left(\mathrm{tr}(Q^2)\right) + \left(\mathrm{tr}(Q^2)\right)^2 & \text{in 2D} \\ -\frac{1}{2}\left(\mathrm{tr}(Q^2)\right) - \frac{1}{3}\left(\mathrm{tr}(Q^3)\right) + \frac{1}{2}\left(\mathrm{tr}(Q^2)\right)^2 & \text{in 3D} \end{cases}$$

Xia, MacLachlan, Atherton, Farrell, Phys. Rev. Lett. 2021

Q-tensor

Choice of $f_n(Q)$ weakly enforces that

$$Q = \boldsymbol{n} \otimes \boldsymbol{n} - \frac{I_d}{d},$$

where $\boldsymbol{n}$ is the same director as in nematic case.

With this, dominant term for density variation is

$$\int_\Omega \left| \mathcal{D}^2 \delta\rho + q^2 \left(Q + \frac{I_d}{d} \right) \delta\rho \right|^2 = \int_\Omega \left| \mathcal{D}^2 \delta\rho + q^2 \boldsymbol{n} \otimes \boldsymbol{n} \delta\rho \right|^2$$

- Energy is quadratic in Hessian of $\delta\rho$
- Expect solutions like $\delta\rho \sim e^{\imath q \boldsymbol{n} \cdot \boldsymbol{x}}$

Discretization and Well-Posedness

Analysis of well-posedness has several pieces

- Fourth-order term in $\delta\rho$
- Coupling between $\delta\rho$ and Q
- Wave-like behaviour
- Penalty terms

We consider a variety of discretizations

- Conforming (too expensive)
- C^0 interior penalty methods (no efficient solvers)
- Mixed formulations (harder theory)

Have variety of results around well-posedness and error estimates

---

A. Hamdan's Ph.D. thesis, in progress

Some simulations

Two 2D simulations, visualize $\delta\rho$:

- Periodic rectangular domain, anchor $\boldsymbol{n}$ to fixed angle, θ_0, at top and bottom of domain. How does lowest-energy solution structure change with θ_0?
- Rectangular domain of aspect ratio τ, anchor $\boldsymbol{n}$ to be horizontal on bottom, vertical on other 3 sides. How does lowest-energy solution change with τ?

One 3D simulation, visualize zero isosurfaces of $\delta\rho$:

- Fix $\boldsymbol{n}$ to be radially oriented on bottom of a box
- Fix $\boldsymbol{n}$ to be tilted, $\pi/12$ from vertical, on top
- Find 3 solutions that are close in energy

Xia, MacLachlan, Atherton, Farrell, Phys. Rev. Lett. 2021

Smectic C Models

Near crystal regime, enter Smectic C phase

- $\boldsymbol{n}$ orients at fixed angle, θ, to layer normal, $\boldsymbol{a}$
- Layer tangent vector, $\boldsymbol{c}$, gives $\boldsymbol{n} = \boldsymbol{a}\cos\theta + \boldsymbol{c}\sin\theta$
- Marked by strong anisotropy in energy coefficients

Elastic energy density is given by

$$\begin{aligned}
&\frac{K_1}{2}(\nabla\cdot\boldsymbol{a})^2 + \frac{K_2}{2}(\nabla\cdot\boldsymbol{c})^2 \\
&+ \frac{K_3}{2}(\boldsymbol{a}\cdot\nabla\times\boldsymbol{c})^2 + \frac{K_4}{2}(\boldsymbol{c}\cdot\nabla\times\boldsymbol{c})^2 + \frac{K_5}{2}((\boldsymbol{a}\times\boldsymbol{c})\cdot\nabla\times\boldsymbol{c})^2 \\
&+ K_6(\nabla\cdot\boldsymbol{a})((\boldsymbol{a}\times\boldsymbol{c})\cdot\nabla\times\boldsymbol{c}) + K_7(\boldsymbol{a}\cdot\nabla\times\boldsymbol{c})(\boldsymbol{c}\cdot\nabla\times\boldsymbol{c}) \\
&+ K_8(\nabla\cdot\boldsymbol{c})((\boldsymbol{a}\times\boldsymbol{c})\cdot\nabla\times\boldsymbol{c}) + K_9(\nabla\cdot\boldsymbol{a})(\nabla\cdot\boldsymbol{c})
\end{aligned}$$

Have $K_1, K_5, K_6 \gg 1$, other constants $\mathcal{O}(1)$

---

with J. Jackaman, in progress

Summary and Future Work

- LC models are complicated, best understood from energy perspective
- Finite-element framework is natural
- Need advanced nonlinear solvers to see interesting physical behaviours
  - Deflation, continuation, damping of Newton, ...
- Also need advanced linear solvers to efficiently compute in parallel
- Working frameworks for nematics, smectic A, and smectic C LCs

Simulations have caught up to known physics, now exploring new questions