A Ginzburg-Landau Type Problem for Nematics with Highly Anisotropic Elastic Term

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Conference in Honor of Bernard Helffer

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$$E = \int (\text{Bulk potential favoring one or more states})$$

$$+$$

$$\int (\text{Elastic energy density penalizing deformations})$$

In a series of projects we have pursued the question:

What happens when certain types of deformations (e.g. stretching, twisting, bending etc.) are penalized much more heavily than others?

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Motivation: nematic/isotropic phase transitions in liquid crystals

A liquid crystal in a nematic state consists of thin molecules that can be characterized by a *director* field $\mathbf{n} : \Omega \to \mathbb{S}^2$. Here $\mathbf{n}(x)$ represents local orientation of nematic molecules near a point $\mathbf{x}$ in the material sample Ω.

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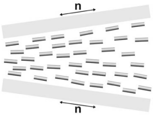
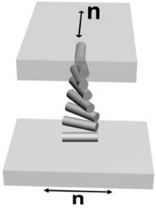
Oseen-Frank Model elastic energy density

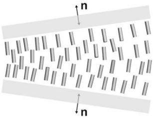
$$f_{OF}(\mathbf{n}, \nabla \mathbf{n}) := \frac{K_1}{2}(\operatorname{div}\mathbf{n})^2 + \frac{K_2}{2}(\operatorname{curl}\mathbf{n}\cdot\mathbf{n})^2 + \frac{K_3}{2}|\operatorname{curl}\mathbf{n}\times\mathbf{n}|^2 + \frac{K_2+K_4}{2}\left(\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2\right)$$



Splay



Twist



Bend

Saddle Splay

Oseen-Frank with strong anchoring:

Minimize

$$\mathcal{F}_{OF}[\mathbf{n}] \quad := \quad \int_\Omega \left\{ \frac{K_1}{2}(\operatorname{div}\mathbf{n})^2 + \frac{K_2}{2}(\operatorname{curl}\mathbf{n}\cdot\mathbf{n})^2 + \frac{K_3}{2}|\operatorname{curl}\mathbf{n}\times\mathbf{n}|^2 \right\}$$

in $H^1(\Omega,\mathbb{S}^2)$ or $H^1(\Omega,\mathbb{S}^1)$ subject to the appropriate Dirichlet boundary data g. Invoking the identity:

$$(\operatorname{div}\mathbf{n})^2 + (\operatorname{curl}\mathbf{n})^2 = |\nabla\mathbf{n}|^2 \; + \; \text{null Lagrangian}$$

and assuming that $K_2 = K_3$ we need only retain two of the elastic terms, say

$$|\nabla\mathbf{n}|^2 \quad \text{and} \quad (\operatorname{div}\mathbf{n})^2.$$

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Relaxed model for thin film nematics

Relax the constraint $\mathbf{n} \in \mathbb{S}^1$ by replacing $\mathbf{n}$ by $\mathbf{u} \in \mathbb{R}^2$ with a penalty for $|\mathbf{u}|$ deviating from 1. Take $\Omega \subset \mathbb{R}^2$, so $u : \Omega \to \mathbb{R}^2$.

Upon rescaling, we arrive at a functional that will be the focus of this talk:

$$\boxed{E_\varepsilon(\mathbf{u}) = \frac{1}{2}\int_\Omega \frac{1}{\varepsilon}(|\mathbf{u}|^2 - 1)^2 + \varepsilon\,|\nabla \mathbf{u}|^2 + L(\operatorname{div}\mathbf{u})^2\,dx.}$$

Here $L > 0$ is independent of $\varepsilon > 0$, whereas $\varepsilon \ll 1$, so splay is penalized much more heavily than bending.

Admissible competitors $\mathbf{u}$ must lie in $H^1(\Omega; \mathbb{R}^2)$ and satisfy an S^1-valued Dirichlet condition

$$\mathbf{u} = g \text{ on } \partial\Omega \quad \text{for some } g \in H^{1/2}(\partial\Omega; S^1).$$

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With this choice of potential favoring S^1 there will not be isotropic regions, hence no nematic/isotropic phase boundaries, but...

We are interested in identifying any other **singular structures** such as vortices and domain walls (both smooth and non-smooth) that arise as $\varepsilon \to 0$.

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Two asymptotic limits for the term $L\int (\mathrm{div}\,\mathrm{u})^2\,\mathrm{dx}$

• Note that if one takes $L = 0$ in E_ε, then this is precisely the famous Brezis-Bethuel-Helein [BBH] problem, multiplied by ε:

$$\boxed{\inf_{\mathbf{u}\in H^1_g(\Omega;\mathbb{R}^2)} E_\varepsilon^{BBH}(u) := \frac{1}{2}\int_\Omega \frac{1}{\varepsilon}(|\mathbf{u}|^2 - 1)^2 + \varepsilon\,|\nabla \mathbf{u}|^2\,dx,}$$

whose minimizers are characterized by Ginzburg-Landau vortices.

• On the other hand, if we formally consider the limit $L \to \infty$ so that competitors $\mathbf{u}$ are required to be divergence-free, then writing $\mathbf{u} = (\nabla v)^\perp$ for some scalar $v : \Omega \to \mathbb{R}$ we find that E_ε takes the form

$$\boxed{E_\varepsilon^{AG}(v) := \frac{1}{2}\int_\Omega \frac{1}{\varepsilon}(|\nabla v|^2 - 1)^2 + \varepsilon\,\left|D^2 v\right|^2\,dx,}$$

which is the well-known Aviles-Giga energy, whose minimizers in the limit $\varepsilon \to 0$ are characterized by wall-type singularities.

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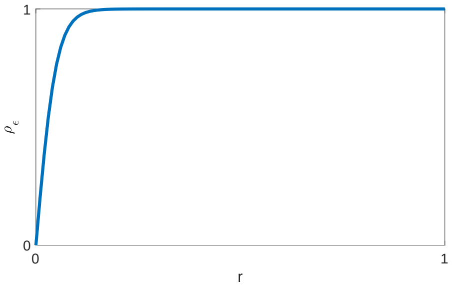
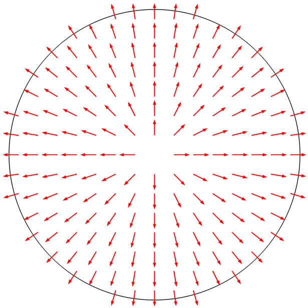
Singular structures in this model: a GL vortex

- Ginzburg-Landau type vortex $u_\varepsilon = \rho_\varepsilon(r)(\cos\theta, \sin\theta)$–expensive!

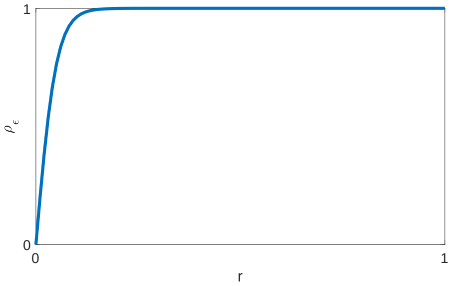


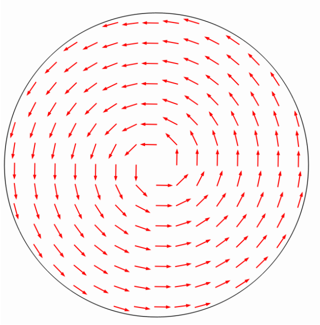


$$L\int_\Omega (\mathrm{div}\, u)^2\, dx \sim L|\ln\varepsilon| \quad \text{so} \quad E_\varepsilon(u_\varepsilon) \to \infty.$$

Singular structures in this model: a zero divergence vortex

- A divergence-free vortex $u_\varepsilon = \rho_\varepsilon(r)(-\sin\theta, \cos\theta)$–cheap!





$$\operatorname{div} u_\varepsilon \equiv 0 \quad \text{so} \quad E_\varepsilon(u_\varepsilon) \sim \varepsilon \int_\Omega |\nabla u|^2 \sim \varepsilon |\ln \varepsilon| \to 0$$

Singular structures: a domain wall

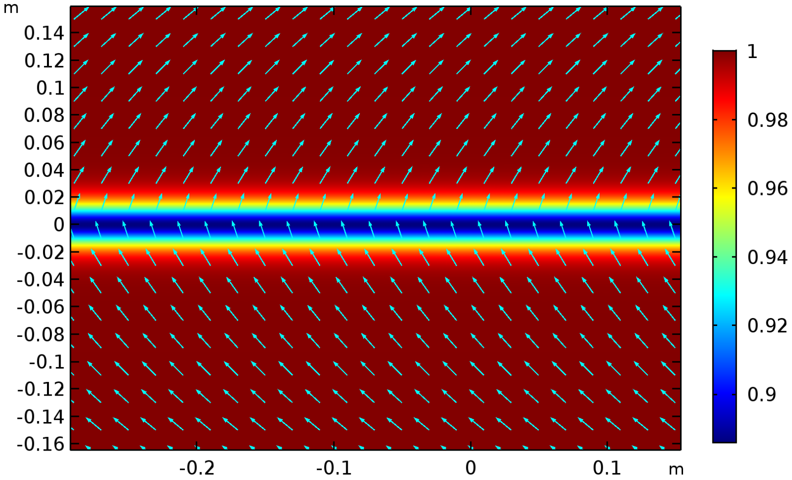


Figure: u and $|u|$.

Note: Continuity of normal component across the (vertical) jump.

The right space of competitors for a limiting problem

Given that energy-bounded sequences $E_\varepsilon(\mathbf{w}_\varepsilon) < C$ satisfy the bounds

$$||\mathrm{div}\,\mathbf{w}_\varepsilon||_{L^2(\Omega)} < C \quad \text{and} \quad \int_\Omega (|\mathbf{w}_\varepsilon|^2 - 1)^2\,dx < C\varepsilon^2,$$

it makes sense to seek a limiting problem defined for

$$\mathbf{u} \in H_{\mathrm{div}}(\Omega; S^1) := \{\mathbf{u} \in L^2(\Omega; S^1) : \ \mathrm{div}\,\mathbf{u} \in L^2(\Omega)\}.$$

Key point: **Functions $\mathbf{u} \in H_{\mathrm{div}}(\Omega; S^1)$ are allowed to have jump discontinuities across a curve provided $\mathbf{u} \cdot \mathbf{n}$ is continuous.**
(In particular, the normal trace is well-defined.)
Since $|\mathbf{u}| = 1$ on either side of the jump, this means across the "jump set" J_u the tangential component simply switches signs:

$$\mathbf{u}^+ \cdot \tau = -\mathbf{u}^- \cdot \tau,$$

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Towards a Γ-Convergence result: Compactness

With only a minor modification of the compactness proof of DeSimone, Kohn, Müller, Otto (2001) for the Aviles-Giga functional, one has:

Theorem

Assume $\{\mathbf{v}_\varepsilon\} \subset H^1(\Omega)$ satisfies the uniform energy bound

$$\sup_{\varepsilon>0} E(\mathbf{v}_\varepsilon) = \sup_{\varepsilon>0} \frac{1}{2}\int_\Omega \frac{1}{\varepsilon}(|\mathbf{v}_\varepsilon|^2 - 1)^2 + \varepsilon\,|\nabla \mathbf{v}_\varepsilon|^2 + L(\operatorname{div}\mathbf{v}_\varepsilon)^2\,dx < \infty.$$

Then there exists a subsequence (still denoted by $\mathbf{v}_\varepsilon$) and a function $\mathbf{v} \in H_{\mathrm{div}}(\Omega; S^1)$ such that $\mathbf{v}_\varepsilon \overset{\triangle}{\rightharpoonup} \mathbf{v}$ defined as

$$\operatorname{div}\mathbf{v}_\varepsilon \rightharpoonup \operatorname{div}\mathbf{v} \quad \textit{weakly in } L^2$$
$$\mathbf{v}_\varepsilon \to \mathbf{v} \quad \textit{in } L^2(\Omega;\mathbb{R}^2) \quad \textit{[DKMO].}$$

Note: Under this convergence, if $\mathbf{v}_\varepsilon = g$ on $\partial\Omega$ then $\mathbf{v}\cdot\mathbf{n} = g\cdot\mathbf{n}$.

Asymptotic cost of a horizontal domain wall along $y = 0$

To smoothly approximate, say, a horizontal wall across which $\mathbf{u}$ jumps from $\big(-\sqrt{1-a^2}, a\big)$ to $\big(\sqrt{1-a^2}, a\big)$ for some $a \in [0,1)$ in an energetically efficient way, a natural ansatz is:

$$\mathbf{u}_\varepsilon(x,y) = \big(\zeta(\frac{y}{\varepsilon}), a\big) \text{ with } \zeta(\pm\infty) = \pm\sqrt{1-a^2}$$

where $a =$ normal (here 2nd) component of $\mathbf{u}(x,0)$.

The optimal such profile $\zeta(y)$ is given by the heteroclinic connection (hyperbolic tangent profile) minimizing

$$F(\zeta) := \int_{-\infty}^{\infty} (\zeta_y)^2 + (1-a^2-\zeta^2)^2\, dy,\ \zeta(x,\pm\infty) \to \pm\sqrt{1-a^2}.$$

A direct calculation yields that in a neighborhood of this construction:

$$E_\varepsilon(\mathbf{u}_\varepsilon) \to \frac{1}{6}\int_{J_u} \left|\mathbf{u}^+ - \mathbf{u}^-\right|^3\, d\mathcal{H}^1$$

where J_u denotes the jump set of $\mathbf{u}$; in this example $J_u = (0,1)\times\{0\}$.

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These types of wall constructions are well-known from earlier studies in many different contexts:

smectic-A liquid crystals, thin film blistering, micromagnetics,...

Within the math community, there are *many* contributors including:

Ambrosio/DeLellis/Mantegazza, Aviles/Giga, Jin/Kohn, Conti/DeLellis, Ignat, James, Poliakovsky, Alouges/Riviere/Serfaty, and ***many*** **others...**

The Γ-limit:

What a uniform energy bound does *not* yield is that the limit lies in BV (cf. example by Ambrosio/De Lellis/Montegazza for Aviles-Giga)

However, we make this assumption and propose a candidate for the Γ-limit: For $\mathbf{u} \in H_{\mathrm{div}}(\Omega; S^1) \cap BV(\Omega; S^1)$ with $\mathbf{u} \cdot \mathbf{n} = g \cdot \mathbf{n}$ on $\partial\Omega$, let $E_0(\mathbf{u})$ be given by

$$E_0(\mathbf{u}) := \frac{1}{6} \int_{J_u \cap \Omega} \left| \mathbf{u}^+ - \mathbf{u}^- \right|^3 \, d\mathcal{H}^1 \quad + \quad \frac{1}{6} \int_{J_u \cap \partial\Omega} \left| \mathbf{u}_{|_{\partial\Omega}} - g \right|^3 \, d\mathcal{H}^1 + \frac{L}{2} \int_\Omega (\operatorname{div} \mathbf{u})^2 \, dx,$$

where $\mathbf{u}^+$ and $\mathbf{u}^-$ denote the traces of $\mathbf{u}$ on $J_u \cap \Omega$, and $\mathbf{u}_{|_{\partial\Omega}}$ denotes the trace of $\mathbf{u}$ along $\partial\Omega$.

Γ-convergence

Theorem

Let $\mathbf{u} \in H_{\mathrm{div}}\left(\Omega; S^1\right) \cap BV\left(\Omega; \mathbb{S}^1\right)$ *with* $\mathbf{u}_{\partial\Omega} \cdot \mathbf{n} = g \cdot \mathbf{n}$ *on* $\partial\Omega$

(i) If $\mathbf{u}_\varepsilon \in H^1_g(\Omega, \mathbb{R}^2)$ *is a sequence of functions such that* $\mathbf{u}_\varepsilon \xrightarrow{\triangle} \mathbf{u}$*, then*

$$\liminf_{\varepsilon \to 0} E_\varepsilon(\mathbf{u}_\varepsilon) \geqslant E_0(\mathbf{u}).$$

(ii) There exists $\mathbf{w}_\varepsilon \in H^1_g(\Omega; \mathbb{R}^2)$ *with* $\mathbf{w}_\varepsilon \xrightarrow{\triangle} \mathbf{u}$ *satisfying*

$$\limsup_{\varepsilon \to 0} E_\varepsilon(\mathbf{w}_\varepsilon) = E_0(\mathbf{u}).$$

The proof uses the ideas from Jin/Kohn and Alouges/Riviere/Serfaty (lower semicontinuity) and Conti/De Lellis (recovery sequence).

Criticality Conditions for E_0

Theorem

Suppose that $\mathbf{u} \in BV(\Omega, \mathbb{S}^1) \cap H_{\mathrm{div}}(\Omega, \mathbb{S}^1)$ *such that* $\mathbf{u}_{\partial\Omega} \cdot \mathbf{n} = g \cdot \mathbf{n}$ *on* $\partial\Omega$ *is a critical point of* E_0*. Denote by* J_u *its jump set. Then*

$$\mathbf{u}^{\perp} \cdot \nabla \mathrm{div}\, \mathbf{u} = 0 \text{ holds weakly on } \Omega \backslash J_u, \text{ where } \mathbf{u}^{\perp} = (-u_2, u_1)\,.$$

Furthermore, if the traces $\mathrm{div}\, \mathbf{u}_+$ *and* $\mathrm{div}\, \mathbf{u}_-$ *on* J_u *are sufficiently smooth, then*

$$L\,[\mathrm{div}\, \mathbf{u}] + 4\big(1 - (\mathbf{u} \cdot \nu_u)^2\big)^{1/2} (\mathbf{u} \cdot \nu_u) = 0 \text{ on } J_u \cap \Omega,$$

where $[a] = a_+ - a_-$ *represents the jump of* a *across* J_u *and* ν_u *is the unit normal to* J_u *pointing from the* $+$ *side of* J_u *to the* $-$ *side.*

One can also derive criticality conditions associated with variations of the jump set itself that involve curvature of J_u.

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A method of characteristics approach in the bulk

Corollary

Suppose $\mathbf{u}$ *is smooth and critical for* E_0*. Then writing* u *locally in terms of a lifting as* $\mathbf{u}(x,y) = \big(\cos\theta(x,y), \sin\theta(x,y)\big)$ *and defining the scalar* $v := \operatorname{div}\mathbf{u}$ *one has that the criticality condition*

$$\mathbf{u}^{\perp} \cdot \nabla \operatorname{div}\mathbf{u} = 0 \text{ on } \Omega \backslash J_u$$

is equivalent to the following system for the two scalars θ *and* v*:*

$$\begin{cases} -\sin\theta\, v_x + \cos\theta\, v_y = 0, \\ -\sin\theta\, \theta_x + \cos\theta\, \theta_y = v. \end{cases}$$

Integrating the characteristic system

$$x_t = -\sin\theta, \quad y_t = \cos\theta, \quad \theta_t = v \quad v_t = 0$$

one finds:

Characteristics are circular arcs that carry constant values of divergence and the curvature of each such circular arc is given by that constant divergence.

In case the divergence is zero, the corresponding characteristic is a straight line.

A basic example: Minimizing E_0 in a periodic strip

We first consider a basic example of a rectangle with periodic boundary conditions on the left and right sides:

Let $\Omega = [-T, T] \times [-H, H]$ and set

$$\begin{cases} g(-T, y) = g(T, y), & y \in [-H, H], \\ g(x, \pm H) = (\pm 1, 0), & x \in [-T, T]. \end{cases}$$

Goals:

• To understand how bulk divergence versus walls contribute to the total energy E_0

• To understand how strongly 1d configurations are favored.

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1D versions of E_ε and E_0

Let

$$\mathcal{A}^0 := \{\mathbf{u} = \mathbf{u}(y) \in H^1((-H,H);\mathbb{R}^2), \mathbf{u}(\pm H) = (\pm 1, 0)\}.$$

and consider the variational problem $\inf_{\mathbf{u}\in\mathcal{A}^0} E_\varepsilon^{1D}(\mathbf{u})$, where

$$\boxed{E_\varepsilon^{1D}(\mathbf{u}) := \frac{1}{2}\int_{-H}^{H} \varepsilon|\mathbf{u}'|^2 + \frac{1}{\varepsilon}(|\mathbf{u}|^2 - 1)^2 + L(u_2')^2\, dy.}$$

and one can prove that the Γ-limit restricted to 1D competitors is:

$$\boxed{E_0^{1D}(u) =: \frac{L}{2}\int_{-H}^{H} (u_2')^2\, dy + \frac{1}{6}\sum_{y_j\in J_{u_1}} \left|[u_1](y_j)\right|^3.}$$

In 1D the jump set only involves jumps in u_1 since $u_2 \in H^1$ and J_{u_1} consists of a set of points $\{y_j\}$.

Minimizers of the 1D Γ-limit

Theorem

(i) *If $L/H < 2$, the problem*

$$\inf_{\mathcal{A}^0} E_0^{1D}(\mathbf{u})$$

has a unique solution $\mathbf{u}^* = (u_1^*, u_2^*)$ where u_1^* has exactly one jump located at $y = 0$ and u_2^* is continuous on $[-H, H]$ and linear on the subintervals $[-H, 0]$ and $[0, H]$. The infimum of the energy is $E_0^{1D}(\mathbf{u}^*) = \frac{L}{H} - \frac{1}{12}\frac{L^3}{H^3}$.

(ii) *If $L/H > 2$ then the minimizer has the form*

$$u^*(y) = \begin{cases} (-1, 0) & \text{for } y \in (-H, y^*], \\ (1, 0) & \text{for } y \in (y^*, H), \end{cases}$$

where $y^* \in [-H, H]$ is arbitrary and the infimum of the energy is $E_0^{1D}(u^*) = 4/3$.

Computations in a rectangle. Is the minimizer 1d?

$L = 0.3, \ H = 0.5, \ T = 0.5, \ \varepsilon = 0.005$

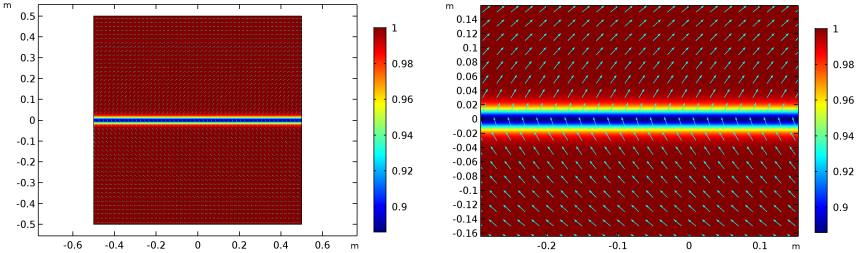

Figure: $|u|$ and u.

The 1d minimizer seems to also be the 2d minimizer.

$L = 0.5, \;\; H = 0.5, \;\; T = 0.3, \;\; \varepsilon = 0.005$

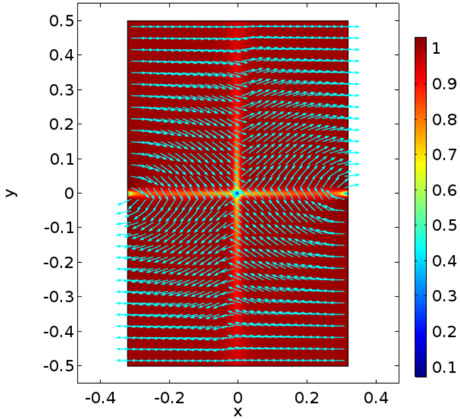

Figure: u and $|u|$.

$L = 0.5,\ \ H = 0.5,\ \ T = 0.3,\ \ \varepsilon = 0.005$

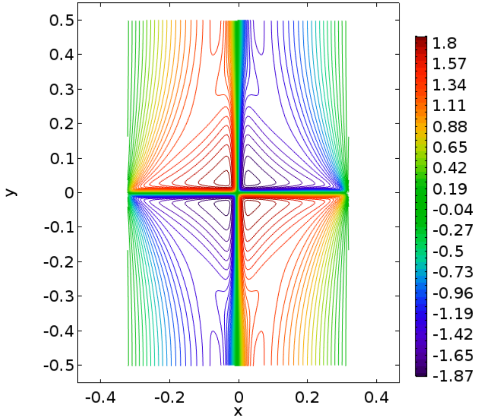

Figure: Level curves for the divergence of u.

Theorem

Consider the minimization problem for E_0 in the rectangle $\Omega = (-T, T) \times (-H, H)$, subject to the boundary conditions $\mathbf{u}(x, \pm H) = (\pm 1, 0)$. There exist constants $L_0 \approx 1.27$ and $L_1 \approx 2.14$ such that whenever $L/H \in (L_0, L_1)$ and $T = H\tilde{T}(L/H)$ where $\tilde{T}(L/H)$ solves a certain algebraic equation, we have

$$\frac{\inf E_0(\mathbf{u})}{2T} < \inf_{\mathcal{A}^0} E_0^{1D}(\mathbf{u}).$$

In a certain parameter regime, the "cross-tie" 2d solution is cheaper than the 1d solution.

Characteristics solution construction

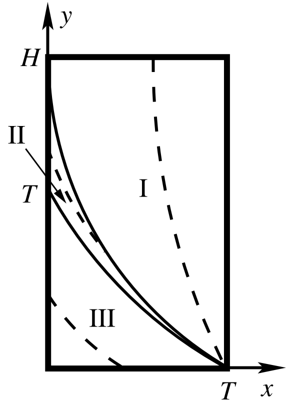

Figure: Regions corresponding to different characteristics families. Typical characteristics for each region are indicated by dashed lines.

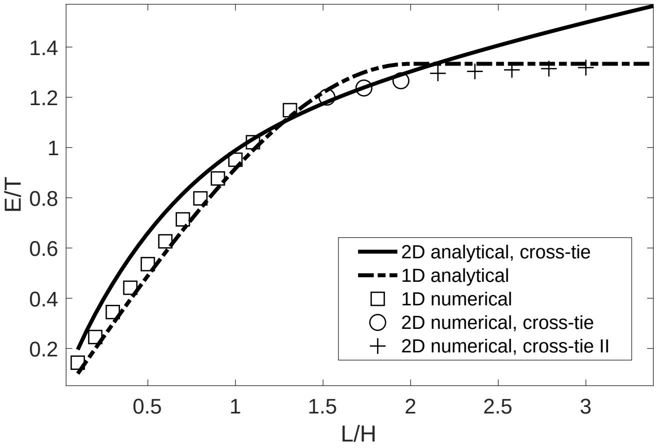

Figure: Energy per unit length.

For L/H between about 1.27 and 2.14 the minimizer is *not* 1D.

Upgrade to a model for nematic/isotropic transitions

Experimentally obtained phase boundaries:

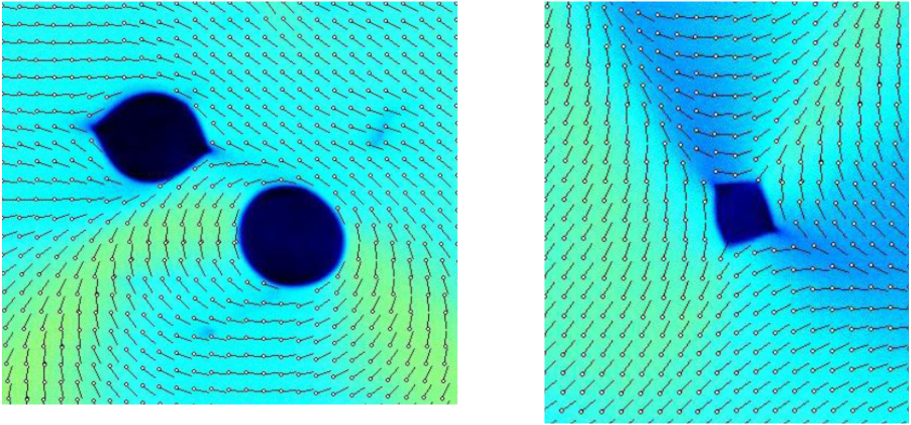

Figure: Isotropic tactoids in a nematic phase. Courtesy of O. D. Lavrentovich

Modeling: Include an extra potential well at the origin

We replace the Ginzburg-Landau potential $(1-|u|^2)^2$ with

$$|u|^2(1-|u|^2)^2$$

and consider the energies

$$\boxed{E_\varepsilon(u) := \frac{1}{2}\int_\Omega \frac{1}{\varepsilon}|u|^2(1-|u|^2)^2 + \varepsilon\,|\nabla u|^2 + L(\operatorname{div} u)^2\,dx.}$$

Correspondence:

$$u \approx 0 \quad \Longleftrightarrow \quad \text{isotropic state}$$

$$|u| \approx 1 \quad \Longleftrightarrow \quad \text{nematic state}$$

Singular Structures: Phase boundaries in addition to walls

In the $\varepsilon \to 0$ limit, in addition to wall singularities involving jumps between two S^1-valued states, now we also have:

<u>Phase boundaries</u> between S^1 nematic and 0 isotropic phases:

When $\mathbf{u}$ jumps between S^1-values and 0, continuity of $\mathbf{u} \cdot \nu$ means:

$\mathbf{u} \cdot \nu = 0$ from the nematic (S^1-valued) side, i.e.

Tangency to the phase boundary is required.

This turns out to be a mechanism for formation of phase boundary singularities. In both our model and in experiments appearance (or non-appearance) of phase boundary singularities related to degree of boundary conditions/far field conditions.

A Conjecture for the Γ-limit

Recall:

$$E_\varepsilon(\mathbf{u}) := \frac{1}{2}\int_\Omega \frac{1}{\varepsilon}|\mathbf{u}|^2(|\mathbf{u}|^2-1)^2 + \varepsilon\,|\nabla \mathbf{u}|^2 + L(\operatorname{div}\mathbf{u})^2\,dx.$$

We have an upper bound construction yielding the energy

$$E_0(\mathbf{u}) = \frac{L}{2}\int_\Omega (\operatorname{div}\,\mathbf{u})^2\,dx + \frac{K(0)}{2}\mathrm{Per}_\Omega(\{|\mathbf{u}|=1\}) + \int_{J_\mathbf{u}\cap\{|\mathbf{u}|=1\}} K(\mathbf{u}\cdot\nu)\,d\mathcal{H}^1,$$

for $\mathbf{u} \in (H_{\mathrm{div}} \cap BV)(\Omega; \mathbb{S}^1 \cup \{0\})$, where $J_\mathbf{u}$ is the jump set, and

$$K(z) := \int_{-\sqrt{1-z^2}}^{\sqrt{1-z^2}} \sqrt{z^2+y^2}\left(1-z^2-y^2\right)\,dy$$

is the asymptotic cost of a 1d transition in the tangential component.

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A lower bound on divergence–good degrees and bad degrees

Theorem

Fix $0 < \rho < \rho' \leqslant 1$, set $A := \{x \in \mathbb{R}^2 : \rho < |x| < \rho'\}$ and let C_t be a circle of radius t centered at the origin. Suppose that $u \in C^1(\overline{A}; \mathbb{R}^2)$ is such that $|u| \geqslant 1/2$ on A and $\deg(u, C_t) = d \neq 0, 1$ for any $t \in [\rho, \rho']$. Then

$$\int_A (\operatorname{div} u)^2 \, dx \geqslant |\pi d \log(\rho'/\rho) + 4|, \qquad d < 0,$$

$$\int_A (\operatorname{div} u)^2 \, dx \geqslant |\pi (d-1) \log(\rho'/\rho) - 4|, \qquad d > 1.$$

- This says that vortices of degree other than 0 or 1 are certainly expensive. Degree 1 vortices may or may not be expensive: e_r is expensive, e_θ is cheap.

Computations with boundary data of degree -2 and -3

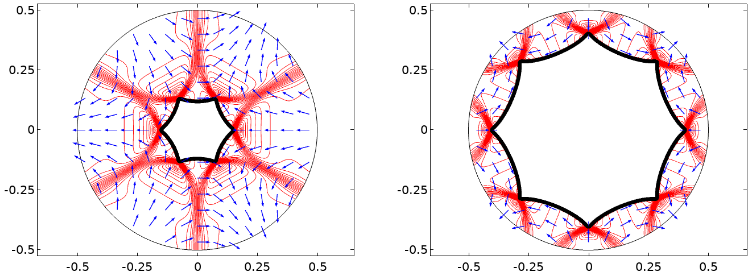

Figure: Notice the walls branching off of the singularities on the phase boundary.