A GINZBURG-LANDAU TYPE PROBLEM FOR NEMATICS WITH HIGHLY ANISOTROPIC ELASTIC TERM

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Suppose that a nematic occupies a thin domain with cross-section \( \Omega \subset \mathbb{R}^2 \) and \( n : \Omega \rightarrow S^1 \). The director field \( n(x) \) represents local orientation of nematic molecules near \( x \in \Omega \).

To formulate a continuum variational theory, need an energy functional that takes into account

- Elastic distortions of the director field \( n \) in \( \Omega \)
- Interactions of the nematic with the walls of the container, i.e. the boundary or anchoring conditions satisfied by the director field \( n \) on \( \partial \Omega \).
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Director-Based Theory–Thin Film Regime

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Oseen-Frank Model

**Oseen-Frank elastic energy density (Frank, 1958):**

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

- **Splay**
- **Twist**
- **Bend**
- **Saddle**
- **Splay**
Example: Oseen-Frank with strong anchoring:

Minimize

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

in $H^1(\Omega, S^1)$ subject to the appropriate Dirichlet boundary data $g$, i.e., $n|_{\partial\Omega} = g$ such as $n|_{\partial\Omega} =$ outer normal for the homeotropic anchoring.

Invoking the identity:

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

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

$$|\nabla n|^2 \quad \text{and} \quad (\text{div} n)^2.$$
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$$F_{OF}[\mathbf{n}] := \int_{\Omega} \left\{ \frac{K_1}{2} (\nabla \cdot \mathbf{n})^2 + \frac{K_2}{2} (\nabla \times \mathbf{n} \cdot \mathbf{n})^2 + \frac{K_3}{2} |\nabla \times \mathbf{n} \times \mathbf{n}|^2 \right\}$$

in $H^1(\Omega, S^1)$ subject to the appropriate Dirichlet boundary data $g$, i.e., $\mathbf{n}|_{\partial \Omega} = g$ such as $\mathbf{n}|_{\partial \Omega} =$ outer normal for the homeotropic anchoring.

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Relaxed model

Relax the constraint \( n \in S^1 \) by replacing \( n \) by \( u \in \mathbb{R}^2 \) with a penalty for \( |u| \) deviating from 1. The resulting functional resembles Ericksen model for a director \( u/|u| \) and variable degree of orientation (scalar) \( |u| \).

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

\[
E_\varepsilon(u) = \frac{1}{2} \int_\Omega \frac{1}{\varepsilon} (|u|^2 - 1)^2 + \varepsilon |\nabla u|^2 + L(\text{div } u)^2 \, dx.
\]

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

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

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

Notation: We’ll write \( u \in H^1_g(\Omega; \mathbb{R}^2) \) for such competitors.
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Motivation for the model

We are interested in capturing singular structures such as vortices and domain walls (both smooth and non-smooth) arising in nematic liquid crystal models that one might associate with a large disparity in the value of the elastic constants.

The model we look at here is a kind of ‘toy problem’ meant to isolate certain key features while for the time being ignoring other complicating factors associated with, say, the full Landau-deGennes Q-tensor theory or with double well potentials.
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Two asymptotic limits for the term $L \int (\text{div } u)^2 \, dx$

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

  $$\inf_{u \in H^1_{g}(\Omega; \mathbb{R}^2)} \frac{1}{2} \int_\Omega \frac{1}{\varepsilon} (|u|^2 - 1)^2 + \varepsilon |\nabla u|^2 \, dx,$$

  whose minimizers are characterized by Ginzburg-Landau vortices.

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

  $$E^{\text{AG}}_\varepsilon (v) := \frac{1}{2} \int_\Omega \frac{1}{\varepsilon} (|\nabla v|^2 - 1)^2 + \varepsilon |D^2 v|^2 \, dx,$$

  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!

\[ L \int_\Omega (\text{div } u)^2 \, dx \sim L|\ln \varepsilon| \quad \text{so} \quad E_\varepsilon(u_\varepsilon) \to \infty. \]
Singular structures in this model: a zero divergence vortex

- A divergence-free vortex \( \mathbf{u}_\varepsilon = \rho_\varepsilon(r)(-\sin \theta, \cos \theta) \)

\[
\text{div } \mathbf{u}_\varepsilon \equiv 0 \quad \text{so} \quad E_\varepsilon(\mathbf{u}_\varepsilon) \sim \varepsilon |\ln \varepsilon| \to 0
\]
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 \( E_\varepsilon(w_\varepsilon) < C \) satisfy the bounds

\[
\| \text{div} \, w_\varepsilon \|_{L^2(\Omega)} < C \quad \text{and} \quad \int_\Omega (|w_\varepsilon|^2 - 1)^2 \, dx < C \varepsilon^2,
\]

it makes sense to seek a limiting problem defined for

\[
u \in H_{\text{div}}(\Omega; S^1) := \{ u \in L^2(\Omega; S^1) : \text{div} \, u \in L^2(\Omega) \}.
\]

**Key point:** Functions \( u \in H_{\text{div}}(\Omega; S^1) \) are allowed to have jump discontinuities across a curve provided \( u \cdot n \) is continuous. (In particular, the normal trace is well-defined.)

Since \( |u| = 1 \) on either side of the jump, this means across the “jump set” the tangential component simply switches signs:

\[
u^+ \cdot \tau = -u^- \cdot \tau,
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where \( u^\pm \) denote the traces on either side of the jump set.
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Towards a $\Gamma$-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 \( \{v_\varepsilon\} \subset H^1(\Omega) \) satisfies the uniform energy bound

\[
\sup_{\varepsilon > 0} E(v_\varepsilon) = \sup_{\varepsilon > 0} \frac{1}{2} \int_\Omega \frac{1}{\varepsilon} (|v|^2 - 1)^2 + \varepsilon |\nabla v|^2 + L(|\text{div} \, v|^2) \, dx < \infty.
\]

Then there exists a subsequence (still denoted by \( v_\varepsilon \)) and a function \( v \in H_{\text{div}}(\Omega; S^1) \) such that \( v_\varepsilon \xrightarrow{\Delta} v \) defined as

\[
\text{div} \, v_\varepsilon \rightharpoonup \text{div} \, v \quad \text{weakly in } L^2 \\
v_\varepsilon \rightharpoonup v \quad \text{in } L^p(\Omega; \mathbb{R}^2) \text{ for all } p < \infty \quad [DKMO].
\]

**Note:** Under this convergence, if \( v_\varepsilon = g \) on \( \partial \Omega \) then \( v \cdot n = g \cdot n \).
Asymptotic cost of a horizontal domain wall along $y = 0$

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

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

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

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

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

A direct calculation yields

$$E_\varepsilon(u_\varepsilon) \to \frac{1}{6} \int_{J_u} |u^+ - u^-|^3 \, d\mathcal{H}^1 + \frac{L}{2} \int_{\Omega} (\text{div } u)^2 \, dx \, dy$$

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

Aviles/Giga, Jin/Kohn, Conti/DeLellis, Ignat, James, Poliakovky, Alouges/Riviere/Serfaty, and many others…
The $\Gamma$-limit:

What a uniform energy bound does \textit{not} yield is that the limit lies in $BV$ (cf. example by Ambrosio/De Lellis/Montegazza)

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

$$E_0(u) := \frac{1}{6} \int_{J_u \cap \Omega} |u^+ - u^-|^3 \, d\mathcal{H}^1 + \frac{1}{6} \int_{J_u \cap \partial\Omega} |u|_{\partial\Omega} - g|^3 \, d\mathcal{H}^1$$

$$+ \frac{L}{2} \int_{\Omega} (\text{div } u)^2 \, dx,$$

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

**Theorem**

Let \( u \in H_{\text{div}}(\Omega; S^1) \cap \text{BV}(\Omega; S^1) \) with \( u_{\partial \Omega} \cdot n = g \) on \( \partial \Omega \)

(i) If \( u_\varepsilon \in H^1_g(\Omega, \mathbb{R}^2) \) is a sequence of functions such that \( u_\varepsilon \rightharpoonup u \), then

\[
\liminf_{\varepsilon \to 0} E_\varepsilon(u_\varepsilon) \geq E_0(u).
\]

(ii) There exists \( w_\varepsilon \in H^1_g(\Omega; \mathbb{R}^2) \) with \( w_\varepsilon \rightharpoonup u \) satisfying

\[
\limsup_{\varepsilon \to 0} E_\varepsilon(w_\varepsilon) = E_0(u).
\]

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

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

Furthermore, if the traces $\text{div} u_+$ and $\text{div} u_-$ on $J_u$ are sufficiently smooth, then

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

where $[a] = a_+ - a_-$ represents the jump of $a$ across $J_u$ and $\nu_u$ 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 $u$ is smooth and critical for $E_0$. Then writing $u$ locally in terms of a lifting as $u(x, y) = (\cos \theta(x, y), \sin \theta(x, y))$ and defining the scalar $v := \text{div } u$ one has that the criticality condition

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

is equivalent to the following system for the two scalars $\theta$ 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

\[ x_t = -\sin \theta, \quad y_t = \cos \theta, \quad \theta_t = \nu \quad \nu_t = 0 \]

one finds:

*Characteristics are circular arcs that carry constant values of divergence and 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.
First example: a periodic strip

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

\[
\begin{aligned}
g(-T, y) &= g(T, y), \quad y \in [-H, H], \\
g(x, \pm H) &= (\pm 1, 0), \quad x \in [-T, T].
\end{aligned}
\]
1D versions of $E_\varepsilon$ and $E_0$

Let

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

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

$$E^{1D}_\varepsilon(u) := \frac{1}{2} \int_{-H}^{H} \varepsilon |u'|^2 + \frac{1}{\varepsilon} (|u|^2 - 1)^2 + L(u'_2)^2 \, dy.$$ 

and the $\Gamma$-limit restricted to 1D competitors:

$$E^{1D}_0(u) := \frac{L}{2} \int_{-H}^{H} (u'_2)^2 \, dy + \frac{1}{6} \sum_{y_j \in J_{u_1}} |[u_1](y_j)|^3.$$ 

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 $\{y_j\}$. 
Improved Compactness in 1D

**Theorem**

Let \( u_\varepsilon = (u_1^{(1)}(y), u_1^{(2)}(y)) \) be an energy-bounded sequence, i.e.

\[
E_1^{1D}(u_\varepsilon) \leq C.
\]

Then, up to extraction of subsequences, one has \( u_1^{(1)} \rightarrow u_1 \) in \( L^3(-H, H) \) for some function \( u_1 \) such that \( u_1^{(3)} \in BV(-H, H) \) and one has \( u_1^{(2)} \rightarrow u_2 \) in \( C^{0,\gamma} \) for all \( \gamma < 1/2 \). Furthermore, \( \left| \langle u_1(y), u_2(y) \rangle \right| = 1 \) a.e.
Minimizers of the 1D Γ-limit

Theorem

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

$$\inf_{A_0} E_{1D}^1(u)$$

has a unique solution $u^* = (u_1^*, u_2^*)$ 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 $E_{1D}^1(u^*) = \frac{L}{H} - \frac{1}{12} \frac{L^3}{H^3}$.

(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 $E_{1D}^1(u^*) = 4/3$. 
$L = 0.3, \ H = 0.5, \ T = 0.5, \ \varepsilon = 0.005$

Figure: $u$ and $|u|$. 
$L = 0.5$, $H = 0.5$, $T = 0.3$, $\varepsilon = 0.005$

Figure: $u$ and $|u|$. 
\( L = 0.5, \quad H = 0.5, \quad T = 0.3, \quad \varepsilon = 0.005 \)

**Figure:** Level curves for the divergence of \( u \).
Consider the minimization problem for $E_0$ in the rectangle $\Omega = (-T, T) \times (-H, H)$, subject to the boundary conditions $u(x, \pm H) = (\pm 1, 0)$. 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

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

Here the infimum on the left is taken over all $u \in H_{\text{div}} (\Omega; S^1) \cap BV(\Omega; S^1)$ such that $u \cdot n = 0$ on the top and bottom sides of the rectangle $y = \pm H$ and $u$ is $2T$-periodic in $x$. 
Figure: Regions corresponding to different characteristics families. Typical characteristics for each region are indicated by dashed lines.
$L = 0.5, \ H = 0.5, \ T = 0.3, \ \varepsilon = 0.005$

**Figure:** Level curves for the divergence of $u$.  

![Level curves for the divergence of $u$.](image)
For $L/H$ between about 1.27 and 2.14 the minimizer is not 1D.
Examples for $\Omega = \mathbb{D}$ (disk) under various boundary conditions

1. Examples where minimizers have no walls:

**Theorem**

For boundary conditions $\mathbf{u} \cdot \mathbf{n} = g \cdot \mathbf{n}$ on $\partial \mathbb{D}$ with

(i) $g = \hat{e}_\theta$ (tangential b.c.) or

(ii) $g = (x, y)$ (hedgehog b.c.)

the global minimizer of $E_0$ in $H_{\text{div}}(\mathbb{D}; S^1) \cap BV(\mathbb{D}; S^1)$ is

(i) $\mathbf{u} \equiv \hat{e}_\theta$ and

(ii) $\mathbf{u}_\pm(r, \theta) = r\hat{e}_r \pm \sqrt{1 - r^2}\hat{e}_\theta$, respectively.

In both examples, there is a divergence-free vortex at the origin and no jump set. In (i) $E_0(\hat{e}_\theta) = 0$.

In (ii) all of the minimizing energy comes from the divergence as the minimizer “unwinds” from $\hat{e}_\theta$ to $\hat{e}_r$. 
Examples for $\Omega = \mathbb{D}$ (disk) under various boundary conditions

II. An example with nontrivial wall structure:

Take as Dirichlet condition: $g(x, y) = (x, -y)$. These degree -1 boundary conditions induce walls.

At least for some parameter regimes of $L$, we can capture these analytically again using the conservation law approach.

We conclude with some numerical experiments with this boundary condition, letting $L$ increase.
Examples for $\Omega = \mathbb{D}$ (disk) under various boundary conditions

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Computed solution for $g(x, y) = (x, -y)$ with $L = 0.2$

Figure: $L = 0.2$. The field $\mathbf{u}$ and level curves of $|\mathbf{u}|$. 
Computed solution for $g(x, y) = (x, -y)$ with $L = 1.0$

**Figure:** $L = 1.0$. The field $\mathbf{u}$ and level curves of $|\mathbf{u}|$. 
Computed solution for $g(x, y) = (x, -y)$ with $L = 1.3$

Figure: $L = 1.3$. The field $\mathbf{u}$ and level curves of $|\mathbf{u}|$. 
Computed solution for $g(x, y) = (x, -y)$ with $L = 2.0$

Figure: $L = 2.0$. The field $\mathbf{u}$ and level curves of $|\mathbf{u}|$. 
Computed solution for $g(x, y) = (x, -y)$ with $L = 10.0$

Figure: $L = 10.0$. The field $u$ and level curves of $|u|$. 