Mathematical Continuum theories of Smectic Liquid Crystals

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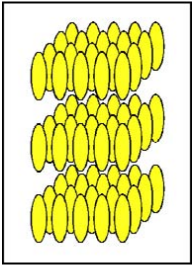
Outline

Liquid crystals

An intermediate phase between fluid and solid (orientationally ordered soft matter)

- Calamitic liquid crystals (rod like molecules)



Arrangement of molecules in a solid crystal

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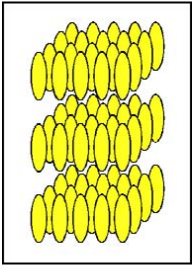

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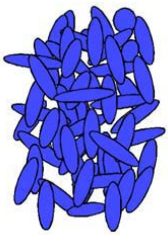

Arrangement of molecules in a liquid

- Molecular director $\mathbf{n}$: average molecular orientation, $|\mathbf{n}| = 1$

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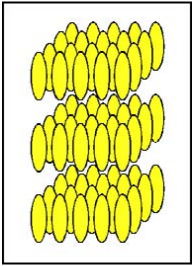

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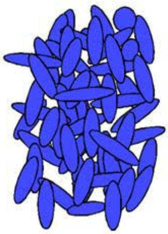

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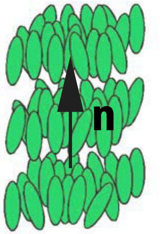


Arrangement of molecules in a liquid crystal

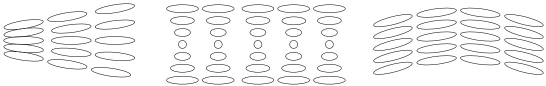
- Molecular director $\mathbf{n}$: average molecular orientation, $|\mathbf{n}| = 1$

Nematic Energy

Frank elastic energy density for nematic LC

$$f_n = K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2 + (K_2 + K_4)(tr(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2)$$

K_1 : splay, $(n_r, n_\theta, n_z) = (1, 0, 0)$
K_2 : twist, $(n_x, n_y, x_z) = (\cos\phi(z), \sin\phi(z), 0)$
K_3 : bend, $(n_r, n_\theta, n_z) = (0, 1, 0)$



Splay **Twist** **Bend**

The last term is null-Lagrangian;

$$tr(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2 = div[(\nabla \mathbf{n})\mathbf{n} - (div\mathbf{n})\mathbf{n}]$$

It depends only on the restriction of $\mathbf{n}$ and its tangential gradient to the boundary $\partial\Omega$.

Cholesteric liquid crystals

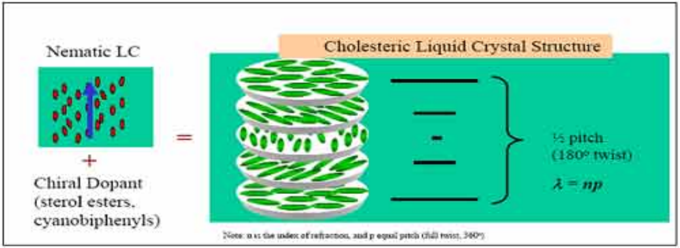
- One constant approximation: $K_1 = K_2 = K_3 = \frac{K}{2} > 0,\ K_4 = 0$

$$f_n = \frac{K}{2}|\nabla \mathbf{n}|^2.$$

- Cholesteric liquid crystals (Chiral nematics, N*)

$$\begin{aligned} f_{n^*} =& K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n} + \tau)^2 + K_3|\mathbf{n}\times(\nabla\times\mathbf{n})|^2 \\ &+ (K_2+K_4)(tr(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2) \end{aligned}$$

$f_{n^*}(\mathbf{n}_\tau) = 0$, where $\mathbf{n}_\tau(\mathbf{x}) = (\cos(\tau z), \sin(\tau z), 0)$.



dye & piements

Boundary conditions

- Strong anchoring condition (Dirichlet Boundary condition)
- Weak anchoring condition : add Rapini-Popoular surface energy

$$F_S = c \int_{\partial\Omega} (\mathbf{n} \cdot \mathbf{e})^2$$

  - If $c < 0$, $\mathbf{n}$ tends to be $\|$ to $\mathbf{e}$, $\mathbf{e}$ is an easy axis.
  - If $c > 0$, $\mathbf{n}$ tends to be $\perp$ to $\mathbf{e}$

Theorem (Hardt, Kinderlehrer, Lin)

Assume that $\partial\Omega$ is a smooth surface, $\mathbf{n}_0$ is smooth, and $K_1, K_2, K_3 > 0$. Then there is a minimizer of F_n in the class

$$\mathcal{A} = \{\mathbf{n} : \Omega \to \mathbb{S}^2, \mathbf{n}|_{\partial\Omega} = \mathbf{n}_0, \int_\Omega |\nabla \mathbf{n}|^2 < \infty\}$$

Defect

- $\mathbf{n}(x)$ may have singularities, eg, $\mathbf{n}_1 = \mathbf{e}_r$: line singularity
  - $\mathbf{n}_1$ satisfies Euler equation associated with the OF energy.
  - But, $\displaystyle\int_{\mathcal{C}} |\nabla \mathbf{n}_1|^2 = \infty$ where $\mathcal{C}$ is a cylinder. What is wrong?
- Oseen-Frank theory is limited: it can only account for point defects but not the more complicated line and surface defects.
- Ericksen theory: the state of the liquid crystal is described by a pair, $(s, n) \in \mathbb{R} \times \mathbb{S}^2$, where s is a real scalar order parameter that measures the degree of orientational ordering.

$$\int_{\Omega} s(x)^2 |\nabla \mathbf{n}|^2 + k|\nabla s|^2$$

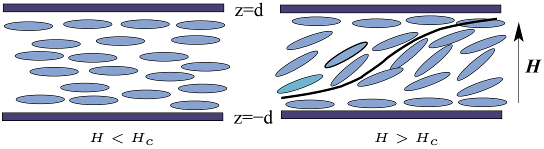
  where k is a material constant. This theory can account for all physically observable defects, but is restricted to uniaxial liquid crystal materials.

Landau-de Gennes theory

- This theory can account for both uniaxial and biaxial phases.
- The state of a nematic liquid crystal is modelled by a symmetric, traceless 3×3 matrix Q , known as the Q-tensor order parameter.
  - Isotropic phase when $Q = 0$
  - Uniaxial phase when $Q = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I)$
  - Biaxial phase when $Q = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I) + r(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3}I)$
- $f = f_e + f_b$ where

$$\begin{aligned} f_e &= \frac{L}{2}|\nabla Q|^2 \\ f_b &= a\,tr(Q^2) - b\,tr(Q^3) + c\,tr(Q^4) \end{aligned}$$

Frederiks effect : Splay geometry



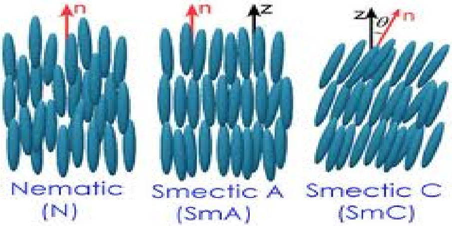
$$f = f_n - \frac{\chi_a}{2}(\mathbf{n}\cdot\mathbf{H})^2$$

- Special class of minimizers: $\mathbf{n} = \cos\theta(z)\mathbf{e}_1 + \sin\theta(z)\mathbf{e}_3$
- $\mathbf{H}_c = \dfrac{\pi}{2d}\sqrt{\dfrac{2K_1}{\chi_a}}$

Smectic Liquid Crystals

- Nematic phase : Orientational order
- Smectic phase : Orientational + 1d Positional order (layer)
  - Smectic A : molecules are perpendicular to the layers
  - Smectic C : molecules are tilted w.r.t. the layer normal
- Phase transitions

$$\text{Liquid} \longleftarrow \text{Nematic} \longleftarrow \text{Smectic} \longleftarrow \text{Solid}$$



Order parameter of Smectic phases

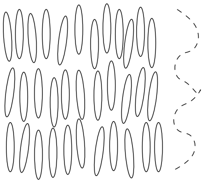
Order parameter $\Psi = \rho e^{iq\phi}$

- $\delta(\mathbf{x}) = \rho_0 + \frac{1}{2}(\Psi(\mathbf{x}) + \Psi^*(\mathbf{x})) = \rho_0 + \rho\cos(q\phi)$: mass density

  where ρ_0: locally uniform molecular mass density

  NEMATIC PHASE IF THE MINIMIZER $\Psi \equiv 0$.

- ϕ : layer position ($\nabla\phi$: layer normal)



Smectic A free energy density

$$f = f_n + f_A$$

deGenne energy

$$f_A = \frac{C}{2}|\nabla\Psi - iq\mathbf{n}\Psi|^2 + \frac{g}{2}(|\Psi|^2 - 1)^2$$

Assuming that $\Psi = \rho e^{i\varphi}$, f_A becomes

$$f_A = |\nabla\rho|^2 + \rho^2|\nabla\varphi - q\mathbf{n}|^2 + \frac{g}{2}(\rho^2 - 1)^2$$

- level sets of φ are layers, $\nabla\varphi \parallel \mathbf{n}$, and $q \approx |\nabla\varphi|$
- $|\nabla\rho|^2$ penalizes the phase transition.
  - $\rho = 1$: smectic phase.
  - $\rho = 0$: nematic phase

Free energy density for chiral smectic C LCs

Modified CHEN-LUBENSKY ENERGY by I.Luk'yanchuk '98

$$f = f_{n^*} + f_s = f_{n^*} + D\left|\mathbf{D}_\mathbf{n}^2\Psi\right|^2 - C_\perp\left|\mathbf{D}_\mathbf{n}\Psi\right|^2 + C_\parallel\left|\mathbf{n}\cdot\mathbf{D}_\mathbf{n}\Psi\right|^2 + r|\Psi|^2 + \frac{g}{2}|\Psi|^4,$$

where $\mathbf{D}_\mathbf{n} = \nabla - iq\mathbf{n}, \quad \mathbf{D}_\mathbf{n}^2\Psi = \mathbf{D}_\mathbf{n}\cdot\mathbf{D}_\mathbf{n}\Psi.$

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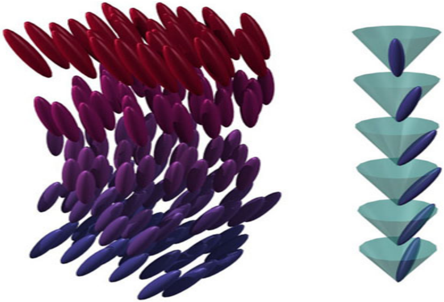
where $\mathbf{D}_\mathbf{n} = \nabla - iq\mathbf{n}, \quad \mathbf{D}_\mathbf{n}^2\Psi = \mathbf{D}_\mathbf{n}\cdot\mathbf{D}_\mathbf{n}\Psi.$

Chiral Smectic C liquid crystal (SmC*)



C.J. Barrett, barrett-group.mcgill.ca

Sign of $C_\perp$

Assuming that $\Psi = e^{i\varphi}$, (away from the phase transition),

$$f_s = D|\nabla\varphi - q\mathbf{n}|^4 + D(\Delta\varphi - q\nabla\cdot\mathbf{n})^2 - C_\perp|\nabla\varphi - q\mathbf{n}|^2 + C_{||}(\mathbf{n}\cdot\nabla\varphi - q)^2$$

deGenne energy

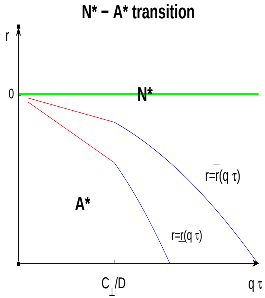
- $C_\perp < 0 : \nabla\varphi = q\mathbf{n} \quad \Rightarrow \quad \boxed{\nabla\varphi \parallel \mathbf{n}} \quad \Rightarrow$ Sm A
  - de Genne energy for Sm A: $f_s = -C_\perp|\nabla\varphi - q\mathbf{n}|^2$
- $C_\perp > 0 : \mathbf{n}\cdot\nabla\varphi = q,\ |\nabla\varphi - q\mathbf{n}|^2 = \dfrac{C_\perp}{2D} \Rightarrow \boxed{\tan^2\alpha = \dfrac{C_\perp}{2Dq^2}},$

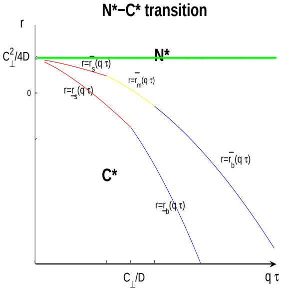
  where α is the tilt angle between the layer normal and the director. $\Rightarrow$ Sm C

Phase transition from N* toward chiral smectic LCs

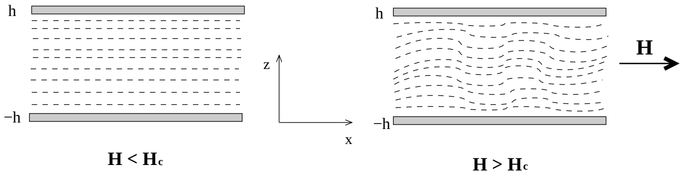
[Joo and Phillips, Comm. Math. Phys. 2007] Phase transition between chiral nematic and smectics: Characterize $\bar{r}$ and $\underline{r}$ as a function of $q\tau$ for which

- $r > \bar{r}$ implies the minimizer $\Psi \equiv 0 \Rightarrow$ Chiral Nematic
- $r < \underline{r}$ implies the minimizer $\Psi \not\equiv 0 \Rightarrow$ Chiral Smectic





Layer Undulations (Helfrich-Hurault effect) in Smectic A



- undeformed state (pure smectic state): $\phi_0 = z, \mathbf{n}_0 = (0, 1)$

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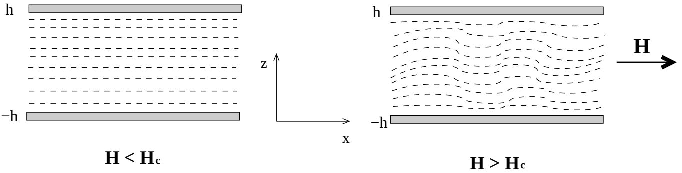

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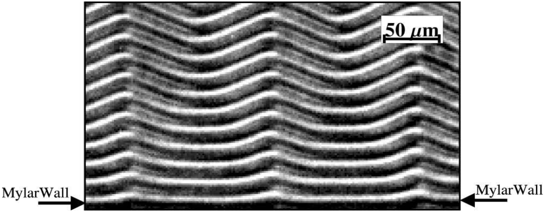
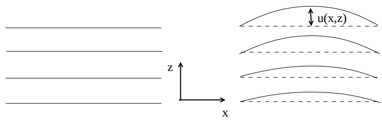
experiment with Cholesteric LCs



(d) Ishikawa and Lavrentovich, PRE 2001

Set $\phi = z - u(x,z)$ where u is the small displacement.

Layer displacement : u(x,z)



Setting $\mathbf{n} \approx (-u_x, 1)$, & strong anchoring

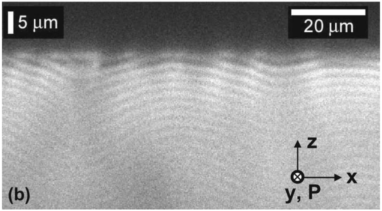
$$\mathcal{F} = \frac{K}{2}(u_{xx})^2 + \frac{B}{2}(u_z)^2 - \frac{\chi_a \sigma^2}{2}(u_x)^2$$

Look for a solution of type $u(x,z) = u_0 \cos(k_z z)\sin(kx)$ for $z \in (-h/2, h/2)$ and find

$$\chi_a \sigma_c^2 = \frac{\pi K_1}{\lambda h}, \quad k^2 = \frac{\pi}{\lambda h}, \quad k_z = \frac{\pi}{h}$$

where $\lambda = \sqrt{K/B}$.

Helfrich-Hurault theory vs. Experiment



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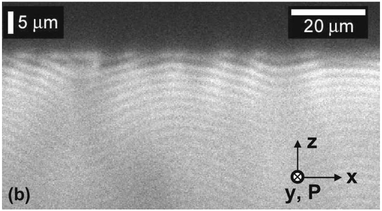

result

In the experiment... *Lavrentovich et al, PRE (2001, 2006)*

- The lower critical field of undulation instability
- Larger layers' displacement
- The displacement of layers immediately adjacent to the bounding plates is nonzero.
- Weakened dependence of the layer shape on the vertical z-coordinate when the field increases well above the threshold.

Free energy

$$\mathcal{G}(\psi,\mathbf{n}) = \int \left(C|\nabla\psi - iq\mathbf{n}\psi|^2 + K|\nabla\mathbf{n}|^2 + \frac{g}{2}(|\psi|^2-1)^2 - \lambda(\mathbf{n}\cdot\mathbf{H})^2 \right) dxdy$$

- $\Omega = (-L,L)\times(-d,d)$
- Undeformed state : $(\psi_0,\theta_0) \equiv (\tilde{c}e^{iqy},0)$ is a trivial critical point of $\mathcal{G}$ where $\tilde{c}\in\mathbb{C}$ such that $|\tilde{c}| = 1$.
- Setting $\mathbf{n} = (\sin\theta,\cos\theta)$,

$$\frac{1}{2}\frac{d^2}{dt^2}\mathcal{G}(\psi_0+t\psi,t\theta)\Big|_{t=0} = \int_\Omega (C|\psi_x - iq\theta\psi_0|^2 + C|\psi_y - iq\psi|^2$$
$$+K|\nabla\theta|^2 + 2g[Re(\psi_0\bar{\psi})]^2 - \lambda|\theta|^2)\,dxdy$$
$$=: \mathcal{L}(\psi,\theta) - \lambda\int_\Omega |\theta|^2\,dxdy$$

Stability of undeformed state

Critical field

$$\lambda_c = \inf_{(\psi,\theta)\in\mathcal{A}} \mathcal{L}(\psi,\theta)$$

where the admissible set $\mathcal{A}$ is given by

$\mathcal{A} = \{(\psi,\theta) \in \mathcal{H}^1(U) \times H^1(U) : \|\theta\|_{L^2(U)} = 1, \theta(x,\pm d) = 0$ for all x,

$U = \mathbb{R}/(-L+2L\mathbb{Z}) \times (-d,d)$.
i.e., periodic boundary condition in the x direction.

- If $\lambda \leq \lambda_c \Rightarrow$ the undeformed state is stable.
- If $\lambda > \lambda_c \Rightarrow$ the undeformed state is unstable.
- Stable bifurcation is possible at $\lambda = \lambda_c$.

Reformulation

Set $\psi = iq\psi_0\varphi$. Then

$$\mathcal{L} = Cq^2|\varphi_x - \theta|^2 + Cq^2|\varphi_y|^2 + K|\nabla\theta|^2 + 2g[-q\Im(\varphi)]^2$$

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We may assume that φ is a real- valued function. Introducing $x = x_{\text{old}}/d, y = y_{\text{old}}/d$, and $\varphi = \varphi_{\text{old}}/d$,

$$\mathcal{L}(\psi, \theta) = \frac{K}{\varepsilon}\int_D \left(\frac{(\varphi_x - \theta)^2}{\varepsilon} + \frac{\varphi_y^2}{\varepsilon} + \varepsilon|\nabla\theta|^2 - \sigma\theta^2\right) dx\, dy$$

where $D = (-c, c) \times (-1, 1)$, $\varepsilon = \dfrac{\sqrt{K}}{qd\sqrt{C}} \ll 1$, and $\sigma = \dfrac{d\lambda}{q\sqrt{CK}}$.

Theorem (Garcia-Cervera, Joo)

$\sigma_c = O(1)$ *for* $\varepsilon \ll 1$.

Fourier series

Represent θ and ϕ by their Fourier series,

$$\theta(x,y) = \sum_{n=-\infty}^{\infty} \theta_n(y)e^{i\mu_n x} \quad \text{and} \quad \varphi(x,y) = \sum_{n=-\infty}^{\infty} \varphi_n(y)e^{i\mu_n x}$$

where $\mu_n = 2\pi n/c$, then the energy becomes

$$\begin{aligned}\mathcal{L}(\varphi,\theta) &= 2c\sum_{n=-\infty}^{\infty}\int_{-1}^{1}\left(\varepsilon|\theta_n'|^2 + \delta|\theta_n|^2 + \frac{1}{\varepsilon}|\theta_n - \phi_n|^2 + \frac{1}{\delta}|\varphi_n'|^2\right)dy. \\ &=: 2c\sum_{n=-\infty}^{\infty} F_\varepsilon(\phi_n,\theta_n,\delta)\end{aligned}$$

where $\delta = \varepsilon\mu_n^2$ and $\phi_n = i\mu_n\varphi_n$. Then one can see that

$$\sigma_c = \inf_n \sigma_n = \inf_n \inf_{(\varphi,\theta)\in\mathcal{B}} \mathcal{F}_\varepsilon(\varphi,\theta,n),$$

where

$$\mathcal{B} = \{(\varphi,\theta) \in \mathcal{H}_0^1(-1,1)\times\mathcal{H}^1(-1,1) : \int_{-1}^{1}|\theta(y)|^2\,dy = 1\}.$$

Problem

$$F_\varepsilon(\theta,\varphi,\delta) := \begin{cases} \int_I \left(\varepsilon\theta'^2 + \frac{1}{\delta}\varphi'^2 + \delta\theta^2 + \frac{1}{\varepsilon}(\theta-\varphi)^2\right) dy & \text{if } (\theta,\varphi,\delta)\in X \\ \infty & \text{else} \end{cases}$$

◂ Γ-Convergence

One can see that $F_\varepsilon(\theta,\varphi,\delta) = F_\varepsilon(-\theta,-\varphi,\delta)$ and a minimizer is either positive or negative in I.

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◂ Γ-Convergence

One can see that $F_\varepsilon(\theta,\varphi,\delta) = F_\varepsilon(-\theta,-\varphi,\delta)$ and a minimizer is either positive or negative in I. Thus we define

$$X_n = \{(\theta,\varphi,\delta)\in W_0^{1,2}(I)\times W^{1,2}(I)\times\mathbb{R} : [\theta]\equiv \int_I \theta \geq 0 \text{ in } I\}$$
$$X_d = \{(\theta,\varphi,\delta)\in X_n : \varphi\in W_0^{1,2}(I)\}.$$

We look for a minimizer of F_ε for $X = X_d$ (Fixed layers at the boundary) or $X = X_n$ (general case) with the constraint

$$\int_I |\theta(y)|^2\,dy = 1.$$

Γ-Convergence

Underlying method: the study of complex minimum problems involving a (small) parameter ε is approximated by a minimum problem where the dependence on this parameter has been averaged out.

The notion of Γ-convergence of energies is designed to guarantee the convergence of minimum problems; i.e.,

$$F_\varepsilon \xrightarrow{\Gamma} F_0 \Rightarrow \min F_\varepsilon := m_\varepsilon \to m_0 := \min F_0.$$

and (almost) minimizers of min F_ε converge to minimizers of F_0.

(Note: compactness of minimizers is given for granted)

Definition of Γ-Convergence

$\{F_\varepsilon\}$ Γ-converges to F ($F_\varepsilon \xrightarrow{\Gamma} F_0$)if

1. (Lower bound inequality) $F(u) \leq \liminf_{\varepsilon \to 0} F_\varepsilon(u_\varepsilon)$ if $u_\varepsilon \to u$
2. (Existence of recovery sequences) for all u there exists $u_\varepsilon \to u$ such that $F(u) = \lim_{\varepsilon \to 0} F_\varepsilon(u_\varepsilon)$.

This convergence has been introduced by De Giorgi in the 1970s.

- (Compactness) Given $\{u_\varepsilon\}$ such that $F_\varepsilon(u_\varepsilon)$ is uniformly bounded, then $\{u_\varepsilon\}$ is relatively compact.

Then every minimizing sequence admits a subsequence approximating a solution of the problem

$$\min\{F(u)\}.$$

Plan - fixed layers on the boundary

1. Show Γ-convergence and compactness

$$F_\varepsilon^d(\theta, \varphi, \delta) \xrightarrow{\Gamma} F_0^d(\theta, \varphi, \delta)$$

▸ F_ε

Plan - fixed layers on the boundary

1. Show Γ-convergence and compactness

$$F^d_\varepsilon(\theta,\varphi,\delta) \xrightarrow{\Gamma} F^d_0(\theta,\varphi,\delta)$$

F_ε

$$:= \begin{cases} \int_I (\delta\theta^2 + \frac{1}{\delta}\theta'^2)\,dy & \text{if } \theta = \varphi \in W^{1,2}_0(I), [\theta] > 0 \\ \infty & \text{else} \end{cases}$$

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F_ε

2. The Γ-limit has a unique minimizer, $(\theta_0, \varphi_0, \delta_0)$;

$\delta_0 = \frac{\pi}{2}, \quad \theta_0(y) = \varphi_0(y) = \cos\frac{\pi}{2}y$

The minimum value of F_0^d is π.

Plan - fixed layers on the boundary

1. Show Γ-convergence and compactness

$$F_\varepsilon^d(\theta,\varphi,\delta) \xrightarrow{\Gamma} F_0^d(\theta,\varphi,\delta)$$

F_ε

$$:= \begin{cases} \int_I (\delta\theta^2 + \frac{1}{\delta}\theta'^2)\,dy & \text{if } \theta = \varphi \in W_0^{1,2}(I), [\theta] > 0 \\ \infty & \text{else} \end{cases}$$

2. The Γ-limit has a unique minimizer, $(\theta_0, \varphi_0, \delta_0)$;

$\delta_0 = \frac{\pi}{2}, \quad \theta_0(y) = \varphi_0(y) = \cos\frac{\pi}{2}y$
The minimum value of F_0^d is π.

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Layer undulations - fixed layers on the cell boundaries

Theorem (Garcia-Cervera and Joo)

Let $(\theta, \varphi, \delta) \in X_d$ *be a minimizer of* F_ε^d *constrained by* $\displaystyle\int_I |\theta|^2\, dy = 1$. *For* $\varepsilon = 1/h \ll 1$, *we have*

$$\mu^2/h \approx \frac{\pi}{2}, \quad F_\varepsilon^d \approx \pi, \quad \textit{and} \quad \int_I |\varphi(y) - \cos\frac{\pi}{2}y|^2\, dy \ll 1.$$

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- The maximum undulation occurs in the middle of the cell $(y = 0)$ and the displacement amplitude decreases as approaching the boundary $(y = \pm h)$.

The results are consistent with the result found in the classic Helfrich-Hurault theory.

General case: Layers are not fixed on the boundary

$$F_\varepsilon^n(\theta,\varphi,\delta) := \begin{cases} \int_I \left(\varepsilon\theta'^2 + \frac{1}{\delta}\varphi'^2 + \delta\theta^2 + \frac{1}{\varepsilon}(\theta-\varphi)^2\right) dy & \text{if } (\theta,\varphi,\delta) \in X_n \\ \infty & \text{else} \end{cases}$$

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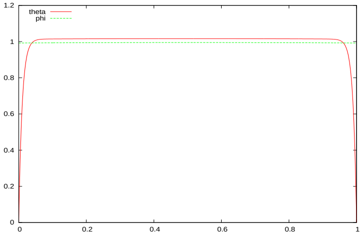

(f) configuration of minimizer of F_ε^n with $\varepsilon = 0.01, \delta = 0.01$

Plan: general case

1. Show Γ-convergence and compactness

$$F_\varepsilon^n(\theta,\varphi,\delta) \xrightarrow{\Gamma} F_0^n(\theta,\varphi,\delta)$$

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Γ-Convergence : Lower semi-continuity

Lemma (Garcia-Cervera and Joo)

For every $(\theta, \varphi, \delta) \in [L^2(I)]^2 \times \mathbb{R}$ *and every sequence* $(\theta_j, \varphi_j, \delta_j) \in X_n$ *such that* $(\theta_j, \varphi_j, \delta_j)$ *converges to* $(\theta, \varphi, \delta)$ *in* $[L^2(I)]^2 \times \mathbb{R}$ *there holds*

$$\liminf_{j \to \infty} F^n_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) \geq F^n_0(\theta, \varphi, \delta),$$

with $\theta \in W^{1,2}(I)$ *and* $\varphi \in W^{1,2}(I)$.

Proof.

- Modify the proof for Allen-Cahn functional with Dirichlet boundary condition. [N.C. Owen, J. Rubinstein and P. Sternberg, Proc. R. Soc. Lond. A, 1990]

$\square$

Γ-convergence : upper bound inequality

Lemma (Garcia-Cervera and Joo)

For any $(\theta, \varphi, \delta) \in X_n$ *with* $\int_I |\theta|^2 \, dz = 1$ *and* $\theta = \varphi$*, there exists a sequence* $(\theta_j, \varphi_j, \delta_j) \in W_0^{1,2}(I) \times W^{1,2}(I) \times \mathbb{R}$ *with* $\int_I |\theta_j|^2 \, dz = 1$*, converging in* $[L^2(I)]^2 \times \mathbb{R}$ *as* $j \to \infty$*, to* $(\theta, \varphi, \delta)$*, and such that*

$$\limsup_{j \to \infty} F^n_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) = F^n_0(\theta, \varphi, \delta).$$

- Take $\varphi_\varepsilon = \varphi$ and $\delta_\varepsilon = \delta$
- For θ_ε;
  - Construct the boundary layer $\rho_\varepsilon(y)$ from singular perturbation.
  - Normalization: $\theta_\varepsilon(y) = \dfrac{\rho_\varepsilon(y)}{\|\rho_\varepsilon\|_{L^2(I)}}$.

Layer Undulations

Theorem (Garcia-Cervera and Joo)

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- The critical field is given by $\kappa_c \approx \dfrac{1}{h}$, lower than $\kappa_c^0 \approx \dfrac{\pi}{h}$.
- Larger undulation displacement, $\dfrac{1}{\mu_n}\phi(y)$ from $\varepsilon\mu_n^2 \approx 0$.

◂ Bifurcation

Bifurcation from simple eigenvalue

- Assumption
  - X, Y are Banach spaces.
  - $F : X \times \mathbb{R} \to Y, C^2$. ($F(u, \lambda) = 0$: Euler equation)
  - $L := F_x(0, \lambda)$ has a simple eigenvalue. (L : the second variation of the energy at a critical point)
- Check general criteria given by Crandall and Rabinowitz.
  - (i) $KerL =< x_0 >$
  - (ii) $RangeL = Y_1$ has codimension 1. (If L:self-adjoint, (i) $\Rightarrow$ (ii))
  - (iii) $F_{\lambda x}(0, \lambda_0)x_0 \notin Y_1$.
- Then there is a bifurcating curve $\{(x(s), \lambda(s)) : |s| < s_0\}$ of zeroes of F intersecting $(0, \lambda)$ only at $(0, \lambda_0)$.
- There are eigenvalues and eigenvectors

$$F_x(x(s), \lambda(s))\omega(s) = \mu(s)\omega(s) \text{ and } F_x(0, \lambda)u(\lambda) = \gamma(\lambda)u(\lambda)$$

- From $\dfrac{dx}{dt} = F(x, \lambda)$, stability of equilibrium solution $(x(s), \lambda(s))$ is determined by the sign of $\mu(s)$.

Example: $\Delta u - u^3 + \lambda u = 0$

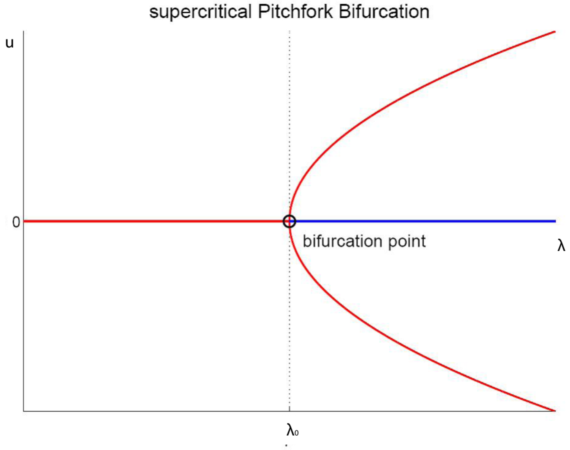
Consider $F(u, \lambda) = \Delta u - u^3 + \lambda u$.

- $u = 0$ is a solution for all λ.
- $F_u(0, \lambda) = \Delta u + \lambda u =: Lu$ has a simple first eigenvalue, λ_0 and corresponding eigenfunction u_0. i.e., $KerL =< u_0 >$.
- Since L is a self-adjoint operator, $KerL = (RangeL)^{\perp}$. Thus, codimension of the range of $F_u(0, \lambda)$ is 1.
- $F_{u\lambda}(0, \lambda_0) = u_0$, but $u_0 \perp rangeL$
- From the theory of Crandall and Rabinowitz, $(0, \lambda_0)$ is a bifurcating point and there is an analytic family of solutions

$$(u(s), \lambda(s)) = (su_0 + s^2 u_2(s), \lambda_0 + s\lambda_2(s))$$

- We can further prove that $\lambda(0) = \lambda'(0) = 0$ and $\lambda''(0) = 2\int u_0^4 > 0$. $\Rightarrow$ Supercritical pitchfork bifurcation!

Example continued: $\Delta u - u^3 + \lambda u = 0$



Eigenvalue problem : formal asymptotic expansion

Result from Γ-Convergence

The frequency of the oscillation is smaller than $O(h^{-1/2})$ from $\varepsilon\mu_n^2 \approx 0$.

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- Standard process for eigenvalue problem
- Formal asymptotic expansion for the derived algebraic equation
- Use results from Γ-convergence theory
- The minimizer of F_ε is obtained; As $\varepsilon \to 0$,
  - $\delta = \varepsilon(2\pi/c)^2 + O(\varepsilon)$ and
  - $\lambda = 1 + (1/2 + 2/3(2\pi/c)^2)\varepsilon + O(\varepsilon^2)$.

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  - $\lambda = 1 + (1/2 + 2/3(2\pi/c)^2)\varepsilon + O(\varepsilon^2)$.
- When $c = L/h = 4$, the wave number is 2.

Linearized problem: simple eigenvalue

For $\sigma = \sigma_c$, except for a discrete set of the domain sizes, the linearized problem

$$\varepsilon\Delta\theta + \frac{1}{\varepsilon}\varphi_x - \frac{1}{\varepsilon}\theta + \sigma\theta = 0$$
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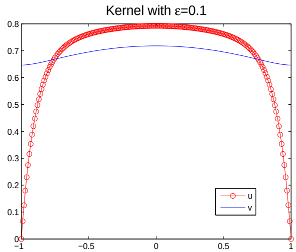
has a solution set spanned by $\{\theta_n(y)\cos\mu_n x, \varphi_n(y)\sin\mu_n x\}$ for some n.



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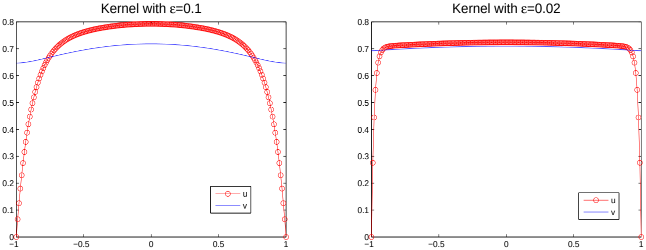

Bifurcation curve

Euler-Lagrange equations: for $\psi = u + iv$, $\mathbf{z} = (u, v, \theta)$

$$\begin{aligned}
F_1(\mathbf{z}, \lambda) &= C[\Delta u + 2q(\sin\theta v_x + \cos\theta v_y) + q(\cos\theta\theta_x - \sin\theta\theta_y)v \\
&\quad -q^2 u] + g(1 - u^2 - v^2)u = 0, \\
F_2(\mathbf{z}, \lambda) &= C[\Delta v - 2q(\sin\theta u_x + \cos\theta u_y) - q(\cos\theta\theta_x - \sin\theta\theta_y)u \\
&\quad -q^2 u] + g(1 - u^2 - v^2)v = 0, \\
F_3(\mathbf{z}, \lambda) &= K\Delta\theta + Cq[\cos\theta(uv_x - vu_x) - \sin\theta(uv_y - vu_y)] \\
&\quad +\lambda\sin\theta\cos\theta = 0.
\end{aligned}$$

Theorem (existence and stability)

There is an $r > 0$ and bifurcation curve of solutions to the system for $s \in (-r, r)$,

$$\psi = \psi_0 + s\psi_1 + \mathcal{O}(s^3), \theta(s) = s^2\theta_1 + \mathcal{O}(s^4), \text{ and } \lambda(s) = \lambda_0 + \mathcal{O}(s^2).$$

Furthermore, the system has only two solutions $\mathbf{z}_0 = (\psi_0, 0)$ and $(\mathbf{z}(s), \sigma(s))$ and the nontrivial solution is stable in a sufficiently small neighborhood of $(\mathbf{z}_0, \lambda_c)$.

Numerical scheme for de Genne energy

Gradient flow

$$\begin{aligned}
\frac{\partial \phi}{\partial t} &= \Delta\phi - \nabla\cdot\mathbf{n} \\
\frac{\partial \mathbf{n}}{\partial t} &= -\mathbf{n}\times\left(\mathbf{n}\times\left(\Delta\mathbf{n} + \nabla\phi - \mathbf{n} + \kappa(\mathbf{n}\cdot\mathbf{h})\mathbf{h}\right)\right).
\end{aligned}$$

where $\mathbf{n}\times(\mathbf{n}\times\frac{\delta G}{\delta \mathbf{n}})$ in the second equation appears as a result of the constraint $|\mathbf{n}| = 1$. Boundary conditions on the top and bottom plates:

$$\mathbf{n} = (0,1) \quad \text{and} \quad \begin{array}{ll} \text{Either} & \phi|_{\pm h} = y \\ \text{or} & \dfrac{\partial\phi}{\partial\nu} = \mathbf{n}\cdot\nu \end{array}$$

Fast Fourier Transform + semi-implicit finite difference method

Layer : the contour map of φ

Fixed layers on the boundaries; The analysis predicts that $\kappa_c^0 \sim \pi/h \sim 0.125$ and the wave number ~ 8 when $h = 25$, $L = 100$.

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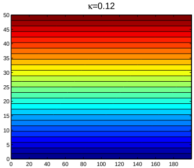

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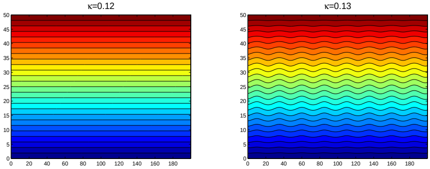

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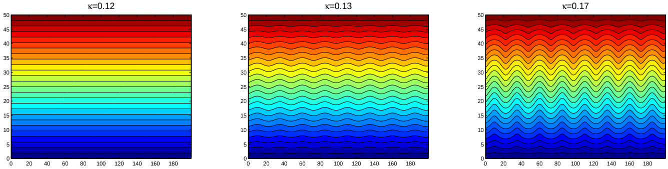

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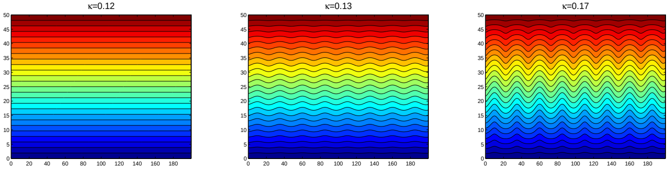

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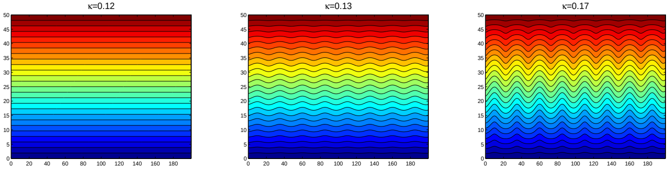

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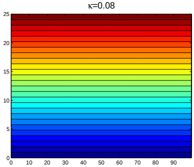

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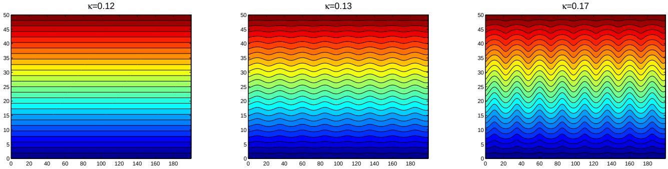

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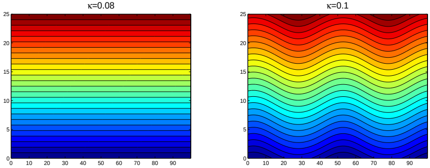

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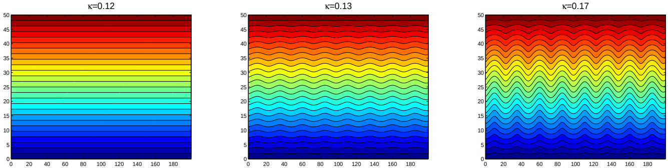

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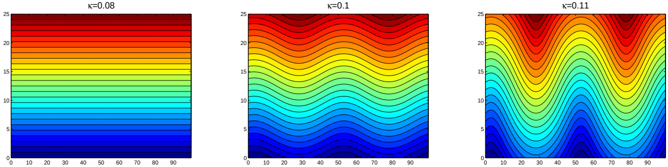
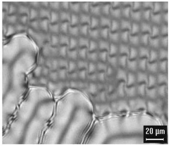


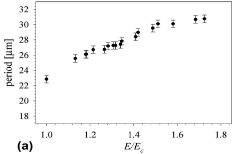
Current/Future work

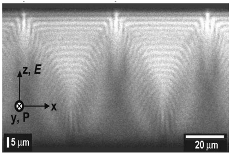
- Extension to Smectic C
- 3d extension - numerical simulation

(a) 

Senyuk, Smalyukh, and Lavrentovich, PRE 2006

- Beyond the critical field





- Q tensor and smectic order parameter