Existence of Surface Smectic States of Liquid Crystals

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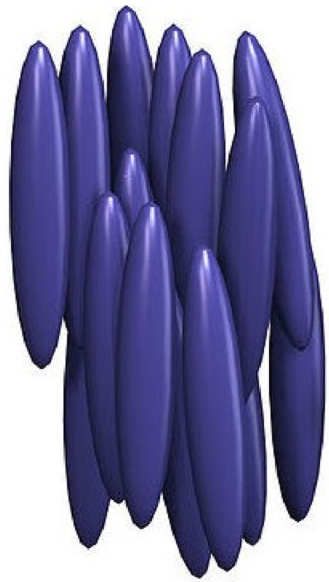
(Joint work with S. Fournais and X.B. Pan)

Nematic/Smectic phases of Liquid crystals



- Phase transition occurs when the temperature crosses a critical value T_{NS}

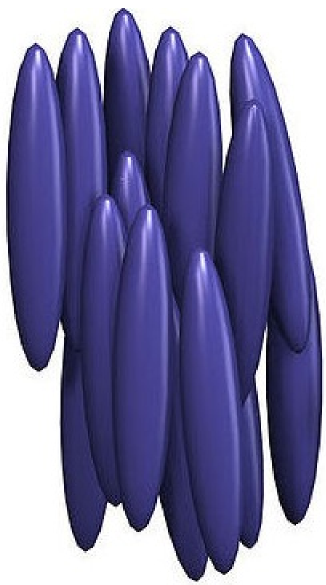
Chiral Nematic/Smectic phases

- The director varies with layers

Elements of **Landau-de Gennes Theory**

- The geometry of the container: $\Omega \subset \mathbb{R}^3$
- The temperature T
- The order parameter ψ : To distinguish between nematic/smectic pahses
- The director $\mathbf{n}$: To define the directional order
- The number of layers q
- The chirality parameter τ : To distinguish between *chiral* and *non-chiral* LC

Elements of **Landau-de Gennes Theory**



$\psi = 0$
$\tau = 0$

$\psi \neq 0$
$\tau = 0$

$\tau \neq 0$
$\mathrm{curl}\,\mathbf{n} \neq 0$

The mathematical set-up

- The director field is constrained: $|\mathbf{n}| = 1$
- $(\psi, \mathbf{n})$ minimizes an energy $\mathcal{E}(\psi, \mathbf{n}) = E_{\mathsf{A}} + E_{\mathsf{N}}$
- Earlier contributions include
  - Bauman-Claderer-Liu-Phillips, ARMA, 2002
  - Y. Almog, CVPDE, 2008
  - Helffer-Pan, JFA, 2008
  - N. Raymond, ADE, 2010

The Nematic energy

This is the functional $E_{\mathsf{N}}(\mathbf{n}) = \mathcal{F}_{\mathsf{N}}(\mathbf{n}) + \mathcal{L}(\mathbf{n})$, where

$$\mathcal{F}_{\mathsf{N}}(\mathbf{n}) = \int_\Omega \left\{ K_1 |\operatorname{div}\mathbf{n}|^2 + K_2 |(\operatorname{curl}\mathbf{n})\cdot\mathbf{n} + \tau|^2 + K_3 |\operatorname{curl}\mathbf{n}\times\mathbf{n}|^2 \right\} dx$$

$$\mathcal{L}(\mathbf{n}) = (K_2 + K_4) \int_\Omega \left(\operatorname{tr}(D\mathbf{n})^2 - |\operatorname{div}\mathbf{n}|^2 \right) dx$$

$$= \text{null Lagrangian}$$

and

$$K_2 > 0,\ K_1, K_3 \geq K_2 + K_4 \geq 0,\ 0 \geq K_4$$

are the elasticity coefficients. Under these assumptions, E_{N} is bounded from below.

Minimizing the Nematic energy

After [Ericksen, 1967] and [BCLP, 2002]

$$\begin{aligned}\mathcal{C}_\tau &= \{\mathbf{n} \ : \ F_{\mathsf{N}}(\mathbf{n}) = 0\} \\ &= \{\mathbf{n} : \operatorname{div}\mathbf{n} = 0 \text{ and } \operatorname{curl}\mathbf{n} + \tau\mathbf{n} = 0\} \\ &= \left\{ N_\tau^Q(\cdot) := Q N_\tau(Q^t \cdot) \ : \ Q \in SO(3) \right\}\end{aligned}$$

where

$$N_\tau(x) = (\cos(\tau x_3), \sin(\tau x_3), 0)$$

The smectic energy

This is the functional

$$E_{\mathsf{A}}(\psi, \mathbf{n}) = \int_{\Omega} |(\nabla - iq\mathbf{n})\psi|^2 - r|\psi|^2 + \frac{g}{2}|\psi|^4 \, dx$$

where

- $g > 0$ is fixed
- $r = T_{\mathsf{NA}} - T$
- T is temperature
- T_{NA} is the critical temperature at $\tau = 0$
- For the pure nematic phase $(\psi = 0, \mathbf{n} = N_\tau)$, $E_{\mathsf{A}}(\psi, \mathbf{n}) = 0$
- The smectic phase is favorable if $E_{\mathsf{A}}(\psi, \mathbf{n}) < 0$

The transition between smectic and nematic phases

- [BCLP, 2002]: $\exists\ \overline{\beta} > \underline{\beta} > 0$ such that, for

$$\tilde{r}(q\tau) = \min(q\tau, (q\tau)^2)$$
$$(\psi, \mathbf{n}) \text{ minimizes } \mathcal{E}(\psi, \mathbf{n}) = E_{\mathsf{A}}(\psi, \mathbf{n}) + E_{\mathsf{N}}(\mathbf{n})$$

(Nematic phase)	*(Smectic phase)*
$r < \overline{\beta}\, \tilde{r}(q\tau) \Rightarrow \psi \equiv 0$	$r > \underline{\beta}\, \tilde{r}(q\tau) \Rightarrow \psi \not\equiv 0$

- *(Critical temperature - large number of layers)* Since $r = T_{\mathsf{NA}} - T$, we obtain $T_{\mathsf{NA}} - T_{\mathsf{C}} \approx q\tau$ for $q\tau \gg 1$

- Refined estimates are given by Raymond

Transformation to (GL) like energy

- Let $\kappa = \sqrt{r}$

- The transformation $\psi \mapsto \frac{\kappa}{g^{1/2}}\psi$ yields

$$E_{\mathsf{A}}(\psi, \mathbf{n}) \mapsto \frac{\kappa^2}{g}\mathcal{G}(\psi, \mathbf{n})$$

- $\mathcal{G}(\psi, \mathbf{n}) = \int_\Omega \left(|(\nabla - iq\mathbf{n})\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 \right) dx$

- Conclusion:
  - We get the functional studied by Helffer-Pan, Raymond,..
  - For $r \approx q\tau$, we get $q\tau \approx \kappa^2$
  - Hereafter, we assume that $q\tau = b\kappa^2$, where $b, \tau > 0$ are fixed constants and $\kappa \gg 1$.

The reduced functional

For (κ, q, τ) fixed, $K_4 = -K_2$ and $(K_1, K_2, K_3) \to \infty$, Helffer-Pan derived the reduced functional

$$\mathcal{G}(\psi, \mathbf{n}) = \int_\Omega \left(|(\nabla - iq\mathbf{n})\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 \right) dx$$

acting on

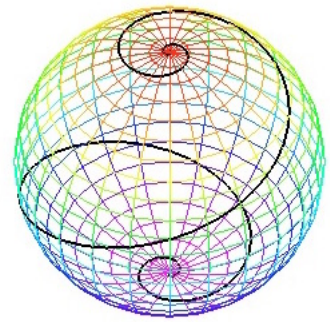
$$(\psi, \mathbf{n}) \in H^1(\Omega; \mathbb{C}) \times \mathcal{C}_\tau$$

Almog proved that for $q\tau = b\kappa^2$, $b > 1$ and $\kappa \gg 1$,

$$|\psi| \le \exp\Big(- \kappa^\epsilon \mathrm{dist}(x, \partial\Omega)\Big)$$

Helffer-Pan obtained further that $|\psi|$ is exponentially small in a boundary region $\partial\Omega \setminus \omega$.

Questions:



- Strength of ψ in the confinement region ?

- Link the results of Almog and Helffer-Pan to the full functional ?

Similar questions were answered for the GL functional [Fournais, K., Persson-Sundqvist, 2013].

The Ginzburg-Landau functional:

- $$GL(\psi, \mathbf{A}) = \int_\Omega \left(|(\nabla - ih_{\text{ex}}\mathbf{A})\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 \right) dx + \int_{\mathbb{R}^3} |\operatorname{curl}(\mathbf{A} - h_{\text{ex}}\mathbf{F})|^2 dx$$

- $\mathbf{F} = \frac{1}{2}(-x_2, x_1, 0)$ and $\operatorname{curl}\mathbf{F} = (0, 0, 1)$

- $\|\mathbf{A} - h_{\text{ex}}\mathbf{F}\|_{C^{0,\alpha}(\Omega)} \lesssim \|\operatorname{curl}(\mathbf{A} - h_{\text{ex}}\mathbf{F})\|_2 + \|(\nabla - ih_{\text{ex}}\mathbf{A})\psi\|_2$

Profile of the director for the full (LdG) energy

Assume that:

- $\kappa \gg 1$ and $q\tau = b\kappa^2$
- $K_1, K_2, K_3 \gg \kappa^2$ and $0 < K_2 + K_4 \approx \kappa^2$
- $(\psi_\kappa, \mathbf{n}_\kappa)$ is a minimizer of LdG functional

Then, $\|\text{div}\mathbf{n}_\kappa\|_2 + \|\,\text{curl}\,\mathbf{n}_\kappa + \tau\mathbf{n}_\kappa\|_2 \lesssim \frac{\kappa}{(K_1+K_2+K_3)^{1/2}} \ll 1$ and $\|D\mathbf{n}_\kappa\|_2 \lesssim 1$.

Furthermore $\mathbf{n}_\kappa \to \mathbf{n}_*$ in $L^p(\Omega;\mathbb{R}^3) \cap W^{1,r}(\Omega;\mathbb{R}^3) \cap L^r(\partial\Omega;\mathbb{R}^3)$, for all $p \in [1,\infty)$ and $r \in [1,2)$, where $\mathbf{n}_* \in \mathcal{C}_\tau$.

Local approximation of the director:

Let $x_0 \in \overline{\Omega}$, $\delta > 0$ and $B_\delta = B(x_0, \delta) \cap \overline{\Omega}$. Then

$$\|\mathbf{n}_\kappa - \mathbf{n}_* - \nabla f_0\|_{L^2(B_\delta)} \lesssim \delta \sqrt{|\ln \delta|} \Big(\|\operatorname{curl} \mathbf{n}_\kappa + \tau \mathbf{n}_\kappa\|_{L^2(Q_\delta)} + \tau \|\mathbf{n}_\kappa - \mathbf{n}_*\|_{L^2(B_\delta)} \Big) + \delta^3$$

But, do we have a good control of $\|\mathbf{n}_\kappa - \mathbf{n}_*\|_{L^2(B_\delta)}$?

Using $|\mathbf{n}_\kappa| = |\mathbf{n}_*| = 1$, we have $\|\mathbf{n}_\kappa - \mathbf{n}_*\|_{L^2(B_\delta)} = \mathcal{O}(\delta^{3/2})$.
This is not enough to control the error that will appear later.

If $\mathbf{n}_\kappa = \mathbf{n}_*$ on $\partial\Omega$, we get $\|\mathbf{n}_\kappa - \mathbf{n}_*\|_{L^2(B_\delta)} \lesssim \Big(\delta \|D(\mathbf{n}_\kappa - \mathbf{n}_*)\|_{L^1(B_\delta)} \Big)^{\frac{1}{2}}$

Construction of the function f_0:

$$\mathbf{a}_\kappa(x) = -\int_\eta^1 s(x-x_0) \times \left(\operatorname{curl} \mathbf{n}_\kappa\right)\Big(s(x-x_0)+x_0\Big)\, ds$$

$$\mathbf{a}_*(x) = -\int_\eta^1 s(x-x_0) \times \left(\operatorname{curl} \mathbf{n}_*\right)\Big(s(x-x_0)+x_0\Big)\, ds$$

$$\mathbf{c}(x) = (\mathbf{n}_\kappa - \mathbf{n}_*)\Big(\eta(x-x_0)+x_0\Big)$$

$$\operatorname{curl}(\mathbf{a}_\kappa - \mathbf{a}_*^0)(x) = \operatorname{curl}(\mathbf{n}_\kappa - \mathbf{n}_*)(x) - \eta \operatorname{curl} \mathbf{c}(x)\,.$$

In a simply connected domain:

$$\mathbf{n}_\kappa - \mathbf{n}_* - \nabla f_0 = \mathbf{a}_\kappa - \mathbf{a}_* + \eta \mathbf{c}$$

Finally, choose $\eta = \delta^{3/2}$.

Why the logarithmic error appears?

By Hölder inequality

$$|\mathbf{a}_\kappa(x)-\mathbf{a}_*(x)|^2 \le \delta^2 \int_\eta^1 s^2 \Big| \Big(\operatorname{curl} \mathbf{n}_\kappa - \operatorname{curl} \mathbf{n}_* \Big) \Big(s(x-x_0)+x_0 \Big) \Big|^2 ds$$

After integration on B_δ, we deduce $(\eta = \delta^{3/2})$

$$\begin{aligned}\int_{B_\delta} |\mathbf{a}_\kappa(x) - \mathbf{a}_*(x)|^2 \, dx &\le \delta^2 \int_\eta^1 \frac{1}{s} \int_{B_\delta} \Big| \Big(\operatorname{curl} \mathbf{n}_\kappa - \operatorname{curl} \mathbf{n}_* \Big)(y) \Big|^2 dy \, ds \\ &\lesssim \delta^2 |\ln \delta| \, \| \operatorname{curl}(\mathbf{n}_\kappa - \mathbf{n}_*)\|^2_{L^2(B_\delta)}\end{aligned}$$

Since $\mathbf{n}_* \in \mathcal{C}_\tau$, $\operatorname{curl} \mathbf{n}_* = -\tau \mathbf{n}_*$. Therefore

$$\| \operatorname{curl}(\mathbf{n}_\kappa - \mathbf{n}_*)\|_2 \le \| \operatorname{curl} \mathbf{n}_\kappa + \tau \mathbf{n}_\kappa\|_2 + \tau \|\mathbf{n}_\kappa - \mathbf{n}_*\|_2$$

Concentration of the order parameter:

Assume that:

- $\kappa \gg 1$; $\quad q\tau = b\kappa^2$; $\quad K_1, K_2, K_3 \gg \kappa^2$
- $(\psi_\kappa, \mathbf{n}_\kappa)$ is a minimizer of LdG functional in the class
  $\mathcal{A} = \{(\psi, \mathbf{n}) \in H^1(\Omega; \mathbb{C}) \times H^1(\Omega; \mathbb{S}^2)\ :\ \exists\ \mathbf{n}_0 \in \mathcal{C}_\tau,\ \mathbf{n} = \mathbf{n}_0 \text{ on } \partial\Omega\}$

Then

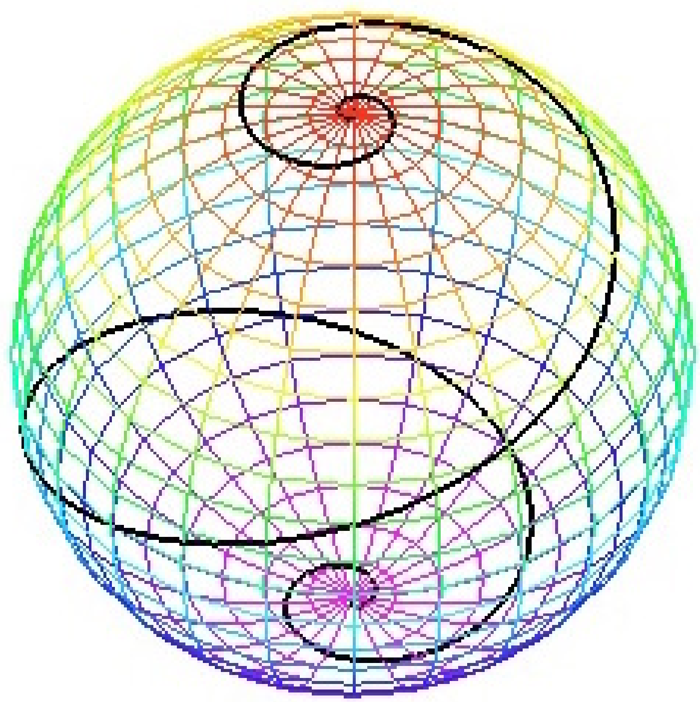
1. $\mathbf{n}_\kappa \to \mathbf{n}_*$ in $L^p(\Omega)$, $p \geq 2$
2. $\kappa|\psi_\kappa|^4\,dx \to -2\sqrt{b}\,\mathfrak{E}\Big(\frac{1}{b}, \nu(x; \mathbf{n}_*)\Big)ds(x)$ in the sense of measures

where

ds is the surface measure on $\partial\Omega$

$\nu(x, \mathbf{n}_*)$ is the acute angle between $\mathbf{n}_*(x)$ and $\partial\Omega$

$\mathfrak{E}(\cdot, \cdot)$ is the surface energy discussed in the talk of Fournais



$\mathfrak{E}(\cdot,\cdot)$ is defined implicitly !

$$\mathfrak{E}(r,\nu) = \lim_{\ell\to+\infty}\left(\frac{1}{4\ell^2}\inf_u G_{r,\ell,\nu}(u)\right) \le 0$$

$$G_{r,\ell,\nu}(u) = \int_{\mathbb{R}_+\times(-\ell,\ell)^2} |(\nabla - i\mathbf{A}_\nu)u|^2 - r|u|^2 + \frac{r}{2}|u|^4$$

$$\mathbf{A}_\nu(x_1,x_2,x_3) = \Big(0,0,x_1\cos(\nu)+x_2\sin(\nu)\Big)$$

$$\mathfrak{E}(r,\nu) < 0 \Longleftrightarrow r > \zeta(\nu)$$

$$\mathfrak{E}(r,\nu) < 0 \iff r > \zeta(\nu)$$

where

- $\zeta(\nu) = \inf \sigma\left(-\Delta + (x_1 \cos\nu + x_2 \sin\nu)^2\right)$ in $L^2(\mathbb{R}^2)$
- $\zeta(\pi/2) = 1$
- $\zeta(0) = \Theta_0 = \inf \sigma\left(-(\nabla - \frac{i}{2}x^\perp)^2\right)$ in $L^2(\mathbb{R}^2_+)$
- $\zeta : [0, \frac{\pi}{2}] \to [\Theta_0, 1]$ is strictly increasing

Concentration of the order parameter:

- $\kappa|\psi_\kappa|^4\,dx \to -2\sqrt{b}\,\mathfrak{E}\Big(\frac{1}{b},\nu(x;\mathbf{n}_*)\Big)ds(x)$

- $\text{supp}\,\mathfrak{E}\Big(\frac{1}{b},\nu(x;\mathbf{n}_*)\Big) = \{x\in\partial\Omega \ : \ \frac{1}{b} > \zeta(\nu(x,\mathbf{n}_*)\}$

- As $b\to\Theta_0^{-1}$, $\text{supp}\,\mathfrak{E}\Big(\frac{1}{b},\nu(x;\mathbf{n}_*)\Big) \to \{\nu(x,\mathbf{n}_*)=0\}$

- As $b\to 1_+$, $\text{supp}\,\mathfrak{E}\Big(\frac{1}{b},\nu(x;\mathbf{n}_*)\Big) \to \partial\Omega$