

Equilibrium Configurations of Nematic Liquid Crystals on a Torus

Antonio Segatti

Dipartimento di Matematica "F. Casorati", Pavia
url: www-dimat.unipv.it/segatti

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M. Snarski (Brown Univ.)
M. Veneroni (Pavia)

preprint, soon

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Liquid crystals

Liquid Crystals are an intermediate state of matter between solids and fluids:

Flow like a fluid but retain some orientational order like solids

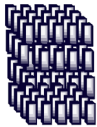
There are three main classes of Liquid Crystals:

Nematic, Smectic, Cholesteric

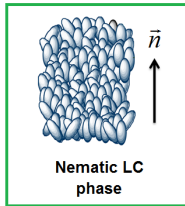
Nematics consist in rod like molecules of length 2-3 nm

The director

The basic mathematical description of the nematic phase is to represent the mean orientation of the molecules through a *unit vector field* $\mathbf{n} = \mathbf{n}(x)$



Crystalline
solid



Nematic LC
phase



Isotropic
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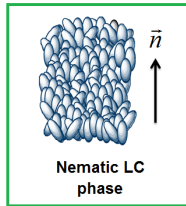
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For the Q -tensor description see DeGennes, Ball, Majumdar, Zarnescu.....many many others

The Oseen-Frank Theory

Consider a region $\Omega \subset \mathbb{R}^3$ occupied by the liquid crystal.

We consider only a static situation in which the fluid velocity is zero.

The Oseen-Frank energy depends on $\mathbf{n} : \Omega \rightarrow \mathbb{S}^2$ and on $\nabla \mathbf{n}$ and has the form

$$\begin{aligned} \mathcal{E}_{OF}(\mathbf{n}) := \frac{1}{2} \int_{\Omega} [& K_1(\operatorname{div} \mathbf{n})^2 + K_2(\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + K_3|\mathbf{n} \times \operatorname{curl} \mathbf{n}|^2 \\ & + (K_2 + K_4)\operatorname{div}((\nabla \mathbf{n})\mathbf{n} - (\operatorname{div} \mathbf{n})\mathbf{n})] \, dx, \end{aligned}$$

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5. the last term is a Null Lagrangian

Mathematical Analysis

Problem: We are interested in the minimization of $\mathcal{E}_{OF}$ in a suitable functional class + suitable boundary conditions

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Non trivial interplay between: Calculus of Variations, PDEs, Topology. In particular: Choice of the boundary conditions $\rightsquigarrow$ topological obstruction to regularity

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See, e.g., Hardt, Kinderlehrer, Lin 1986 (and many many others):

Existence, (Partial) Regularity results, dimension of the singular set

The one constant approximation

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$\mathbf{n} : \Omega \rightarrow \mathbb{S}^2$ solves

$$-\Delta \mathbf{n} = |\nabla \mathbf{n}|^2 \mathbf{n} \text{ in } \Omega$$

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Towards a surface theory....

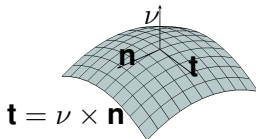
Let S be a compact, orientable, regular surface in $\mathbb{R}^3$.

- ν is the (unit) normal vector field
- For $\mathbf{u}$ tangent, $\mathfrak{B}\mathbf{u} := -\nabla_{\mathbf{u}}\nu$ is the Shape operator ($\mathfrak{B}$ is linear and self-adjoint)

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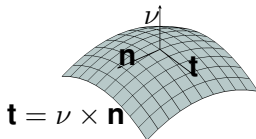
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- $\kappa_{\mathbf{n}}$, $\kappa_{\mathbf{t}}$ geodesic curvature of (flux lines) of $\mathbf{n}$ and of $\mathbf{t}$



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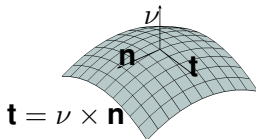
Poincaré-Hopf Th.: For any smooth unit vector field $\mathbf{v}$ there holds

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$\rightsquigarrow$ Unavoidable defects for some choices of S .

Surface Differential Operators 1

Let $\mathbf{u}, \mathbf{v}$ be tangent vector fields on S , $D_{\mathbf{v}}\mathbf{u} := \mathbb{P}\nabla_{\mathbf{v}}\mathbf{u}$ is the covariant derivative of $\mathbf{u}$ ($\mathbb{P}$ projection on the tangent). Recall the Gauss Relation $\nabla_{\mathbf{v}}\mathbf{u} = D_{\mathbf{v}}\mathbf{u} + (\mathfrak{B}\mathbf{u}, \mathbf{v})\nu$.

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$$\begin{aligned}\nabla_S \mathbf{u}[\mathbf{v}] &:= \nabla_{\mathbb{P}\mathbf{v}}\mathbf{u}, \\ \text{i.e. } \nabla_S \mathbf{u} &:= \nabla \mathbf{u} \mathbb{P}\end{aligned}$$

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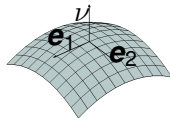
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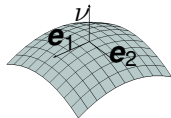
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$$\nabla_S \mathbf{u} = \begin{pmatrix} \cdots & \cdots & 0 \\ \cdots & \cdots & 0 \\ \cdots & \cdots & 0 \end{pmatrix}, D\mathbf{u} = \begin{pmatrix} \cdots & \cdots & 0 \\ \cdots & \cdots & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Surface Differential Operators (Contd.)

For a tangent vector field $\mathbf{u}$, we define the

- surface divergence, that is $\text{div}_S \mathbf{u} := \text{tr} \nabla_S \mathbf{u} = \text{tr} D\mathbf{u}$

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$$|\nabla_s \mathbf{n}|^2 = \underbrace{|D\mathbf{n}|^2}_{\text{Intrinsic}} + \underbrace{|\mathfrak{B}\mathbf{n}|^2}_{\text{Extrinsic}} = \kappa_{\mathbf{f}}^2 + \kappa_{\mathbf{n}}^2 + c_{\mathbf{n}}^2 + \tau_{\mathbf{n}}^2$$

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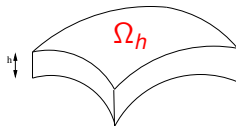
$$|\nabla_s \mathbf{n}|^2 = |D\mathbf{n}|^2 + |\mathfrak{B}\mathbf{n}|^2 = \kappa_{\mathbf{t}}^2 + \underbrace{\kappa_{\mathbf{n}}^2 + c_{\mathbf{n}}^2}_{\mathfrak{K}_{\mathbf{n}}^2} + \tau_{\mathbf{n}}^2$$

- note that $\kappa_{\mathbf{n}}^2 + c_{\mathbf{n}}^2 = \mathfrak{K}_{\mathbf{n}}^2$ with $\mathfrak{K}_{\mathbf{n}}$ the curvature of the flux line of $\mathbf{n}$

Surface energy

For any $h > 0$ consider Ω_h

Napoli & Vergori P.R.E. 2012



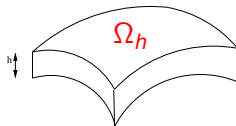
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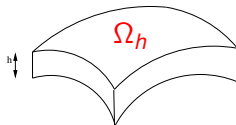
$$\mathcal{E}_{OF}(\mathbf{n}) := \frac{1}{2h} \int_{\Omega_h} [K_1(\operatorname{div} \mathbf{n})^2 + K_2(\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + K_3|\mathbf{n} \times \operatorname{curl} \mathbf{n}|^2] \, dx,$$

- For a fixed (smooth) $\mathbf{n} : \Omega_h \rightarrow \mathbb{S}^2$
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↓ for $h \rightarrow 0$

$$\mathfrak{E}_{OF}(\mathbf{n}_s) := \frac{1}{2} \int_S [K_1(\operatorname{div}_S \mathbf{n}_s)^2 + K_2(\mathbf{n}_s \cdot \operatorname{curl}_S \mathbf{n}_s)^2 + K_3|\mathbf{n}_s \times \operatorname{curl}_S \mathbf{n}_s|^2] dS$$

- For a fixed (smooth) $\mathbf{n} : \Omega_h \rightarrow \mathbb{S}^2$
- Rescale with $h > 0$
- IF $\mathbf{n}$ is ind. of the thickness direction and $\mathbf{n} \cdot \nu = 0$ ($\rightsquigarrow$ the saddle-splay term can be neglected). $\mathbf{n}_s := \mathbf{n}|_S$, $\mathbf{n}_s$ **unit tangent vector field**

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$$\mathfrak{E}_{OF}(\mathbf{n}) = \frac{K}{2} \int_S (|D\mathbf{n}|^2 + |\mathfrak{B}\mathbf{n}|^2) dS \qquad \mathfrak{E}_{OF}^{\text{intr}}(\mathbf{n}) = \frac{K}{2} \int_S |D\mathbf{n}|^2 dS$$

See Napoli & Vergori P.R.L. 2012 for a discussion on the cylinder

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$$-\Delta_g \mathbf{n} + \mathfrak{B}^2 \mathbf{n} = |D\mathbf{n}|^2 \mathbf{n} + |\mathfrak{B}\mathbf{n}|^2 \mathbf{n}$$

Δ_g is the rough Laplacian

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(via **direct method of Calculus of Variations**)

The Torus

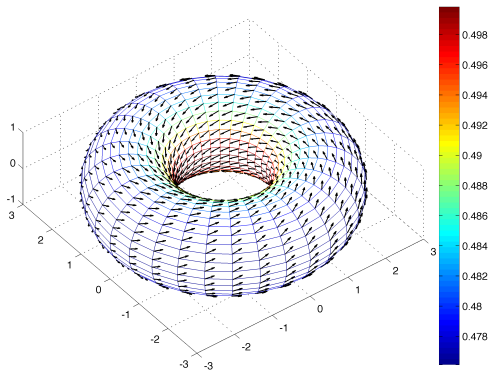
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Poincaré Hopf Theorem:

$$\sum_{j \in J} \text{index}_{x_j} \mathbf{v} = 0$$

for smooth vector fields $\mathbf{v}$



$$\alpha := \angle(\mathbf{n}, \mathbf{e}_1), \quad \alpha \equiv \pi/3$$

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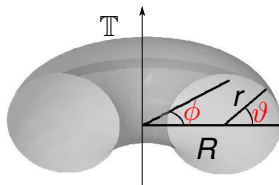
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Important quantity: R/r

We represent $\mathbf{u} \in H_{tan}^1(U; \mathbb{S}^2)$ ($U \subset \mathbb{T}^2$ open and simply connected) as

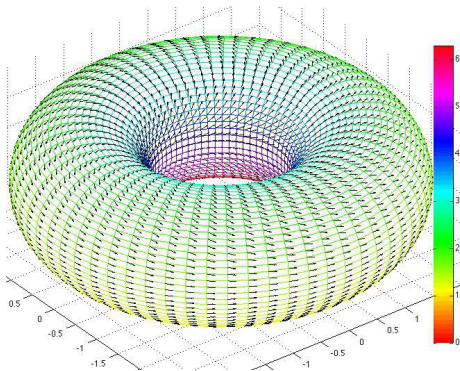
$$\mathbf{u} = \cos \alpha \mathbf{e}_1 + \sin \alpha \mathbf{e}_2$$

$\alpha \in H^1(U; \mathbb{R})$ is the angle between $\mathbf{u}$ and the (direction of the) meridian line of curvature $\mathbf{e}_1$.

Winding Number

Given $\mathbf{n} \in H_{tan}^1(\mathbb{T}; \mathbb{S}^2)$, the **winding number** $d(\mathbf{n}) \in \mathbb{Z} \times \mathbb{Z}$ measures how many times $\mathbf{n}$ "wraps around $\mathbb{T}$ ".

- $d(\mathbf{n})$ is invariant under homotopy

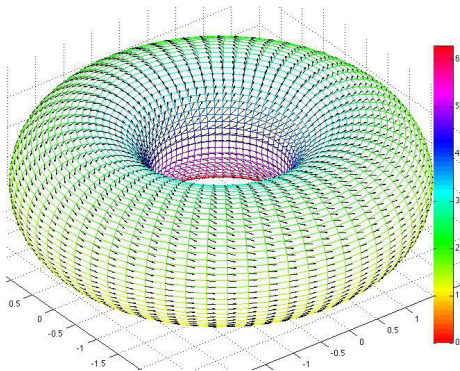


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- $d(\mathbf{n})$ is invariant under homotopy
- If $d(\mathbf{n}) \neq (0, 0)$ the α -representation is only local



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Global α representation 1

For any $h \in \mathbb{Z} \times \mathbb{Z}$ set $((e^1, e^2)$ basis of $\mathbb{R}^2$)

$$\mathcal{A}_h := \left\{ \alpha \in H_{loc}^1(\mathbb{R}^2) : \alpha(x + 2\pi e^j) = \alpha(x) + 2\pi(h \cdot e^j), \forall x \in \mathbb{R}^2 \right\}$$

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- $\forall h \in \mathbb{Z}^2 \exists$ smooth (odd) solution $\alpha = u + \psi_h$ with u periodic (via Schauder Fixed Point argument)

Gradient Flow of $\mathfrak{E}_{OF}(\alpha)$

$$\partial_t \alpha - \Delta_s \alpha - \frac{1}{2}(c_1^2(x) - c_2^2(x)) \sin(2\alpha) = 0 \text{ in } \mathbb{R}^2 \times (0, +\infty)$$

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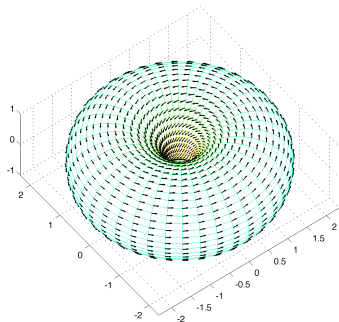
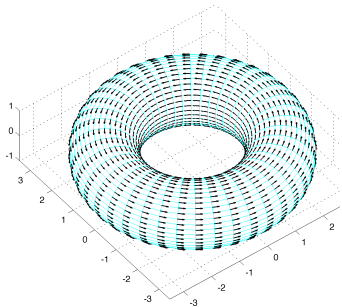
- Well posedness of smooth solutions
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- Conservation of the winding number in the evolution:

$$(d(\mathbf{n}_0) = h \Rightarrow d(\mathbf{n}(t)) = h) \longleftrightarrow (\alpha_0 \in \mathcal{A}_h \Rightarrow \alpha(t) \in \mathcal{A}_h)$$

Some pictures...

Discretization (finite differences in space/time) of

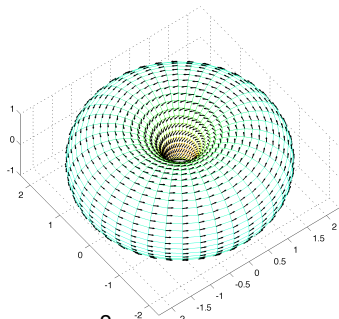
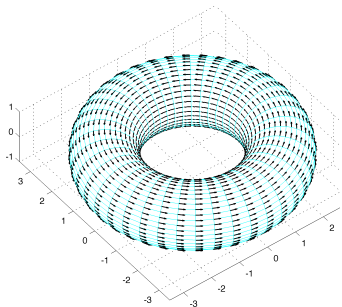
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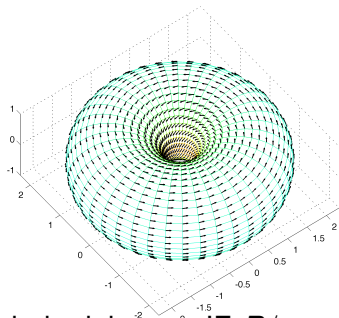
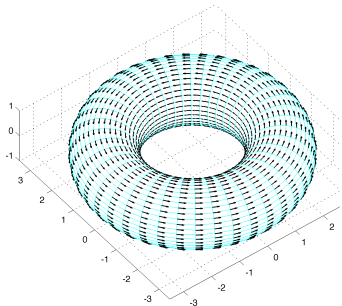


(Left: $R/r = 2.5$, $\alpha = \pi/2$, $\mathfrak{E}_{OF}(\alpha) = 11.96\pi^2$). (Right: $R/r = 1.33$, $\mathfrak{E}_{OF}(\alpha) = 9.95\pi^2 < \mathfrak{E}_{OF}(\pi/2) = 10.22\pi^2$).

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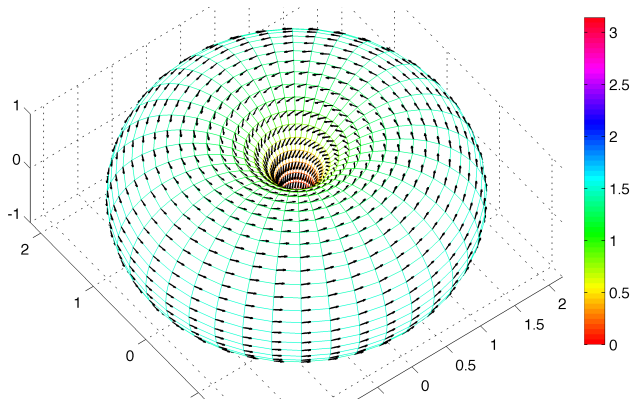
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$\Rightarrow$ IF $R/r > 2$, then $\alpha = \pi/2$ is a global minimum.² IF $R/r < 2/\sqrt{3}$ then $\mathfrak{E}_{OF}(\alpha \equiv 0) < \mathfrak{E}_{OF}(\alpha \equiv \pi/2)$

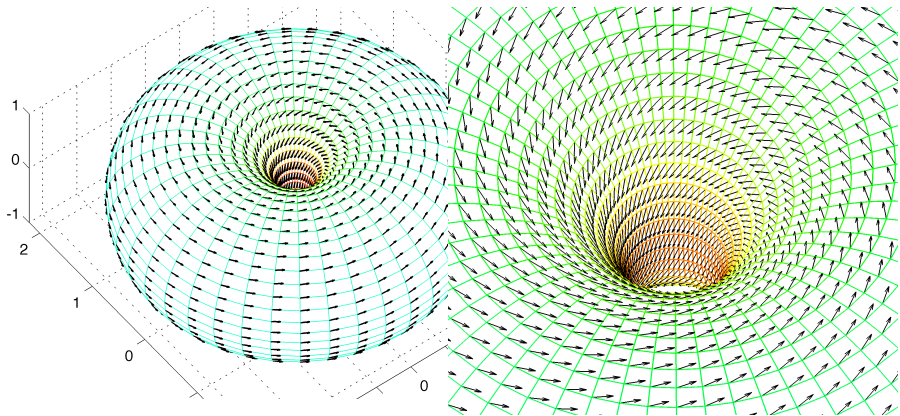
Some Pictures II

What happens for $R/r \in (2/\sqrt{3}, 2]$? Set $R/r = 1.2$: $\mathbf{n}$ in the inner part of $\mathbb{T}$ bends to follow the geodesics along $\mathbf{e}_1$



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R/r	1.2	1.3	1.4	1.5	1.6	1.7	1.8
$\frac{\mathfrak{E}_{OF}(\pi/2)}{\pi^2}$	11.557	10.413	9.912	9.707	9.666	9.726	9.854
$\frac{\mathfrak{E}_{OF}(\alpha^*)}{\pi^2}$	10.696	10.056	9.812	9.705	9.666	9.726	9.854

Comparison between the energy ($/\pi^2$) of the constant solution $\alpha = \pi/2$ and values of the numerical solution α^* , for different ratios R/r and with fixed index 0.

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Numerics says that $b^* \in [1.51, 1.52]$

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Any constant is a solution

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