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 many phases of Liquid Crystals:
Nematic, Smectic, Cholesteric, Blue, …

Liquid Crystals

The Nematic phase:

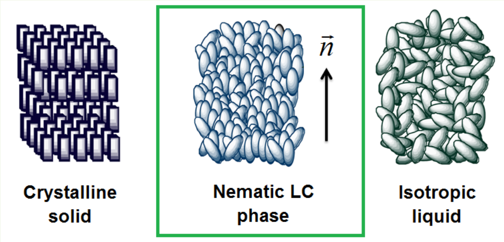


Figure : Garcia-Amorós, Velasco. In *Advanced Elastomers - Technology, Properties and Applications*, 2012.

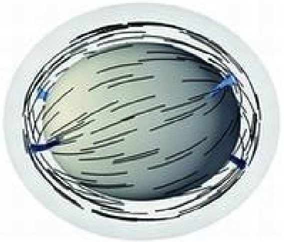
- Mostly uniaxial (rods - cylinders)
- No positional order (random centers of mass)
- Long-range directional order (parallel long axes)

Basic mathematical description: represent the mean orientation through a unit vector field, *the director*, $\mathbf{n} : \Omega \to \mathbb{S}^2$

(Alternative description: order tensors (5 degrees of freedom))

Nematic shells

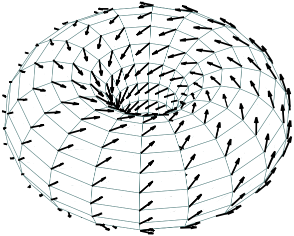
- Physics:



Thin films of nematic liquid crystal coating a small particle with tangent anchoring

[Figure: Bates, Skačej, Zannoni. Defects and ordering in nematic coatings on uniaxial and biaxial colloids. *Soft Matter*, 2010.]

- Model:



Compact surface $\Sigma \subset \mathbb{R}^3$.

Director:

$$\mathbf{n} : \Sigma \to \mathbb{S}^2 \quad \text{with} \quad \mathbf{n}(x) \in T_x\Sigma$$

Energy models

3D director theory, in a domain $\Omega \subset \mathbb{R}^3$

- Frank - Oseen - Zocher elastic energy

One-constant approximation

$$W(\mathbf{n}) = \frac{k}{2} \int_\Omega |\nabla \mathbf{n}|^2 \, \mathrm{d}x$$

2D director theory, on a surface $\Sigma \subset \mathbb{R}^3$

Intrinsic surface energy

$$W_{in}(\mathbf{n}) = \frac{k}{2} \int_\Sigma |\mathrm{D}\mathbf{n}|^2 \, \mathrm{d}S$$

Extrinsic surface energy

$$W_{ex}(\mathbf{n}) = \frac{k}{2} \int_\Sigma |\nabla_s \mathbf{n}|^2 \, \mathrm{d}S$$

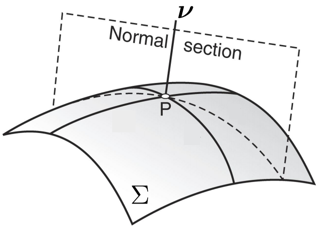
Intrinsic energy: Straley, *Phys. Rev. A*, 1971; Helfrich and Prost, *Phys. Rev. A*, 1988; Lubensky and Prost, *J. Phys. II France*, 1992.

Extrinsic energy: Napoli and Vergori, *Phys. Rev. Lett.*, 2012.

Plan

1. Understand the difference between the two models
2. Study existence of minimizers and gradient flow of W_{in} and W_{ex}
   $\Rightarrow$ Topological constraints
3. Parametrize a specific surface (the axisymmetric torus) and obtain a precise description of local and global minimizers
4. Numerical experiments

Curvatures



Notation:

- $\boldsymbol{\nu}$: normal vector to Σ
- c_1, c_2: principal curvatures, i.e., eigenvalues of $-\mathrm{d}\boldsymbol{\nu} \sim \begin{bmatrix} c_1 & 0 \\ 0 & c_2 \end{bmatrix}$
- Shape operator:

$$T_p\Sigma \to T_p\Sigma, \quad X \mapsto -\mathrm{d}\boldsymbol{\nu}(X)$$

- Scalar 2nd fundamental form:

$$h : T_p\Sigma \times T_p\Sigma \to \mathbb{R}, \quad h(X,Y) = \langle -\mathrm{d}\boldsymbol{\nu}(X), Y \rangle$$

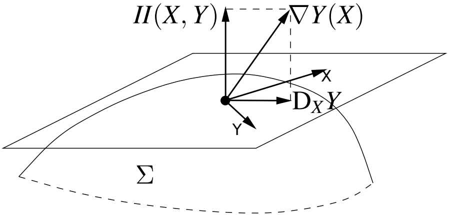
- Vector 2nd fundamental form:

$$II : T_p\Sigma \times T_p\Sigma \to N_p\Sigma, \quad II(X,Y) = h(X,Y)\boldsymbol{\nu}$$

Energy models

X, Y tangent fields on Σ, extended to $\mathbb{R}^3$

Idea: **Decompose $\nabla Y(X)$**



Orthogonal decomposition:

$$\mathbb{R}^3 = T_p\Sigma \oplus N_p\Sigma$$

Gauss formula:

$$\nabla Y(X) = D_X Y + II(X, Y)$$

Define

- $P :=$ orthogonal projection on $T_p\Sigma$
- $\nabla_s Y := \nabla Y \circ P \quad (\neq P \circ \nabla Y = DY)$

$$|\nabla_s \mathbf{n}|^2 = |D\mathbf{n}|^2 + |d\boldsymbol{\nu}(\mathbf{n})|^2$$

Functional framework

$$W_{ex}(\mathbf{n}) = \frac{1}{2}\int_{\Sigma} \left\{ |\mathrm{D}\mathbf{n}|^2 + |\mathrm{d}\boldsymbol{\nu}(\mathbf{n})|^2 \right\} \mathrm{d}S$$

Define the Hilbert spaces

$$L^2_{\tan}(\Sigma) := \left\{ \mathbf{u} \in L^2(\Sigma;\mathbb{R}^3) : \mathbf{u}(x) \in T_x\Sigma \ \text{ a.e.} \right\}$$
$$H^1_{\tan}(\Sigma) := \left\{ \mathbf{u} \in L^2_{\tan}(\Sigma) : |\mathrm{D}_i \mathbf{u}^j| \in L^2(\Sigma) \right\}$$

Objective: minimize W_{ex} on

$$H^1_{\tan}(\Sigma;\mathbb{S}^2) := \left\{ \mathbf{u} \in H^1_{\tan}(\Sigma) : |\mathbf{u}| = 1 \ \text{ a.e.} \right\}$$

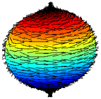
Problem:

- $H^1_{\tan}(\Sigma;\mathbb{S}^2)$ might be empty

Topological constraints

The hairy ball Theorem

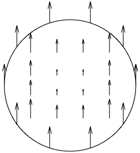
"There is no continuous unit-norm vector field on $\mathbb{S}^2$"



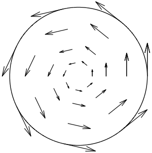
More generally, if v is a smooth vector field on the compact oriented manifold Σ, with finitely many zeroes $x_1, \ldots, x_m$, then

$$\sum_{j=1}^{m} \mathrm{ind}_j(v) = \chi(\Sigma) \qquad \text{(Poincaré-Hopf Theorem)}$$

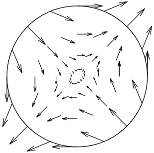
- $\mathrm{ind}_j(v)$, "index of v in x_j" = number of windings of $v/|v|$ around x_j
- $\chi(\Sigma)$, "Euler characteristic of Σ" = # Faces - # Edges + # Vertices



$\mathrm{ind}_0(v) = 0$



$\mathrm{ind}_0(v) = 1$



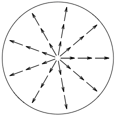
$\mathrm{ind}_0(v) = -1$

Topological constraints

- On a sphere: $\chi(\mathbb{S}^2) = 2 \quad \rightarrow \quad$ e.g. two zeros of index 1, ...
  $\Rightarrow$ no continuous norm-1 fields on $\mathbb{S}^2$
- On a torus: $\chi(\mathbb{T}^2) = 0$
  $\Rightarrow$ possible continuous norm-1 fields on $\mathbb{T}^2$
- On a genus-g surface Σ: $\chi(\Sigma) = 2 - 2g$
  if $g \neq 1 \Rightarrow$ no continuous norm-1 fields on Σ

Poincaré-Hopf does not apply directly: $H^1_{\tan}(\Sigma) \not\subseteq C^0_{\tan}(\Sigma)$...
...still:

$v(\mathbf{x}) := \dfrac{\mathbf{x}}{|\mathbf{x}|}$ on $B_1 \backslash \{0\}$



$\longrightarrow \quad |\nabla v(\mathbf{x})|^2 = \dfrac{1}{|\mathbf{x}|^2}$

$$\int_{B_1 \backslash B_\varepsilon} |\nabla v(\mathbf{x})|^2 \mathrm{d}\mathbf{x} = \int_0^{2\pi} \int_\varepsilon^1 \frac{1}{\rho^2} \rho \, \mathrm{d}\rho \, \mathrm{d}\theta = -2\pi \ln(\varepsilon) \xrightarrow{\varepsilon \searrow 0} +\infty$$

$\Rightarrow v \notin H^1(B_1)$

Summary (1)

- Poincaré-Hopf Theorem suggests that

  if $\chi(\Sigma) \neq 0$, unit-norm vector fields on Σ must have defects.

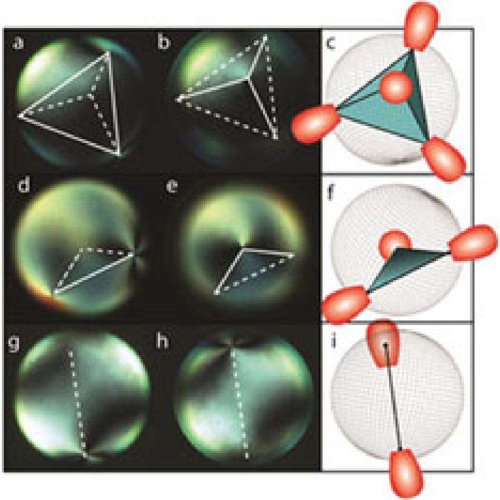
- Simple defects just fail to be H^1

Theorem

Let Σ be a compact smooth surface without boundary. Then

$$H^1_{\tan}(\Sigma; \mathbb{S}^2) \neq \emptyset \quad \Leftrightarrow \quad \chi(\Sigma) = 0.$$

Defects on a sphere



http://www.ec2m.espci.fr/spip.php?rubrique18 - ESPCI ParisTech

Well-posedness

Results

- Stationary problem:

  There exists $\mathbf{n} \in H^1_{\tan}(\Sigma; \mathbb{S}^2)$ which minimizes

$$W_{ex}(\mathbf{n}) = \frac{1}{2} \int_\Sigma \left\{ |\mathrm{D}\mathbf{n}|^2 + |\mathrm{d}\boldsymbol{\nu}(\mathbf{n})|^2 \right\} \mathrm{d}S.$$

- Gradient-flow:

$$\partial_t \mathbf{n} = -\nabla W_{ex}(\mathbf{n}) \qquad \text{on } (0, +\infty) \times \Sigma.$$

  Given $\mathbf{n}_0 \in H^1_{\tan}(\Sigma; \mathbb{S}^2)$, there exists

$$\mathbf{n} \in L^\infty(0, +\infty; H^1_{\tan}(\Sigma; \mathbb{S}^2)), \quad \partial_t \mathbf{n} \in L^2(0, +\infty; L^2_{\tan}(\Sigma))$$

  which solves

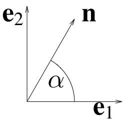
$$\begin{aligned} \partial_t \mathbf{n} - \Delta_g \mathbf{n} + \mathrm{d}\boldsymbol{\nu}^2(\mathbf{n}) &= \left(|\mathrm{D}\mathbf{n}|^2 + |\mathrm{d}\boldsymbol{\nu}(\mathbf{n})|^2 \right) \mathbf{n} && \text{a.e. in } \Sigma \times (0, +\infty), \\ \mathbf{n}(0) &= \mathbf{n}_0 && \text{a.e. in } \Sigma. \end{aligned}$$

α-representation

Given an orthonormal frame $\{\mathbf{e}_1, \mathbf{e}_2\}$, represent the director by the angle α

such that

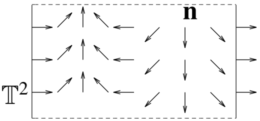
$$\mathbf{n} = \cos(\alpha)\mathbf{e}_1 + \sin(\alpha)\mathbf{e}_2 \qquad (*)$$



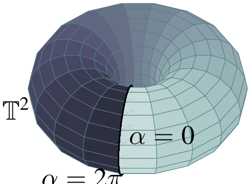
Locally possible.

Globally, $\alpha : \Sigma \to \mathbb{R}$ satisfying (*), may not exist

Example:



$\longrightarrow$



α-representation

Parametrization:

Given

- $\mathbf{n} \in H^1_{\tan}(\Sigma; \mathbb{S}^2)$
- a parametrization
  $Q := [0, 2\pi] \times [0, 2\pi] \xrightarrow{X} \Sigma$
- a global orthonormal frame $\{\mathbf{e}_1, \mathbf{e}_2\}$ (on Q)

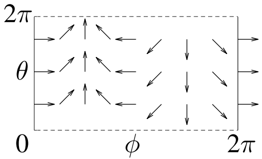
there is $\alpha \in H^1(Q)$:

$$\begin{array}{ccc} \Sigma & \xrightarrow{\mathbf{n}} & \mathbb{S}^2 \\ X \uparrow & & \cos(\alpha)\mathbf{e}_1 + \sin(\alpha)\mathbf{e}_2 \\ Q & & \end{array}$$

α-representation

If $\alpha \in H^1(Q)$ is a representation of $\mathbf{n} \in H^1_{\tan}(\mathbb{T}^2; \mathbb{S}^2)$, there exists $(m_1, m_2) \in \mathbb{Z} \times \mathbb{Z}$ such that

- $\alpha_{|\{\theta=0\}} = \alpha_{|\{\theta=2\pi\}} + 2\pi m_1$
- $\alpha_{|\{\phi=0\}} = \alpha_{|\{\phi=2\pi\}} + 2\pi m_2$



Correspondence between

Fundamental group of $\mathbb{T}^2$

$(\mathbb{Z} \times \mathbb{Z})$

Windings of vector fields $\mathbf{n}$

Boundary conditions for angles α

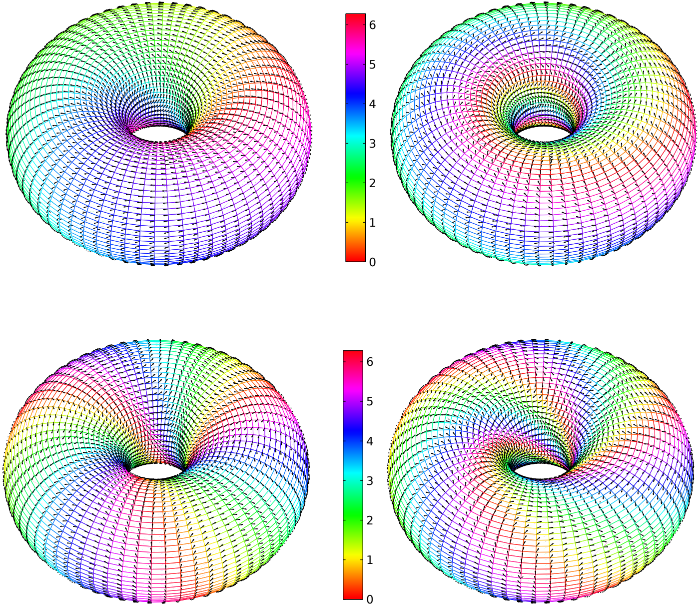
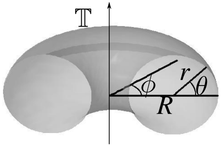


Figure : In clockwise order, from top-left corner: index (1,1), (1,3), (3,3), (3,1). The colour represents the angle $\alpha \mod 2\pi$, the arrows represent the vector field $\mathbf{n}$.

Surface differential operators on the torus

Let $Q := [0, 2\pi] \times [0, 2\pi] \subset \mathbb{R}^2$, and let $X : Q \to \mathbb{R}^3$ be

$$X(\theta, \phi) = \begin{pmatrix} (R + r\cos\theta)\cos\phi \\ (R + r\cos\theta)\sin\phi \\ r\sin\theta \end{pmatrix}$$



$$\begin{aligned} \nabla_s \alpha = g^{ii}\partial_i \alpha &= \frac{\partial_\theta \alpha}{r^2} X_\theta + \frac{\partial_\phi \alpha}{(R + r\cos\theta)^2} X_\phi \\ &= \frac{\partial_\theta \alpha}{r}\mathbf{e}_1 + \frac{\partial_\phi \alpha}{R + r\cos\theta}\mathbf{e}_2, \end{aligned}$$

$$\begin{aligned} \Delta_s = \frac{1}{\sqrt{g}}\partial_i(\sqrt{g} g^{ij}\partial_j) &= \frac{1}{\sqrt{g}}\left(\partial_\theta\left(\sqrt{g}\frac{1}{r^2}\partial_\theta\right) + \partial_\phi\left(\sqrt{g}\frac{1}{(R + r\cos\theta)^2}\partial_\phi\right)\right) \\ &= \frac{1}{r^2}\partial^2_{\theta\theta} - \frac{\sin\theta}{r(R + r\cos\theta)}\partial_\theta + \frac{1}{(R + r\cos\theta)^2}\partial^2_{\phi\phi}. \end{aligned}$$

α-representation

Translate the energies:

$$W_{in}(\mathbf{n}) = \int_\Sigma |D\mathbf{n}|^2 \mathrm{d}S = \int_Q |\nabla_s \alpha|^2 \mathrm{d}S + const(R/r)$$

$$W_{ex}(\mathbf{n}) = \int_\Sigma |\nabla_s \mathbf{n}|^2 \mathrm{d}S = \int_Q \left\{ |\nabla_s \alpha|^2 + \eta \cos(2\alpha) \right\} \mathrm{d}S + const(R/r)$$

where $\eta = \frac{c_1^2 - c_2^2}{2}$.
For $\alpha \equiv const$ on Q,

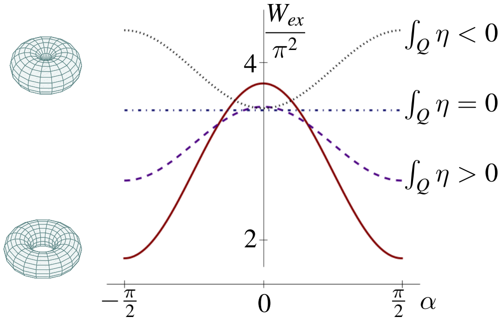


Figure : The ratio of the radii $\mu = R/r$ is : $\mu = 1.1$ (dotted line),

Local minimizers

- Energy:

$$W_{ex}(\mathbf{n}) = \frac{1}{2}\int_Q \left\{|\nabla_s \alpha|^2 + \eta\cos(2\alpha)\right\} \mathrm{d}S$$

  Features: not convex, not coercive

- Euler-Lagrange equation:

$$\Delta_s \alpha + \eta \sin(2\alpha) = 0 \quad \text{on } Q$$

  with $(2\pi m_1, 2\pi m_2)$-periodic boundary conditions
  (Notation: $\alpha \in H^1_{\mathbf{m}}(Q), \quad \mathbf{m} = (m_1, m_2) \in \mathbb{Z} \times \mathbb{Z}$).

Decompose $\alpha \in H^1_{\mathbf{m}}(Q)$ into:

$$\alpha = u + \psi_{\mathbf{m}} \qquad \text{with } \boxed{u \in H^1_{per}(Q)} \quad \text{and} \quad \boxed{\psi_{\mathbf{m}} \in H^1_{\mathbf{m}}(Q),\ \Delta_s \psi_{\mathbf{m}} = 0}$$

From $\quad -\Delta_g \mathbf{n} + \mathrm{d}\boldsymbol{\nu}^2(\mathbf{n}) = \left(|\mathrm{D}\mathbf{n}|^2 + |\mathrm{d}\boldsymbol{\nu}(\mathbf{n})|^2\right)\mathbf{n}$

to

$$\mathcal{A}u = f(u) \quad + \text{ periodic b.c.}$$

Results

Stationary problem:

Given $\mathbf{m} = (m_1, m_2) \in \mathbb{Z} \times \mathbb{Z}$, let $\mu := R/r$

1. $$\psi_{\mathbf{m}}(\theta, \phi) := m_1 \sqrt{\mu^2 - 1} \int_0^\theta \frac{1}{\mu + \cos(s)} \mathrm{d}s + m_2 \phi.$$
2. there exists a classical solution $\alpha \in H^1_{\mathbf{m}}(Q) \cap C^\infty(Q)$. Moreover, α is odd on any line passing through the origin.

Gradient flow:

If $u_0 \in H^2_{per}(Q)$, then there is a unique

$$u \in C^0([0,T]; H^2_{per}(Q)) \cap C^1([0,T]; L^2(Q))$$

such that

$$\partial_t u(t) - \Delta_s u(t) = \eta \sin(2u(t) + 2\psi_{\mathbf{m}}), \qquad u(0) = u_0,$$

$$\sup |u| < C \qquad \text{and} \qquad \sup_{T>0} \left\{ \|\partial_t u\|_{L^2(0,T;L^2(Q))} + \|\nabla_s u(T)\|_{L^2(Q)} \right\} \leq C.$$

Results

Reconstruct $\mathbf{n}$:

1. Let

$$\alpha(t,x) := u(t,x) + \psi_{\mathbf{m}}(x), \qquad \alpha(t) \in H^1_{\mathbf{m}}(Q)$$

   As $t \to +\infty$, $\alpha(t) \to$ solution of E.L. eq.

2. Let

$$\mathbf{n}(t,x) := \cos\alpha(t,x)\mathbf{e}_1(x) + \sin\alpha(t,x)\mathbf{e}_2(x)$$

   $\mathbf{n}$ has constant winding along the flow.

Numerical experiments

Discretize the gradient flow, choose $\alpha_0 \in H^1_{per}(Q)$

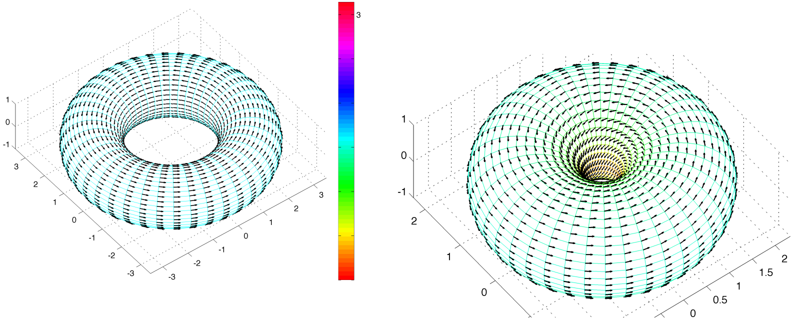


Figure : Numerical solution of the gradient flow. $R/r = 2.5$ (left); $R/r = 1.33$ (right). Colour code: angle $\alpha \in [0, \pi]$; arrows: vector field $\mathbf{n}$.

Numerical experiments

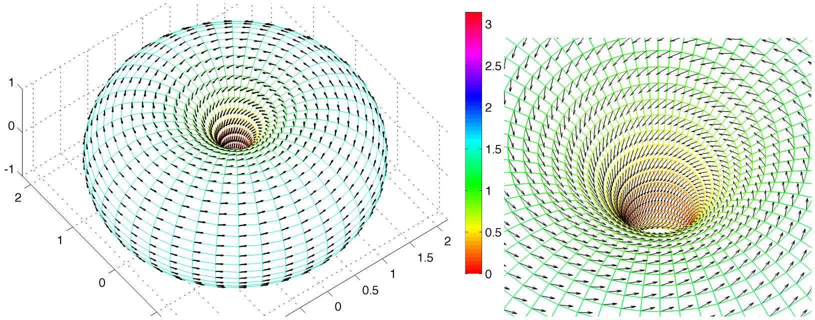
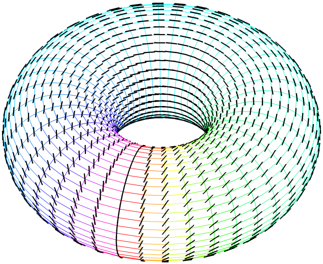
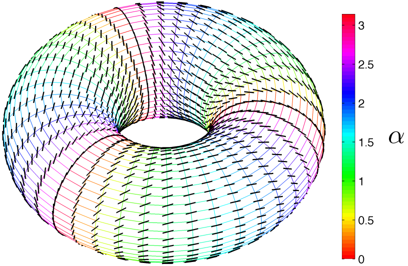


Figure : Configuration of the scalar field α and of the vector field $\mathbf{n}$ of a numerical solution to the gradient flow, for $R/r = 1.2$ (left). Zoom-in of the central region of the same fields (right).

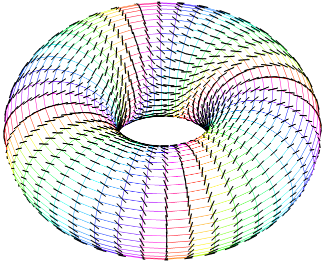
Numerical experiments – identifying **+n** and -**n**



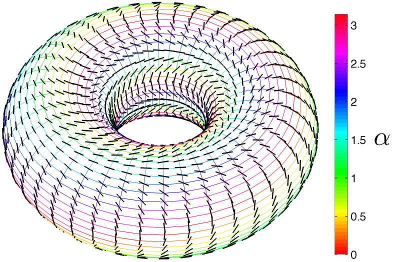
$\mathbf{m} = (0, 1), \quad W_{ex} = 10.93$



$\mathbf{m} = (0, 3), \quad W_{ex} = 14.01$



$\mathbf{m} = (1, 4), \quad W_{ex} = 17.15$



$\mathbf{m} = (4, 1), \quad W_{ex} = 23.02$

References:

- A. Segatti, M. Snarski, M. Veneroni.
  Equilibrium configurations of nematic liquid crystals on a torus.
  Physical Review E, 90(1):012501 (2014).
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  Analysis of a variational model for nematic shells.
  Preprint Isaac Newton Institute for Mathematical Sciences, Cambridge, no. NI14037–FRB, (2014). To appear in *Mathematical Models and Methods in Applied Sciences*

Thank you for your attention !!