Equilibrium configurations of nematic liquid crystals on surfaces

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The Nematic phase:

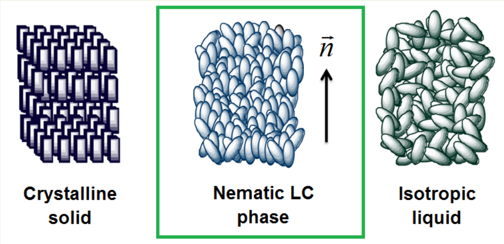


Figure: Garcia-Amorós, Velasco. In *Advanced Elastomers - Technology, Properties and Applications*, 2012.

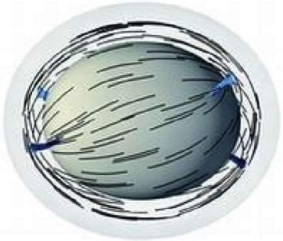
- Mostly uniaxial (rods - cylinders)
- No positional order (random centers of mass)
- Long-range directional order (parallel long axes)

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

(Alternative description: order tensor, $s\left(\mathbf{u} \otimes \mathbf{u} - \frac{1}{3} Id\right)$)

Nematic shells

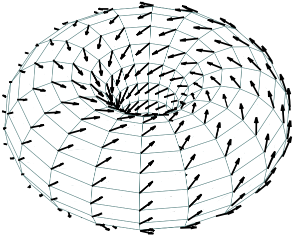
- Physics:



Thin films of nematic liquid crystal coating a small particle

[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 density
  (Distortion free energy density)

$$w(\mathbf{n}) = \frac{k_1}{2}(\operatorname{div}\mathbf{n})^2 + \frac{k_2}{2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + \frac{k_3}{2}|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2$$

$$+(k_2 + k_{24})\operatorname{div}((\nabla\mathbf{n})\mathbf{n} - \mathbf{n}\operatorname{div}\mathbf{n})$$

One-constant approximation

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

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

Intrinsic surface energy

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

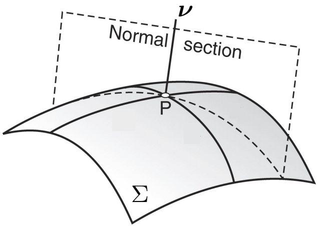
Extrinsic surface energy

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

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.

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:

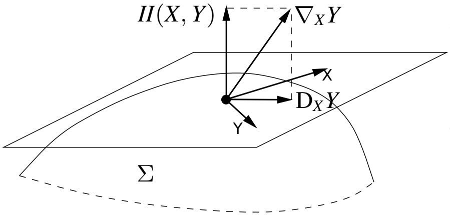
$$h : T_p\Sigma \times T_p\Sigma \to \mathbb{R}, \quad h(X, Y) = \langle -\mathrm{d}\boldsymbol{\nu}(X), Y \rangle$$

- 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 $\mathbb{R}^3$
$\nabla_X Y$= covariant derivation of Y in direction X, i.e. $(\nabla Y)X = \frac{\partial Y^i}{\partial x^j} X^j$



Orthogonal decomposition:

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

Gauss formula:

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

Define

- $P :=$ orthogonal projection on $T_p\Sigma$
- $\nabla_s Y := \nabla Y \circ P$

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

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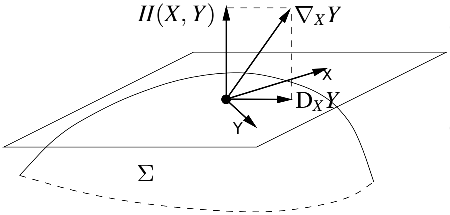

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Plan

1. Relationship between functional framework and topology of Σ
2. Existence of minimizers and gradient flow of W_{ex}
3. Parametrize a specific surface (the axisymmetric torus) and obtain precise description of local and global minimizers

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

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

Note:

- $H^1_{\tan}(\Sigma;\mathbb{S}^2)$ is a weakly closed subset of $H^1_{\tan}(\Sigma)$

Claim:

- $H^1_{\tan}(\Sigma;\mathbb{S}^2)$ is empty, unless genus(Σ)=1

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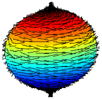
Topological constraints

The hairy ball Theorem

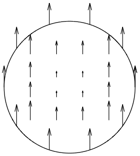
"There is no continuous unit-norm vector field on $\mathbb{S}^2$"



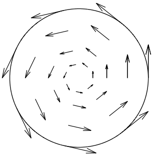
More generally, if v is a smooth vector field on the compact oriented manifold Σ, with finitely many zeroes $x_1, \ldots, x_m$, then

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

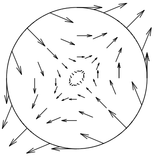
- $\mathrm{ind}_j(v)$, "index of v in x_j" = number of windings of $v/|v|$ around x_j
- $\chi(\Sigma)$, "Euler characteristic of Σ" = # Faces - # Edges + # Vertices



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



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



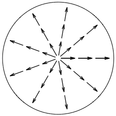
$\mathrm{ind}_0(v) = -1$

Topological constraints

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

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

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



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

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

$v \notin H^1(B_1)$, but $|\nabla v| \in L^p(B_1)$ for all $1 \leq p < 2$.

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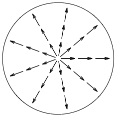

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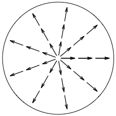

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Summary (1)

- 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, embedded in $\mathbb{R}^3$. Then

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

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Well-posedness

Results

- Stationary problem:

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

- Gradient-flow:

  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

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

Well-posedness

Sketch:

- Relax: instead of solving

$$\partial_t \mathbf{n} = -\nabla W_{ex}(\mathbf{n}), \qquad \text{on } |\mathbf{n}| = 1,$$

  solve

$$\partial_t \mathbf{n}^\varepsilon = -\nabla \left(W_{ex}(\mathbf{n}^\varepsilon) + \frac{1}{4\varepsilon^2} \int_\Sigma (|\mathbf{n}^\varepsilon|^2 - 1)^2 \mathrm{d}S \right).$$

- Recover the quadratic terms $|\mathrm{D}\mathbf{n}|^2\mathbf{n} + \ldots$ with the *Chen-Struwe trick for harmonic maps*:

$$-\Delta \mathbf{n} = |\mathrm{D}\mathbf{n}|^2 \mathbf{n} \qquad \Rightarrow \qquad \begin{cases} -\Delta \mathbf{n} & = \lambda \mathbf{n}, \\ \lambda & = |\mathrm{D}\mathbf{n}|^2 \end{cases}$$

  if $|\mathbf{n}| = 1$,

$$\Delta \mathbf{n} \times \mathbf{n} = 0 \qquad \Rightarrow \qquad \begin{cases} -\Delta \mathbf{n} & = \lambda \mathbf{n}, \\ \lambda & = -\Delta \mathbf{n} \cdot \mathbf{n} = |\mathrm{D}\mathbf{n}|^2 \end{cases}$$

- Apply the trick to $(\partial_t \mathbf{n}^\varepsilon - \Delta_g \mathbf{n}^\varepsilon + \mathrm{d}\nu(\mathbf{n}^\varepsilon)) \times \mathbf{n}^\varepsilon$

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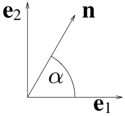
Given an orthonormal frame $\{\mathbf{e}_1, \mathbf{e}_2\}$, represent the director by the angle α such that

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

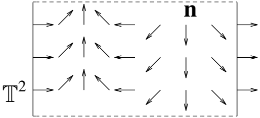


Note: locally it is always possible.

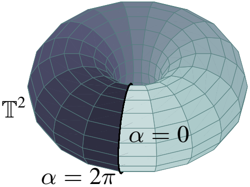
Question:

Given $\mathbf{n} \in H^1_{\tan}(\Sigma; \mathbb{S}^2)$, is it possible to find a global orthonormal frame $\{\mathbf{e}_1, \mathbf{e}_2\}$ and $\alpha \in H^1(\Sigma; \mathbb{R})$ satisfying (*)?

(No) Example:



$\longrightarrow$



α-representation

Answer:

Given

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

it is possible to find and $\alpha \in H^1(Q)$ satisfying

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

Sketch:

- define

$$\omega := \frac{x\,dy - y\,dx}{x^2 + y^2} \qquad \text{on } \mathbb{R}^2 \setminus \{\mathbf{0}\}.$$

- fix $p_0 \in \Sigma$, define

$$\alpha(p) := \alpha_0 + \int_\gamma \mathbf{n}^*\omega \qquad (\gamma: \text{ path connecting } p_0 \text{ and } p)$$

- α is well-defined if and only if $\int_\gamma \mathbf{n}^*\omega = 0$ on loops

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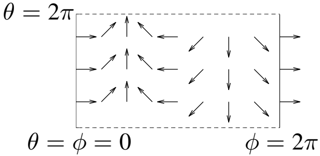
α-representation

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

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



Correspondence between classes in

Fundamental group of $\mathbb{T}^2$
Loops / Homotopy classes

Fields $\mathbf{n} \in H^1_{\tan}(\mathbb{T}^2;\mathbb{S}^2)$
/ degree on generators

$H^1(Q)$ "periodic" functions α / boundary conditions

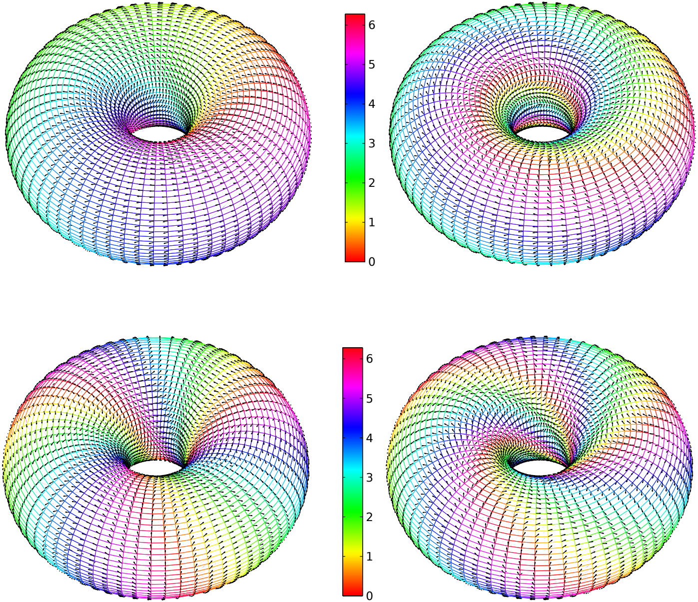


Figure: In clockwise order, from top-left corner: index (1,1), (1,3), (3,3), (3,1). The colour represents the angle $\alpha \mod 2\pi$, the arrows represent the vector field $\mathbf{n}$.

α-representation

Translate the energies:

$$W_{in}(\mathbf{n}) = \frac{1}{2}\int_{\Sigma} |\mathrm{D}\mathbf{n}|^2 \mathrm{d}S = \frac{1}{2}\int_{Q} |\nabla_s \alpha|^2 \mathrm{d}S + M_{in}(R/r)$$

$$W_{ex}(\mathbf{n}) = \frac{1}{2}\int_{\Sigma} |\nabla_s \mathbf{n}|^2 \mathrm{d}S = \frac{1}{2}\int_{Q} \left\{ |\nabla_s \alpha|^2 + \eta \cos(2\alpha) \right\} \mathrm{d}S + M_{ex}(R/r)$$

where M_{in}, M_{ex} are constant in α and $\eta = \frac{c_1^2 - c_2^2}{2}$.
For $\alpha \equiv const$ on Q,

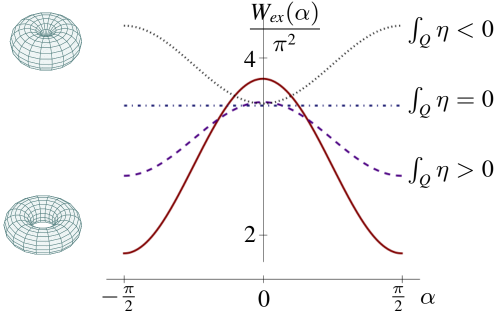
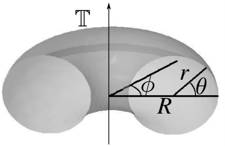


Figure: The ratio of the radii $\mu = R/r$ is : $\mu = 1.1$ (dotted line), $\mu = 2/\sqrt{3}$ (dashed dotted line), $R/r = 1.25$ (dashed line), $R/r = 1.6$ (continuous line).

Explicit forms of 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

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



$$\nabla_s \alpha = g^{ii}\partial_i \alpha = \frac{1}{r^2}(\partial_\theta \alpha)X_\theta + \frac{1}{(R + r\cos\theta)^2}(\partial_\phi \alpha)X_\phi$$
$$= \frac{1}{r}(\partial_\theta \alpha)\mathbf{e}_1 + \frac{1}{R + r\cos\theta}(\partial_\phi \alpha)\mathbf{e}_2,$$

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

Local minimizers

- Energy:

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

Features: <u>not convex</u>, <u>not coercive</u>

- 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:

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

Reduced problem: given $\mathbf{m}$,

1. build $\psi_{\mathbf{m}} \in H^1_{\mathbf{m}}(Q)$
2. find $u \in H^1_{per}(Q)$ such that

$$\Delta_s u + \eta \sin(2u + 2\psi_{\mathbf{m}}) = 0$$

Local minimizers

- Energy:

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

  Features: not convex, not coercive

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$$\Delta_s u + \eta \sin(2u + 2\psi_{\mathbf{m}}) = 0$$

α-flow

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

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

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

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α-flow

1. Reconstruct (i)

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

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

2. Reconstruct (ii):

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

has constant winding **m** along the flow.

Numerical experiments

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

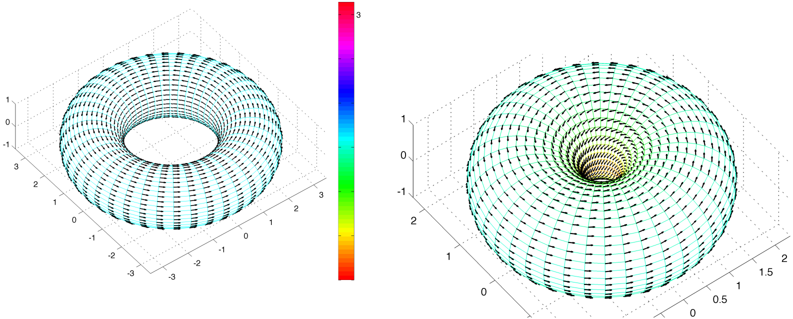


Figure: Configuration of a numerical solution α of the gradient flow. Left $R/r = 2.5$; right: $R/r = 1.33$. The colour represents the angle $\alpha \in [0, \pi]$, the arrows represent the vector field $\mathbf{n}$.

Numerical experiments

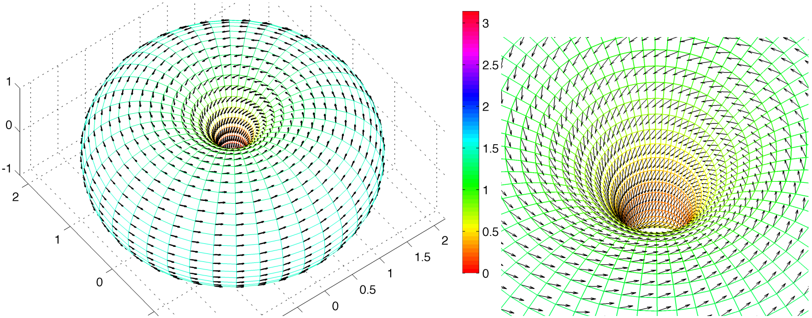
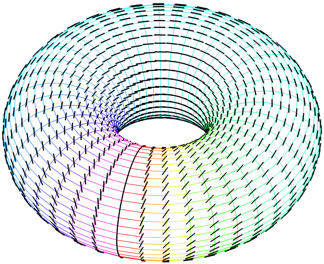
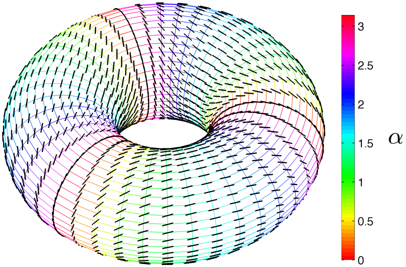


Figure: Configuration of the scalar field α and of the vector field $\mathbf{n}$ of a numerical solution to the the gradient flow, for $R/r = 1.2$ (left). Zoom-in of the central region of the same fields (right).

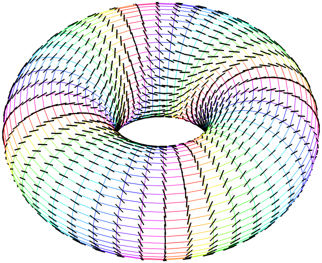
Numerical experiments – identifying +**n** and -**n**



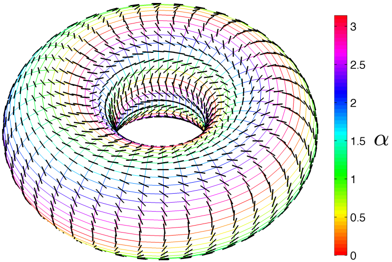
$\mathbf{m} = (0, 1), \quad W = 10.93$



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



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



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