

Minimizers of the Landau-de Gennes energy around a spherical colloid particle

Lia Bronsard

McMaster University

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- Director $n(x)$, $|n(x)| = 1$ indicates local axis of preference: gives on average the direction of alignment.



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 $\implies n : \Omega \rightarrow \mathbb{R}P^2$.

Harmonic Maps to S^2 (or $\mathbb{R}P^2$)

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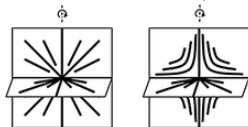
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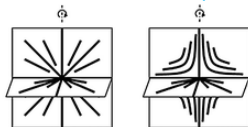
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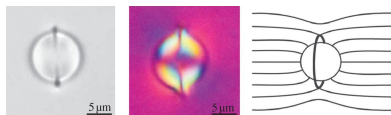
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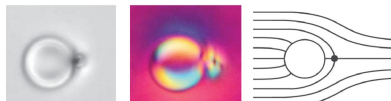
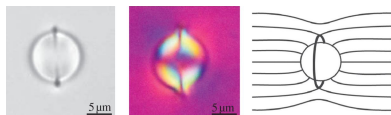


- ▶ Hardt-Kinderlehrer-Lin (1986): for Oseen-Frank, min are real analytic except for a closed set Z , $\mathcal{H}^1(Z) = 0$.

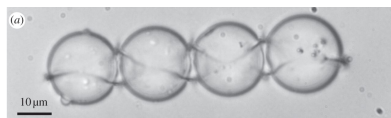
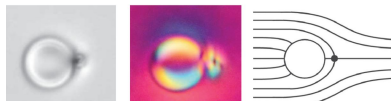
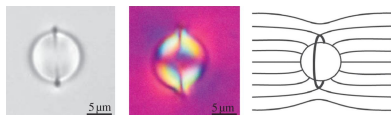
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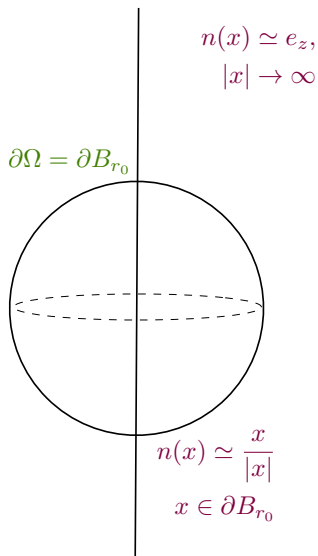
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I. Musevic, M. Skarabot and M. Ravnik, *Phil Trans Roy Soc A*, 2013

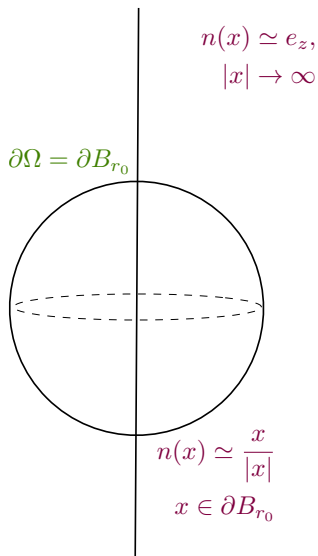
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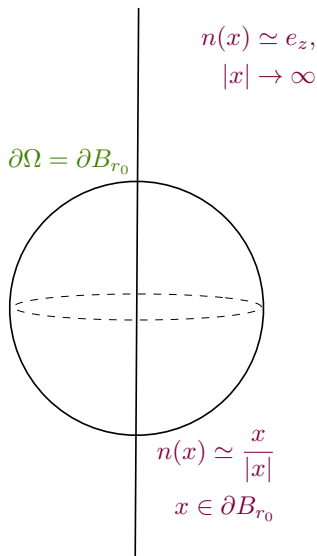
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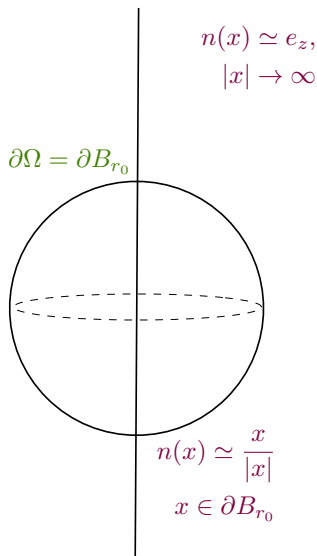
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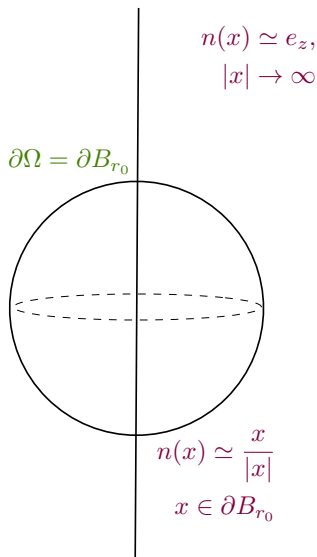
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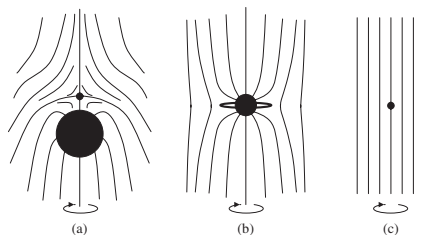
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 - ▶ **Weak anchoring**, via surface energy, $\frac{\gamma}{2} \int_{\partial B_{r_0}} |n - e_r|^2 dS$

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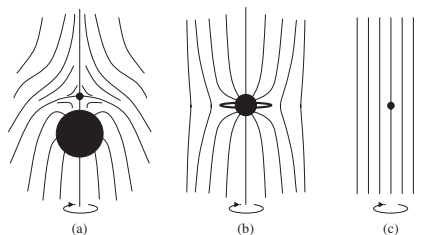
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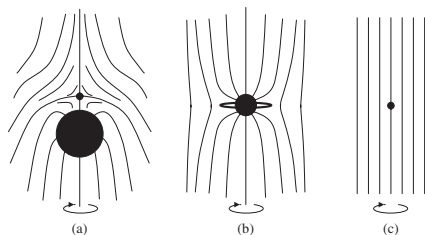


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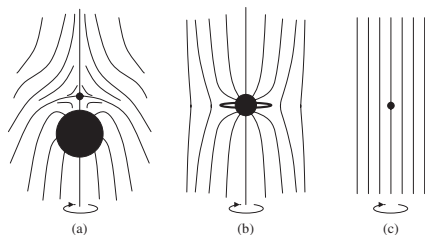


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- (c) For small r_0 and low \mathcal{W} , no singular structure at all.

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 - ▶ But harmonic map/Oseen-Frank has no fixed length scale; cannot distinguish different radii.
- New approach: embed the harmonic map problem in a larger family of variational problems with a natural length scale. The harmonic maps may be recovered in an appropriate limit.

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- **Isotropic** Q-tensor: all eigenvalues are equal, so $Q = 0$. No preferred direction, the liquid crystal has no alignment or ordering.

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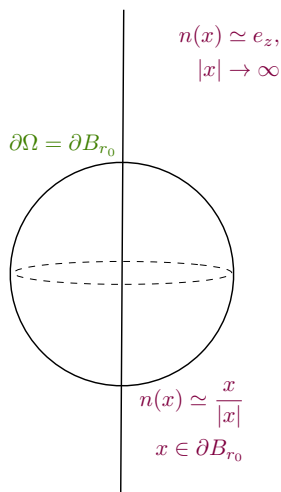
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- Analogy: Ginzburg–Landau model, a relaxation of the \mathcal{S}^1 -harmonic map problem:

$$\int_{\Omega} \left[\frac{\epsilon^2}{2} |\nabla u|^2 + (|u|^2 - 1)^2 \right], u : \Omega \rightarrow \mathbb{C}$$

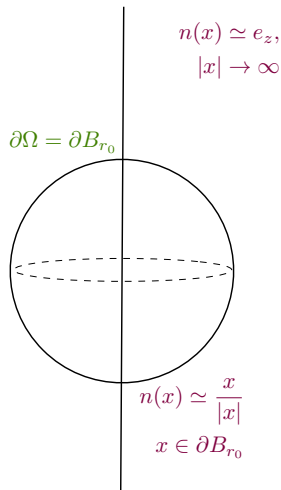
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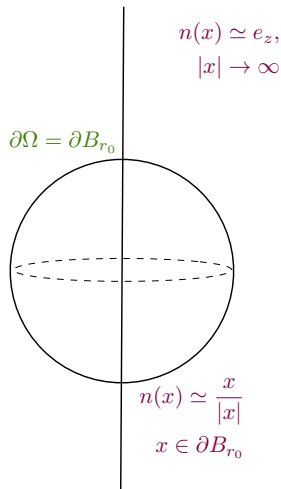
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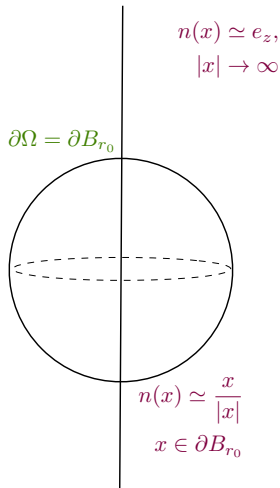
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The spherical colloid, joint work with S. Alama and X. Lamy.

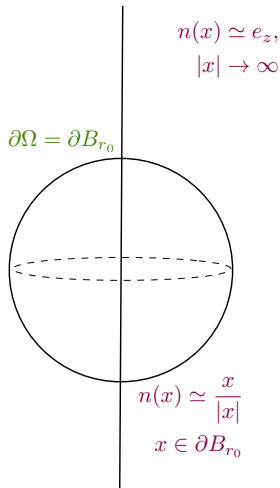
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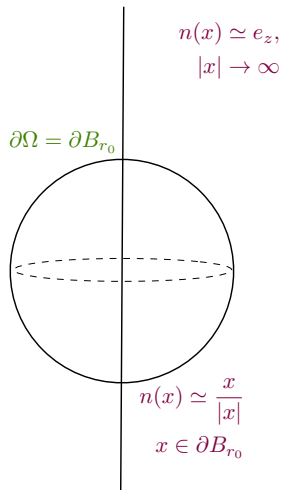
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 - ▶ $\implies \frac{\hat{L}}{\hat{W}} \frac{\partial Q}{\partial \nu} = Q_s - Q$ on ∂B_{r_0} .

Two scaling limits

First rescale by the particle radius r_0 ; $\Omega = \mathbb{R}^3 \setminus B_1(0)$,

$$\mathcal{F}(Q) = \int_{\Omega} \left[\frac{\hat{L}}{2r_0^2} |\nabla Q|^2 + f(Q) \right] dx + \frac{\hat{W}}{2r_0} \int_{\partial B_1} |Q_s - Q|^2 dA.$$

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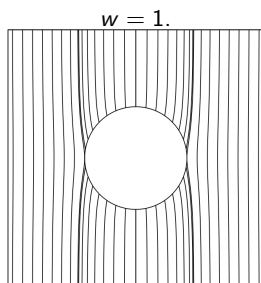
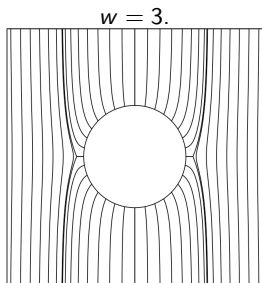
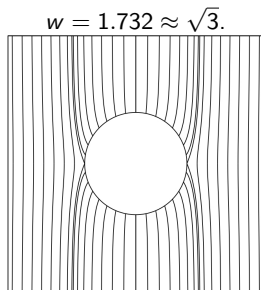
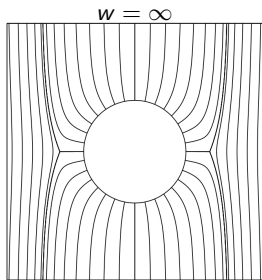
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- At eigenvalue crossing $\lambda_1 = \lambda_2$, eigenvectors exchange \implies **discontinuous director!**
- This occurs along a circle, $(r_w, \theta, 0)$, with r_w root of:

$$r^3 - \frac{w}{1+w} r^2 - \frac{w}{3+w} = 0.$$

The Saturn Ring



Colloidal cuboids (homeotropic)

"Superellipsoid"

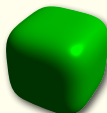
$$\left(\frac{x}{b}\right)^{2p} + \left(\frac{y}{b}\right)^{2p} + \left(\frac{z}{a}\right)^{2p} = 1$$

Aspect ratio: a/b .

"Sharpness": p .



$p = 1$



$p = 2$

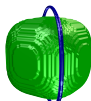


$p = 10$

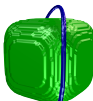
$a/b = 1$



$p = 1$



1.5



2



2.5



3



10

Beller, Gharbi & Liu, *Soft Matter*, 2015, 11, 1078

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 - ▶ [Hardt-Lin \(1986\)](#) For any N , $\exists g : \partial B_1(0) \rightarrow \mathbb{S}^2$ with degree zero such that the *minimizing* harmonic map has N defects in $B_1(0)$.

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Theorem

For any sequence of axisymmetric minimizers with $L \rightarrow 0$, a subsequence converges to a map $Q_(x) = s_*(n(x) \otimes n(x) - I/3)$, locally uniformly in $\overline{\Omega} \setminus \{p_0\}$. Here n minimizes the Dirichlet energy in Ω , among axially symmetric \mathbb{S}^2 -valued maps satisfying the boundary conditions*

$$n = e_r \text{ on } \partial B_1, \quad \text{and} \quad \int_{\Omega} \frac{(n_1)^2 + (n_2)^2}{|x|^2} dx < \infty,$$

*and n is analytic away from **exactly one point defect** p_0 , located on the axis of symmetry.*

Why only one singularity?

- Use cylindrical coords (ρ, θ, z) in $\Omega = \mathbb{R}^3 \setminus B_1$; by axial symmetry,
 - ▶ it suffices to consider the cross-section Ω_{cyl} with $\theta = 0$;
 - ▶ Ω_{cyl} is **simply connected**, so the director n is oriented;
 - ▶ $n \in \mathbb{S}^2$ is determined by the spherical angle $\phi = \psi(\rho, z)$,

$$n = \sin \psi(\rho, z) e_\rho + \cos \psi(\rho, z) e_z$$

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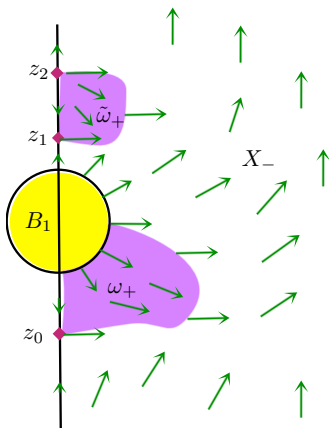
- Harmonic map energy, integrated in a cross-section Ω_{cyl} :

$$E(\psi) = \int_{\Omega_{cyl}} \left[|\partial_\rho \psi|^2 + |\partial_z \psi|^2 + \frac{1}{\rho^2} \sin^2 \psi \right] \rho d\rho dz$$

- Single nonlinear PDE,

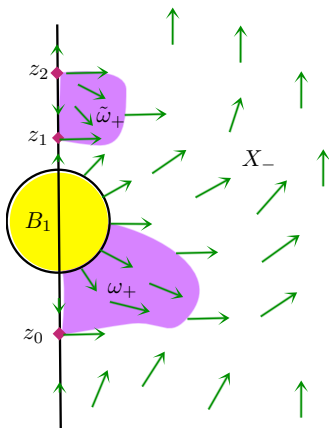
$$\partial_z^2 \psi + \partial_\rho^2 \psi + \frac{1}{\rho} \partial_\rho \psi = \frac{1}{2\rho^2} \sin(2\psi) \quad \text{in } \Omega_{cyl}$$

Key observation: $X_- = \{\psi(\rho, z) < \frac{\pi}{2}\}$ and $X_+ = \{\psi(\rho, z) > \frac{\pi}{2}\}$ are both connected.

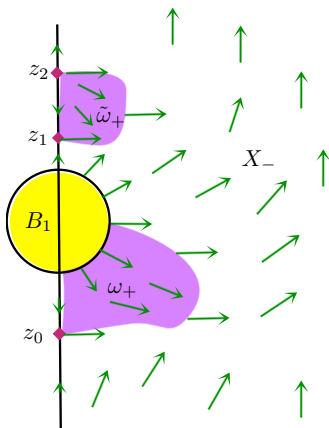


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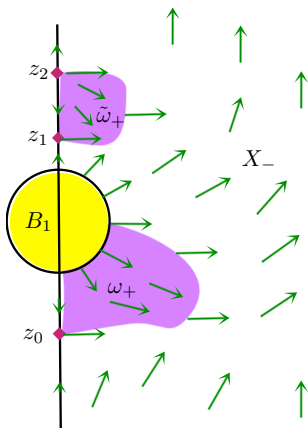


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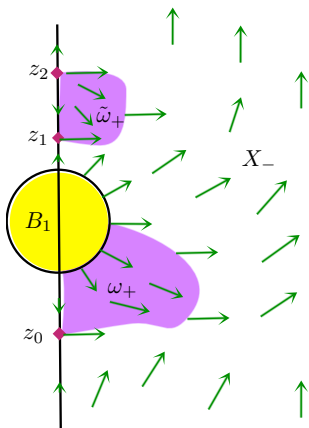
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- If X_+ has a component $\tilde{\omega}_+$ whose boundary is disjoint from ∂B_1 , replace ψ in $\tilde{\omega}_+$ by $\tilde{\psi}(\rho, z) = \pi - \psi(\rho, z)$;
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- X_{\pm} connected + topological argument \implies exactly one defect!