Electrostatic self-interactions of hopfions and skyrmions in liquid crystals

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Motivation

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- Non-polar director field $\vec{n}(\vec{x}) \in \mathbb{RP}^2 \cong S^2/\mathbb{Z}_2$
- Hopfions $\vec{n} : S^3 \to \mathbb{RP}^2$ and skyrmions $\vec{n} : S^2 \to \mathbb{RP}^2$
- Presence of topological defects cause orientational distortions $\longrightarrow$ non-uniform strain
- Flexoelectric effect: electric polarization response $\vec{P}_f(\vec{n})$ $\longrightarrow$ induced electric field $\vec{E}(\vec{n})$
- Associated electrostatic self-energy $\propto \vec{E}(\vec{n}) \cdot \vec{P}_f(\vec{n})$ $\longrightarrow$ back-reaction on $\vec{n}$
- How to include this electrostatic self-interaction and back-reaction?
- Analogous to demagnetization in chiral magnets (depolarization)

Chiral liquid crystals

Isotropic elastic liquid crystal

- Frank-Oseen free energy is $$E_{\mathrm{FO}} = \frac{1}{2}K \int_{\mathbb{R}^3} \mathrm{d}^3x |\nabla \vec{n}|^2$$
- Energy minimizers are solutions of Laplace equation $\Delta \vec{n} = \vec{0}$
- Metastable inhomogeneous solutions found by Belavin and Polyakov[1] in ferromagnets
- More insight can be gained by considering elastic modes
- Decompose director gradient tensor into these normal modes[2] $(\vec{B}, T, S, \mathbf{\Delta})$

$$\partial_i n_j = -n_i B_j + \frac{1}{2} T \epsilon_{ijk} n_k + \frac{1}{2} S(\delta_{ij} - n_i n_j) + \Delta_{ij}$$

[1] A.A. Belavin and A.M. Polyakov, *Metastable states of two-dimensional isotropic ferromagnets*, Pis'ma Zh. E´ksp. Teor. Fiz. **22** (1975) 503
[2] J.V. Selinger, *Interpretation of saddle-splay and the Oseen-Frank free energy in liquid crystals*, Liq. Cryst. Rev. **6** (2018) 129

Bend

$$\partial_i n_j = \boxed{-n_i B_j} + \frac{1}{2} T \epsilon_{ijk} n_k + \frac{1}{2} S(\delta_{ij} - n_i n_j) + \Delta_{ij}$$

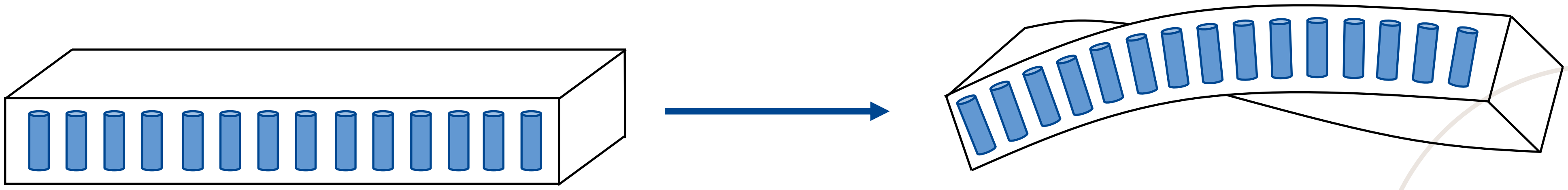
- Standard bend vector $\vec{B} = -(\vec{n} \cdot \vec{\nabla})\vec{n} = \vec{n} \times (\vec{\nabla} \times \vec{n})$
- Invariant under $\vec{n} \mapsto -\vec{n}$

- Elastic bend energy $|\vec{B}|^2 = [\vec{n} \times (\vec{\nabla} \times \vec{n})]^2$

Twist

$$\partial_i n_j = -n_i B_j + \boxed{\frac{1}{2} T \epsilon_{ijk} n_k} + \frac{1}{2} S(\delta_{ij} - n_i n_j) + \Delta_{ij}$$

- Pseudoscalar twist $T = \vec{n} \cdot (\vec{\nabla} \times \vec{n})$
- Invariant under $\vec{n} \mapsto -\vec{n}$



- Elastic twist energy $T^2 = [\vec{n} \cdot (\vec{\nabla} \times \vec{n})]^2$

Splay

$$\partial_i n_j = -n_i B_j + \frac{1}{2} T \epsilon_{ijk} n_k + \boxed{\frac{1}{2} S(\delta_{ij} - n_i n_j)} + \Delta_{ij}$$

- Standard scalar splay $S = \vec{\nabla} \cdot \vec{n}$
- Invariant under $\vec{n} \mapsto -\vec{n}$

- Elastic splay energy $|S\vec{n}|^2 = (\vec{\nabla} \cdot \vec{n})^2$

Nematic liquid crystal (NLC)

- Isotropic Frank-Oseen free energy for a NLC is

$$E_{\mathrm{FO}} = \frac{1}{2} K \int_{\mathbb{R}^3} \mathrm{d}^3 x \left\{ S^2 + T^2 + |\vec{B}|^2 \right\}$$

- Modes cost elastic free energy
- Energy cost of splay, twist and bend deformations are equivalent
- Energy of anisotropic NLC:

$$E_{\mathrm{FO}} = \int_{\Omega} \mathrm{d}^3 x \left\{ \frac{K_1}{2} (\vec{\nabla} \cdot \vec{n})^2 + \frac{K_2}{2} \left[\vec{n} \cdot (\vec{\nabla} \times \vec{n}) \right]^2 + \frac{K_3}{2} \left[\vec{n} \times (\vec{\nabla} \times \vec{n}) \right]^2 \right\}$$

- Can introduce enantiomorphy into the system $\longrightarrow$ **chiral** liquid crystals

Chiral liquid crystal (CLC)

- Molecular chirality characterized by (pseudoscalar) cholesteric twist $q_0 = \dfrac{2\pi}{p}$
- Enantiomorphy introduced via twist $T \mapsto T + q_0$ [3]
- Frank-Oseen free energy picks up 1st order term

$$F_{\mathrm{FO}} = \int_\Omega \mathrm{d}^3x \left\{ \frac{K_1}{2}(\vec{\nabla}\cdot\vec{n})^2 + \frac{K_2}{2}\left[\vec{n}\cdot(\vec{\nabla}\times\vec{n})\right]^2 + \frac{K_3}{2}\left[\vec{n}\times\vec{\nabla}\times\vec{n}\right]^2 + K_2 q_0 \boxed{\left[\vec{n}\cdot(\vec{\nabla}\times\vec{n})\right]} + V(\vec{n}) \right\}$$

- Equivalent to **DMI** term in chiral magnets arising from Dresselhaus SOC

  ⟶ Mechanism responsible for stabilization of bulk skyrmions

  ⟶ Favours Bloch modulations

[3] P.M. Chaikin and T.C. Lubensky, *Principles of Condensed Matter Physics*, Cambridge University Press (1995)

Experimental realization

- CLCs placed between parallel plates with separation d
- System restricted to confined geometry[4]

$$\Omega = \left\{ (x,y,z) \in \mathbb{R}^3 \; : \; |z| \leq \frac{d}{2} \right\}$$

- Apply potential difference U $\longrightarrow$ external electric field $\vec{E}_{\text{ext}} = \left(0, 0, \frac{U}{d}\right)$
- CLCs are dielectric materials

$$\mathcal{E}_{\text{elec}} = -\frac{\epsilon_0 \Delta\epsilon}{2} (\vec{E}_{\text{ext}} \cdot \vec{n})^2$$

- Can impose strong homeotropic anchoring $\vec{n}(x,y,z = \pm d/2) = \vec{n}_{\uparrow}$
- Mimicked in 2D systems by including Rapini-Papoular homeotropic surface anchoring potential[5]

$$\mathcal{E}_{\text{anch}} = -\frac{1}{2} W_0 n_z^2$$

Effective surface anchoring strength

[4] S. Afghah and J.V. Selinger, *Theory of helicoids and skyrmions in confined cholesteric liquid crystals*, Phys. Rev. E **96** (2017) 012708
[5] A. Rapini and M. Papoular, *Distorsion d'une lamelle nématique sous champ magnétique conditions d'ancrage aux parois*, Le J. Phys. Colloq. **30**, C4 (1969)

Electrostatic self-interaction

Flexoelectric polarization

- **Flexoelectricity**: coupling between electrical polarization and <u>non-uniform</u> strain
- Orientational distortions $\longrightarrow$ macroscopic electric polarization $\vec{P}_f$
- Fix splay, induce polarization:

$$F = \frac{1}{2}K_1\left|\vec{n}(\vec{\nabla}\cdot\vec{n}) - c_1\vec{P}\right|^2 + \frac{1}{2}\mu|\vec{P}|^2 \quad\longrightarrow\quad \frac{\delta F}{\delta \vec{P}} = \vec{0} \Rightarrow \vec{P} = \left(\frac{c_1 K_1}{c_1^2 K_1 + \mu}\right)(\vec{\nabla}\cdot\vec{n})\vec{n}$$

- Fix bend, induce polarization:

$$F = \frac{1}{2}K_3\left|[\vec{n}\times(\vec{\nabla}\times\vec{n})] - c_3\vec{P}\right|^2 + \frac{1}{2}\mu|\vec{P}|^2 \quad\longrightarrow\quad \frac{\delta F}{\delta \vec{P}} = \vec{0} \Rightarrow \vec{P} = \left(\frac{c_3 K_3}{c_3^2 K_3 + \mu}\right)[\vec{n}\times(\vec{\nabla}\times\vec{n})]$$

- Polarization caused by mechanical curvature (**flexion**) of director (flexoelectric)[6,7]:

$$\boxed{\vec{P}_f = e_1\left[(\vec{\nabla}\cdot\vec{n})\vec{n}\right] + e_3\left[\vec{n}\times(\vec{\nabla}\times\vec{n})\right]}$$

[6] R.B. Meyer, *Piezoelectric effects in liquid crystals*, Phys. Rev. Lett. **22** (1969) 918
[7] J.S. Patel and R.B. Meyer, *Flexoelectric electro-optics of a cholesteric liquid crystal*, Phys. Rev. Lett. **58** (1987) 1538

Electrostatic potential

$$\vec{P}_f = e_1 \left[(\vec{\nabla} \cdot \vec{n})\vec{n} \right] + e_3 \left[\vec{n} \times (\vec{\nabla} \times \vec{n}) \right]$$

- Flexoelectric polarization induces continuous electric **dipole** moment distribution $\vec{P}_f$
- Associated electric scalar potential

$$\varphi(\vec{x}) = \frac{1}{4\pi\epsilon_0} \int_\Omega \mathrm{d}^3\vec{y} \left\{ \frac{\vec{P}_f(\vec{y}) \cdot (\vec{x} - \vec{y})}{|\vec{x} - \vec{y}|^3} \right\}$$

- Green's function for Laplacian on $\mathbb{R}^3$

$$G(\vec{x}, \vec{y}) = \frac{1}{4\pi|\vec{x} - \vec{y}|}, \qquad \Delta_{\vec{x}} G(\vec{x}, \vec{y}) = \delta(\vec{x} - \vec{y})$$

- Identity: $\vec{\nabla}_{\vec{x}} \left(\frac{1}{|\vec{x} - \vec{y}|} \right) = -\frac{\vec{x} - \vec{y}}{|\vec{x} - \vec{y}|^3} \longrightarrow \varphi(\vec{x}) = -\frac{1}{\epsilon_0} \int_\Omega \mathrm{d}^3\vec{y} \left\{ \vec{P}_f(\vec{y}) \cdot \vec{\nabla}_{\vec{x}} G(\vec{x}, \vec{y}) \right\}$

- **Electrostatic potential** satisfies the **Poisson equation**[8] $\boxed{\Delta\varphi = -\nabla^2\varphi = -\frac{1}{\epsilon_0} \vec{\nabla} \cdot \vec{P}_f}$
- Gauss' law $\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}$

$\boxed{\rho = -\vec{\nabla} \cdot \vec{P}_f}$ electric charge density

[8] J. Yang, Y. Zou, W. Tang, J. Li, M. Huang and S. Aya, *Spontaneous electric-polarization topology in confined ferroelectric nematics*, Nat Commun **13** (2022) 7806

Flexoelectric self-energy

$$\boxed{\Delta\varphi = -\frac{1}{\epsilon_0}\vec{\nabla}\cdot\vec{P}_f}$$

- Energy of a continuous dipole density distribution[9]

$$F_{\text{flexo}} = -\frac{1}{2}\int_{\Omega} \mathrm{d}^3x\,\vec{E}(\vec{x})\cdot\vec{P}_f(\vec{x}) = \frac{1}{2}\int_{\Omega}\mathrm{d}^3x\,\vec{P}_f\cdot\vec{\nabla}\varphi$$

- More useful to express the flexoelectric energy as

$$F_{\text{flexo}} = -\frac{1}{2}\int_{\Omega}\mathrm{d}^3\vec{x}\,\boxed{\left(\vec{\nabla}\cdot\vec{P}_f\right)}\varphi + \cancel{\frac{1}{2}\int_{\partial\Omega}\mathrm{d}\vec{s}\cdot\left(\varphi\vec{P}_f\right)} = \frac{\epsilon_0}{2}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{x}\,\varphi\Delta\varphi$$

- In all cases we consider, surface term vanishes
- Coincides with the electrostatic self-energy of the charge distribution $\rho = -(\nabla\cdot\vec{P}_f)$

$$F_{\text{flexo}} = \frac{\epsilon_0}{2}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{x}\,\varphi\Delta\varphi = \frac{\epsilon_0}{2}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{x}\,|\vec{\nabla}\varphi|^2 = \frac{\epsilon_0}{2}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{x}\,|\vec{E}|^2$$

[9] L.M. Blinov, Structure and Properties of Liquid Crystals, Springer Dordrecht (2011)

Rescaling F_{flexo}

- Length and energy scales: $L_0 = \frac{1}{q_0}\frac{K_1}{K_2}$, $E_0 = \frac{1}{q_0}\frac{K_1^2}{K_2}$
- Scalar potential $\varphi = \lambda\hat{\varphi}$
- Flexoelectric energy and Poisson equation under rescaling

Adimensional polarization

$$\boxed{\vec{P} = (\vec{\nabla}_{\hat{x}}\cdot\vec{n})\vec{n} + \frac{e_3}{e_1}(\vec{n}\times[\vec{\nabla}_{\hat{x}}\times\vec{n}])}$$

$$\hat{F}_{\text{flexo}} = \frac{1}{2}\boxed{\frac{L_0\lambda^2\epsilon_0}{E_0}}\int_\Omega \mathrm{d}^3\hat{x}\,\hat{\varphi}\Delta_{\hat{x}}\hat{\varphi} \qquad \Delta_{\hat{x}}\hat{\varphi} = -\boxed{\frac{e_1}{\epsilon_0\lambda}}\vec{\nabla}_{\hat{x}}\cdot\boxed{\vec{P}}$$

- Dimensionless vacuum permittivity $\epsilon = \boxed{\frac{L_0\lambda^2\epsilon_0}{E_0}} = \left(\boxed{\frac{e_1}{\epsilon_0\lambda}}\right)^{-1}$ $\longrightarrow$ $\lambda = \frac{K_1}{e_1}$

- Necessary rescaling is

$$\hat{F}_{\text{flexo}} = \frac{\epsilon}{2}\int_\Omega \mathrm{d}^3\hat{x}\,\hat{\varphi}\Delta_{\hat{x}}\hat{\varphi}, \quad \Delta_{\hat{x}}\hat{\varphi} = -\frac{1}{\epsilon}\vec{\nabla}_{\hat{x}}\cdot\vec{P}, \quad \epsilon = \frac{K_1\epsilon_0}{e_1^2}$$

Scale invariance of F_{flexo}

- Derrick scaling $\vec{x} \mapsto \vec{x}' = \mu \vec{x}$
- Director rescales as $\vec{n}_\mu = \vec{n}(\mu \vec{x})$

$\longrightarrow$ Polarization $\vec{P}_\mu = \mu \left(\vec{\nabla}' \cdot \vec{n}(\mu \vec{x}) \right) \vec{n}(\mu \vec{x}) + \mu \frac{e_3}{e_1} \left(\vec{n}(\mu \vec{x}) \times \vec{\nabla}' \times \vec{n}(\mu \vec{x}) \right) = \mu \vec{P}(\mu \vec{x})$

- Poisson equation: $\Delta' \varphi_\mu = -\frac{1}{\mu \epsilon} \nabla' \cdot \vec{P}_\mu = -\frac{1}{\epsilon} \nabla' \cdot \vec{P}(\mu \vec{x}) = \Delta' \varphi(\mu \vec{x})$

- Scalar potential must scale as $\varphi_\mu(\vec{x}) = \varphi(\mu \vec{x})$
- In **two dimensions**, the flexoelectric Frank-Oseen energy rescales as

$$F_{\text{FFO}}(\mu) = F_{\text{Dirichlet}} + \frac{1}{\mu} F_{\text{DMI}} + \frac{1}{\mu^2} F_{\text{potential}} + \boxed{F_{\text{flexo}}}$$

Conformally invariant

First variation of F_{flexo}

- First variation is

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = \frac{\epsilon}{2}\int_{\mathbb{R}^2} \mathrm{d}^2x \left(\boxed{\dot\varphi\Delta\varphi} + \varphi\Delta\dot\varphi\right)$$

- Potential does not have compact support

$$\boxed{\int_{\mathbb{R}^2} \mathrm{d}^2x\, \dot\varphi\Delta\varphi = \int_{\mathbb{R}^2} \mathrm{d}^2x\, \varphi\Delta\dot\varphi - \boxed{\oint_{\partial B_\infty(0)} \mathrm{d}\vec{s}\cdot\left(\varphi\vec\nabla\dot\varphi - \dot\varphi\vec\nabla\varphi\right)}}$$

- Does have $1/r$ localization

$$\longrightarrow \boxed{\lim_{R\to\infty} \frac{\epsilon}{2}\int_{\partial B_R(0)} (\dot\varphi \star \mathrm{d}\varphi - \varphi\star\mathrm{d}\dot\varphi) = \lim_{R\to\infty}\frac{\epsilon R}{2}\int_0^{2\pi}(\dot\varphi\varphi_r - \varphi\dot\varphi_r)\mathrm{d}\theta = 0}$$

- First variation reduces to

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = \epsilon\int_\Omega \mathrm{d}^3x\, \varphi\boxed{\Delta\dot\varphi}$$

Need to compute

First variation of F_{flexo}

- First variation is $$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = \epsilon \int_\Omega \mathrm{d}^3x\, \varphi \boxed{\Delta\dot{\varphi}}$$
- Poisson equation variation $$\boxed{\Delta\dot{\varphi} = -\frac{1}{\epsilon}\vec{\nabla}\cdot\left(\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\vec{P}(\vec{n}_t)\right)}$$
- Flexoelectric variation becomes

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = -\int_{\mathbb{R}^2} \mathrm{d}^2x\, \varphi\vec{\nabla}\cdot\left(\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\vec{P}(\vec{n}_t)\right) = \int_{\mathbb{R}^2} \mathrm{d}^2x\, \vec{\nabla}\varphi\cdot\left(\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\vec{P}(\vec{n}_t)\right)$$

$$= \int_{\mathbb{R}^2} \mathrm{d}^2x\, \left(\boxed{\operatorname{grad}_{\vec{n}} F_{\text{flexo}}}\right)\cdot\boxed{\vec{\varepsilon}} \qquad \boxed{\vec{\varepsilon} = \partial_t\vec{n}_t|_{t=0}}$$

$$\boxed{\operatorname{grad}_{\vec{n}} F_{\text{flexo}} = \frac{e_3}{e_1}\left[\left((\vec{\nabla}\times\vec{n})\times\vec{\nabla}\varphi\right) + \left(\vec{\nabla}\times(\vec{\nabla}\varphi\times\vec{n})\right)\right] - \vec{\nabla}(\vec{\nabla}\varphi\cdot\vec{n}) + (\vec{\nabla}\cdot\vec{n})\vec{\nabla}\varphi}$$

Numerical method

Relation to chiral magnets

- Stability of 2D skyrmions in chiral liquid crystals arises from **same mechanism** responsible for the existence of skyrmions in **chiral magnetic** systems[10]
- One constant approximation $K_i = K$
- Vector identity for unit vector $\vec{n}$[11]:

$$(\nabla \vec{n})^2 = \left(\vec{\nabla} \cdot \vec{n}\right)^2 + \left(\vec{n} \cdot \vec{\nabla} \times \vec{n}\right)^2 + (\vec{n} \times \vec{\nabla} \times \vec{n})^2 + \vec{\nabla} \cdot \left[(\vec{n} \cdot \vec{\nabla})\vec{n} - (\vec{\nabla} \cdot \vec{n})\vec{n}\right]$$

- Frank-Oseen energy reduces to chiral magnet energy with Dresselhaus DMI

$$F_{\mathrm{FO}} = \int_{\mathbb{R}^2} \mathrm{d}^2 x \left\{ \frac{1}{2} (\nabla \vec{n})^2 + \left[\vec{n} \cdot (\vec{\nabla} \times \vec{n})\right] + \frac{1}{q_0^2} \frac{1}{K} V(\vec{n}) \right\}$$

[10] A.O. Leonov, I.E. Dragunov, U.K. Rößler and A.N. Bogdanov, *Theory of skyrmion states in liquid crystals*, Phys. Rev. E **90** (2014) 042502
[11] A. Hubert and R. Schäfer, *Magnetic Domains*, Springer Berlin, Heidelberg (2014)

Numerical problem

- Director field $\vec{n}(\vec{x}) \in \mathbb{RP}^2$
- Topological solitons are **minimizers** of the adimensional flexoelectric Frank-Oseen energy

$$F_{\mathrm{FFO}}[\vec{n}] = \int_\Omega \mathrm{d}^3x \left\{ \frac{1}{2}(\nabla\vec{n})^2 + \left[\vec{n}\cdot(\vec{\nabla}\times\vec{n})\right] + \frac{1}{q_0^2}\frac{1}{K}V(\vec{n}) + \frac{1}{2}\vec{P}\cdot\vec{\nabla}\varphi \right\}$$

- Electrostatic potential subject to constraint

$$\begin{cases} \Delta\varphi = -\frac{1}{\epsilon}\vec{\nabla}\cdot\vec{P} & \text{in}\,\Omega, \\ \Delta\varphi = 0 & \text{in}\,\mathbb{R}^3/\Omega. \end{cases} \qquad \Omega = \left\{ (x,y,z) \in \mathbb{R}^3 \,:\, |z| \leq \frac{d}{2} \right\}$$

- Adimensional self-induced polarization is

$$\vec{P} = (\vec{\nabla}\cdot\vec{n})\vec{n} + \frac{e_3}{e_1}\left[\vec{n}\times(\vec{\nabla}\times\vec{n})\right]$$

Electrostatic potential constraint

- Flexoelectric self-interaction introduces **non-locality** into minimization problem
- Reformulate problem as unconstrained optimization problem[12]: minimize the functional

$$F(\varphi) = \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}^3x\, |\mathrm{d}\varphi|^2 + \frac{1}{\epsilon}\int_{\Omega} \mathrm{d}^3x\, \varphi\left(\vec{\nabla}\cdot\vec{P}\right)$$

- Director $\vec{n}$ is fixed

  ⟶ So is divergence of polarization

$$\vec{\nabla}\cdot\vec{P} = \frac{e_3}{e_1}\left[(\vec{\nabla}\times\vec{n})^2 - \vec{n}\cdot[\vec{\nabla}(\vec{\nabla}\cdot\vec{n})] + \vec{n}\cdot\nabla^2\vec{n}\right] + (\vec{\nabla}\cdot\vec{n})^2 + \vec{n}\cdot[\vec{\nabla}(\vec{\nabla}\cdot\vec{n})]$$

- Approach: non-linear conjugate gradient method with line search strategy[13]
- Conjugate stepsize determined using Polak-Ribiere-Polyak method

[12] P. Leask and M. Speight, *Magnetostatic self-interactions of bulk magnetic skyrmion textures in chiral ferromagnets*, In preparation (2025)
[13] D. Harland, P. Leask and M. Speight, *Skyrmion crystals stabilized by ω-mesons*, J. High Energ. Phys. **06** (2024) 116

Arrested Newton flow

- Accelerated gradient descent with flow arresting criteria
- Starting from rest $\partial_t \vec{n}_t|_{t=0} = \vec{0}$
- Solve for motion of a particle in the configuration space under the potential F_{FFO}

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{n}_t = -\mathrm{grad}_{\vec{n}}\left(F_{\mathrm{FO}} + F_{\mathrm{flexo}}\right)[\vec{n}_t]$$

- Reduce problem to coupled system of 1st order ODEs
- Solve coupled system simultaneously with 4th order Runge-Kutta method
- Flow arresting: if $F_{\mathrm{FFO}}(t+\delta t) > F_{\mathrm{FFO}}(t) \longrightarrow$ set $\partial_t \vec{n}(t+\delta t) = \vec{0}$ and restart flow
- Convergence criteria: $\|F_{\mathrm{FFO}}(\vec{n})\|_\infty < 10^{-6}$

Algorithm summary

1. Perform step of ANF method for director field $\vec{n}$ using 4th order Runge-Kutta method
2. Solve Poisson's equation for electric potential φ using NCGD with PRP method
3. Compute total energy of the configuration $(\vec{n}_i, \varphi_i)$ and compare to the energy of the previous configuration $(\vec{n}_{i-1}, \varphi_{i-1})$. If energy has increased, arrest the flow
4. Check convergence criteria: $\|F_{\mathrm{FFO}}(\vec{n})\|_\infty < 10^{-6}$. If the convergence criteria has been satisfied, then stop the algorithm
5. Repeat the process (return to step 1)

Liquid crystal skyrmions

Twist favoured Bloch skyrmions

- In chiral magnets, demagnetizing magnetic potential satisfies $\Delta\psi = -\mu_0 M_s \vec{\nabla} \cdot \vec{n}$
- Dresselhaus DMI favours Bloch skyrmions $\longrightarrow$ $\vec{n}_{\text{Bloch}}(r,\theta) = \sin f(r)\vec{e}_\theta + \cos f(r)\vec{e}_z$
- Bloch skyrmions in chiral magnets are solenoidal $\vec{\nabla} \cdot \vec{n}_{\text{Bloch}} = 0$

  $\longrightarrow$ **Unaffected** by magnetostatic self-interaction

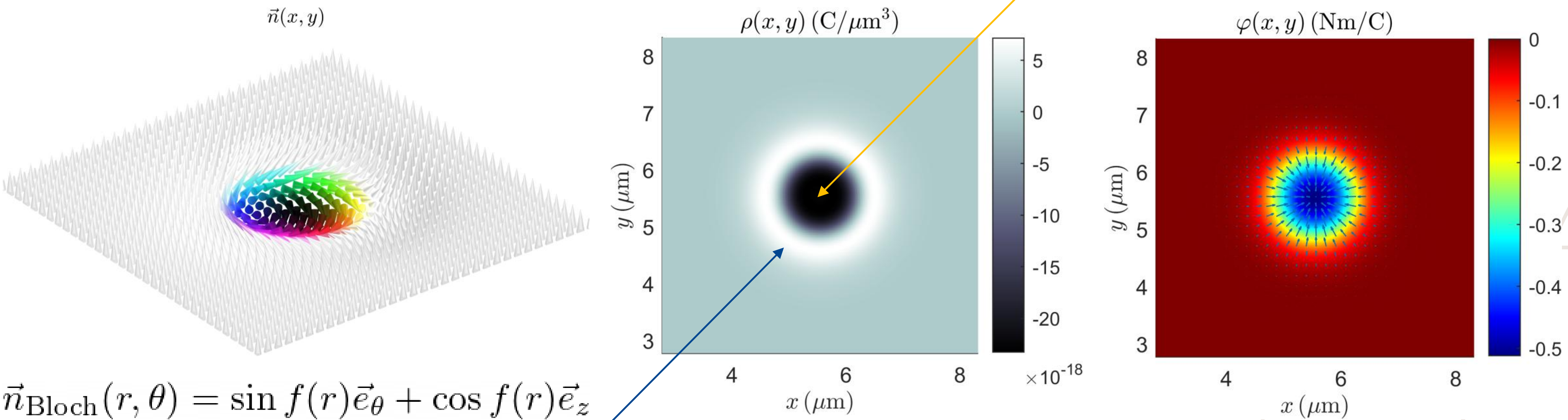
- Chiral liquid crystals: Bloch ansatz is solenoidal, associated polarization <u>is not</u>

$$\vec{P}_{\text{Bloch}} = \frac{e_3}{e_1}\frac{1}{r}\sin^2 f(r)\vec{e}_r \quad \longrightarrow \quad \vec{\nabla} \cdot \vec{P}_{\text{Bloch}} = \frac{e_3}{e_1}\frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r}\sin 2f(r) \neq 0$$

  $\longrightarrow$ Bloch skyrmions in liquid crystals are **affected** by electrostatic self-interaction

Twist favoured Bloch skyrmions $(e_1 = e_3)$

Negatively charged core



$$\vec{n}_{\text{Bloch}}(r,\theta) = \sin f(r)\vec{e}_\theta + \cos f(r)\vec{e}_z$$

Outer ring of positive charge

$$\rho = -\vec{\nabla}\cdot\vec{P}_f = \epsilon_0 \Delta\varphi$$

$$\vec{P}_f = e_1\left[(\vec{\nabla}\cdot\vec{n})\vec{n}\right] + e_3\left[\vec{n}\times(\vec{\nabla}\times\vec{n})\right]$$

Splay and bend favoured liquid crystals

- Nematic liquid crystal $F_{\mathrm{FO}} = \frac{1}{2}K\int_{\Omega}\mathrm{d}^3x\left\{|\vec{S}|^2 + T^2 + |\vec{B}|^2\right\}$

  $\vec{S} = \vec{n}(\vec{\nabla}\cdot\vec{n})$ Splay vector

- Introduce enantiomorphy $\longrightarrow$ Chiral (twist favoured) liquid crystal

$$F_{\mathrm{FO}} = \frac{1}{2}K\int_{\Omega}\mathrm{d}^3x\left\{|\vec{S}|^2 + (T+q_0)^2 + |\vec{B}|^2\right\}$$

- What about splay and bend favoured liquid crystals?

$$F = \frac{K}{2}\int_{\mathbb{R}^3}\mathrm{d}^3x\left\{(\vec{S}+\vec{S}_0)^2 + T^2 + (\vec{B}+\vec{B}_0)^2\right\}$$

- For convenience, consider $\vec{S}_0 = \vec{B}_0 = q_0\vec{e}_3$

DMI from Rashba SOC

$$\longrightarrow \quad F = \int_{\mathbb{R}^3}\mathrm{d}^3x\left\{\frac{K}{2}(\nabla\vec{n})^2 + Kq_0\boxed{[n_z(\vec{\nabla}\cdot\vec{n}) - \vec{n}\cdot\vec{\nabla}n_z]} + V(\vec{n})\right\}$$

Splay and bend favoured Néel skyrmions

- Adimensional splay and bend favoured liquid crystals

$$F = \int_{\mathbb{R}^2} \mathrm{d}^2x \left\{ \frac{1}{2}(\nabla\vec{n})^2 + \boxed{\left[n_z(\vec{\nabla}\cdot\vec{n}) - \vec{n}\cdot\vec{\nabla}n_z \right]} + \frac{1}{q_0^2}\frac{1}{K}V(\vec{n}) + \frac{\epsilon}{2}\varphi\Delta\varphi \right\}$$

- **Rashba DMI** term prefers **Néel** hedgehog skyrmions $\longrightarrow$ $\vec{n}_{\text{Néel}}(r,\theta) = \sin f(r)\vec{e}_r + \cos f(r)\vec{e}_z$
- Unlike Bloch polarization, Néel polarization picks up out-of-plane component

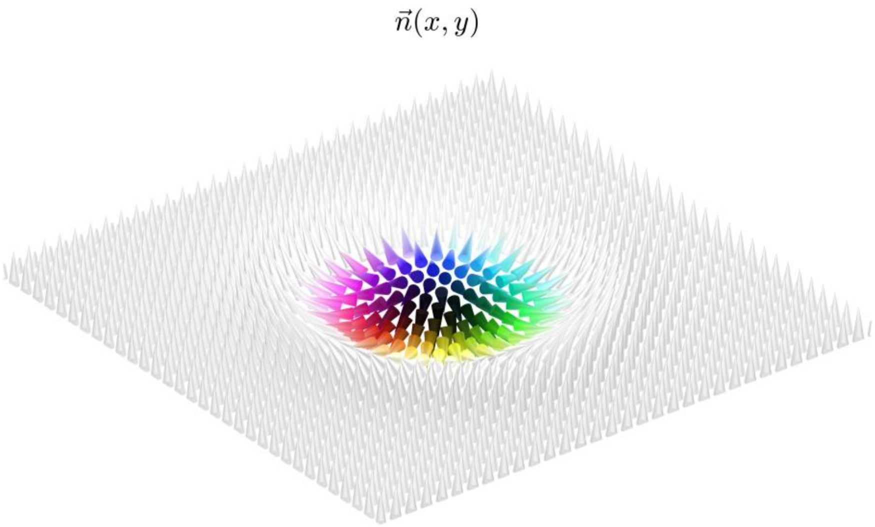
$$\vec{P}_{\text{Néel}} = \left[\frac{1}{r}\sin^2 f(r) + \left(1 - \frac{e_3}{e_1}\right)\frac{1}{2}\sin 2f(r)\frac{\mathrm{d}f}{\mathrm{d}r} \right]\vec{e}_r + \left[\frac{1}{2r}\sin 2f(r) + \left(\cos^2 f(r) + \frac{e_3}{e_1}\sin^2 f(r)\right)\frac{\mathrm{d}f}{\mathrm{d}r} \right]\vec{e}_z$$

- Equal flexoelectric coefficients $e_1 = e_3 \quad \Rightarrow \quad \vec{\nabla}\cdot\vec{P}_{\text{Bloch}} = \vec{\nabla}\cdot\vec{P}_{\text{Néel}} = \frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r}\sin 2f(r)$
- Flexoelectric Bloch and Néel skyrmions equivalent for $e_1 = e_3$

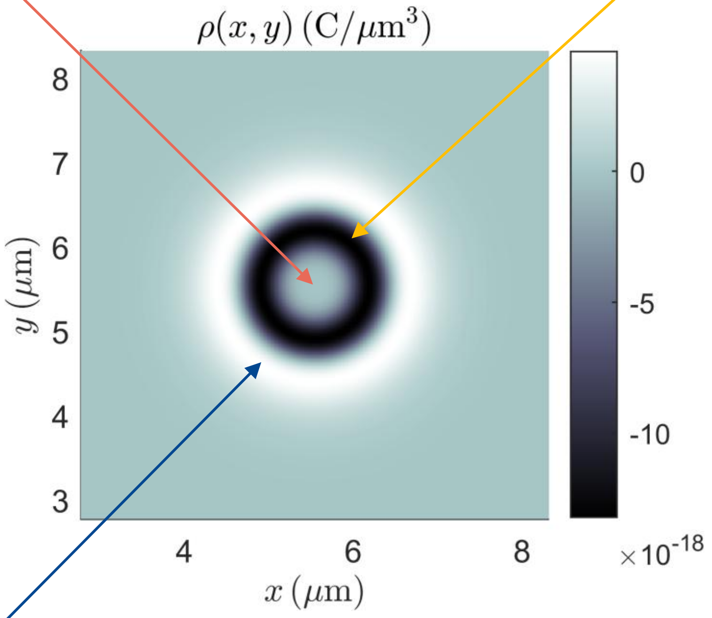
Splay and bend favoured Néel skyrmions $(e_1 < e_3)$

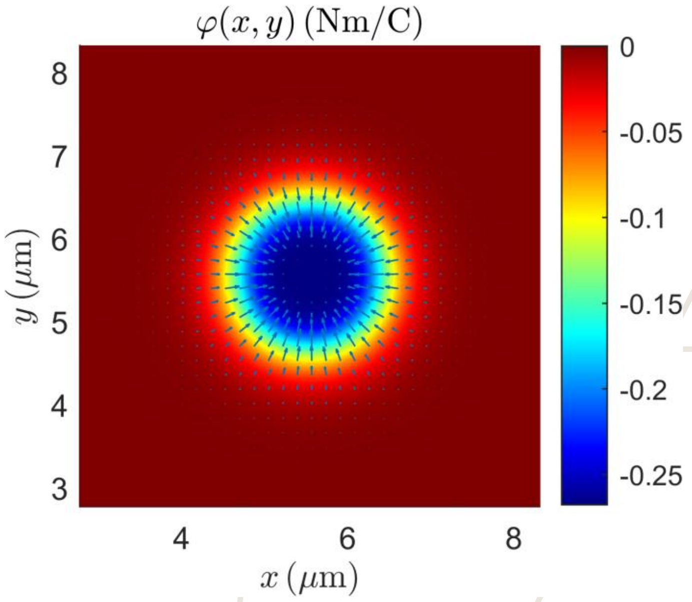
Neutral core

Inner ring of negative charge



$$\vec{n}_{\text{Néel}}(r,\theta) = \sin f(r)\vec{e}_r + \cos f(r)\vec{e}_z$$





Outer ring of positive charge

$$\rho = -\vec{\nabla} \cdot \vec{P}_f = \epsilon_0 \Delta \varphi$$

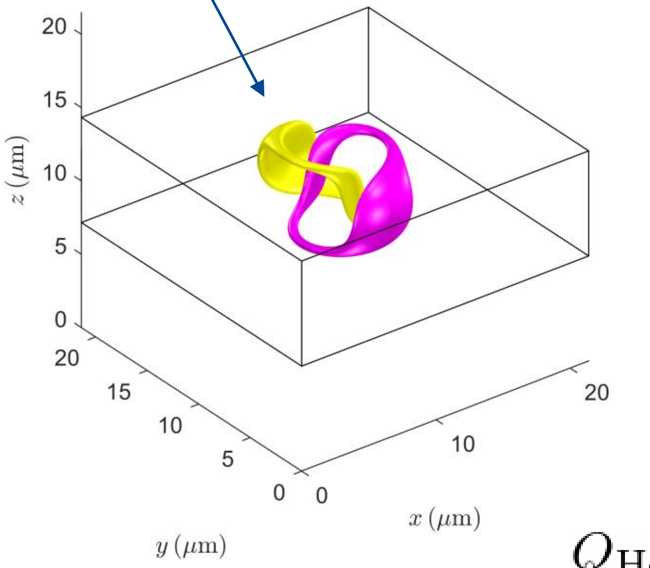
$$\vec{P}_f = e_1 \left[(\vec{\nabla} \cdot \vec{n})\vec{n}\right] + e_3 \left[\vec{n} \times (\vec{\nabla} \times \vec{n})\right]$$

Liquid crystal hopfions

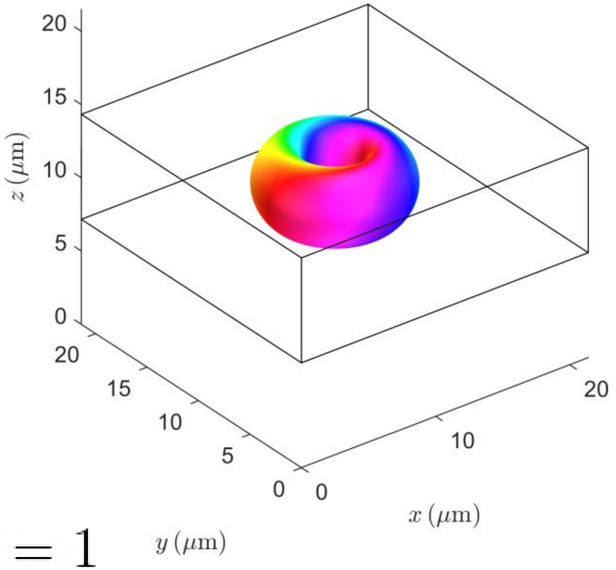
Hopfions

- Can be interpreted as a **twisted skyrmion string**, forming a **closed loop** in real space
- They comprise inter-linked closed-loop preimages of constant $\vec{n}(x,y,z)$
- **Linking** of closed-loop preimages of anti-podal points in $S^2/\mathbb{Z}_2 \cong \mathbb{RP}^2$ defines Hopf index

$n_1(x,y,z) = \pm 0.9$



$n_3(x,y,z) = 0$



$$\boxed{Q_{\text{Hopf}} \in \pi_3(\mathbb{RP}^2) = \pi_3(S^2) = \mathbb{Z}}$$

$$Q_{\text{Hopf}} = 1$$

Hopfions

- Explicit Hopf index[14]: $Q_{\mathrm{Hopf}} = \dfrac{1}{32\pi^2}\displaystyle\int_\Omega \mathrm{d}^3x\, \epsilon^{ijk} A_i \boxed{F_{jk}}$
- Introduce vector potential $\vec{A}$ such that $F_{ij} = \epsilon^{abc} n_a \partial_i n_b \partial_j n_c = \dfrac{1}{2}(\partial_i A_j - \partial_j A_i)$
- Hopfion ansatz with Hopf index $Q_{\mathrm{Hopf}} = 1$[15,16]:

$$\vec{n}_{\mathrm{Hopf}}(r,\theta,z) = \left(\frac{4\Sigma r\left(\Theta\cos\theta - (\Lambda-1)\sin\theta\right)}{(1+\Lambda)^2}, \frac{4\Sigma r\left(\Theta\sin\theta + (\Lambda-1)\cos\theta\right)}{(1+\Lambda)^2}, 1 - \frac{8\Sigma^2 r^2}{(1+\Lambda)^2}\right)$$

- The three functions introduced are[15]

$$\Theta(z) = \tan\left(\frac{\pi z}{d}\right), \Sigma(r,z) = \frac{1}{d}\left[1 + \left(\frac{2z}{d}\right)^2\right]\sec\left(\frac{\pi r}{2d}\right), \Lambda(r,z) = \Sigma^2 r^2 + \frac{\Theta^2}{4}.$$

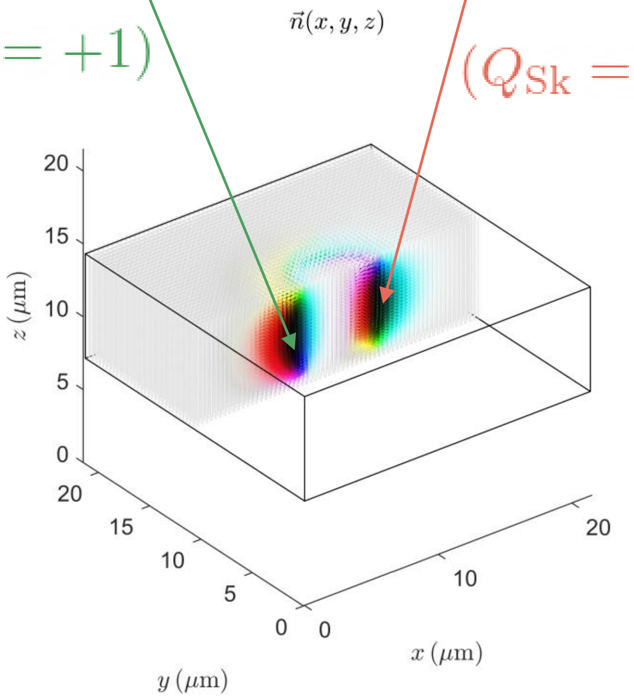
[14] J. Hietarinta, J. Palmu, J. Jäykkä and P. Pakkanen, *Scattering of knotted vortices (Hopfions) in the Faddeev–Skyrme model*, New J. Phys. **14** (2012) 013013
[15] P. Sutcliffe, *Hopfions in chiral magnets*, J. Phys. A: Math. Theor. **51** (2018) 375401
[16] J. Hietarinta and P. Salo, *Faddeev-Hopf knots: dynamics of linked un-knots*, Phys. Lett. B **451** (1999) 60

Hopfion structure

Skyrmion twisting as it winds around the hopfion core, changing from an in-plane skyrmion to an out-of-plane antiskyrmion

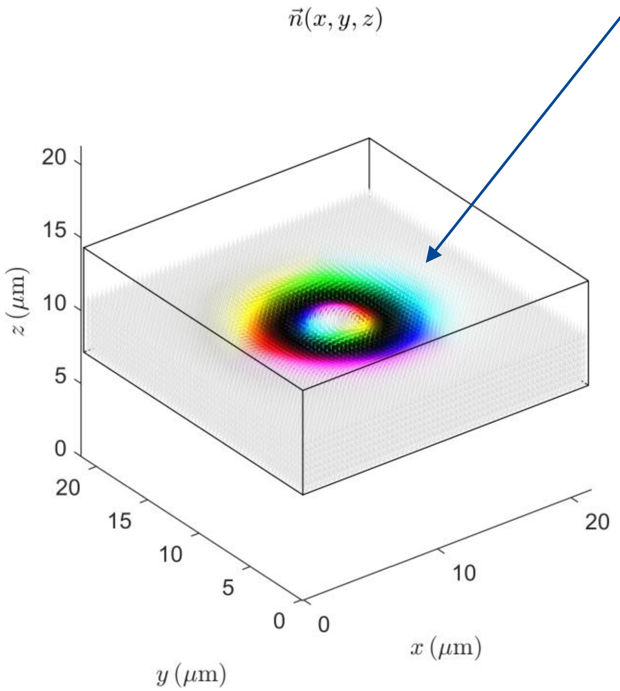
$(Q_{\mathrm{Sk}} = +1)$

$(Q_{\mathrm{Sk}} = -1)$



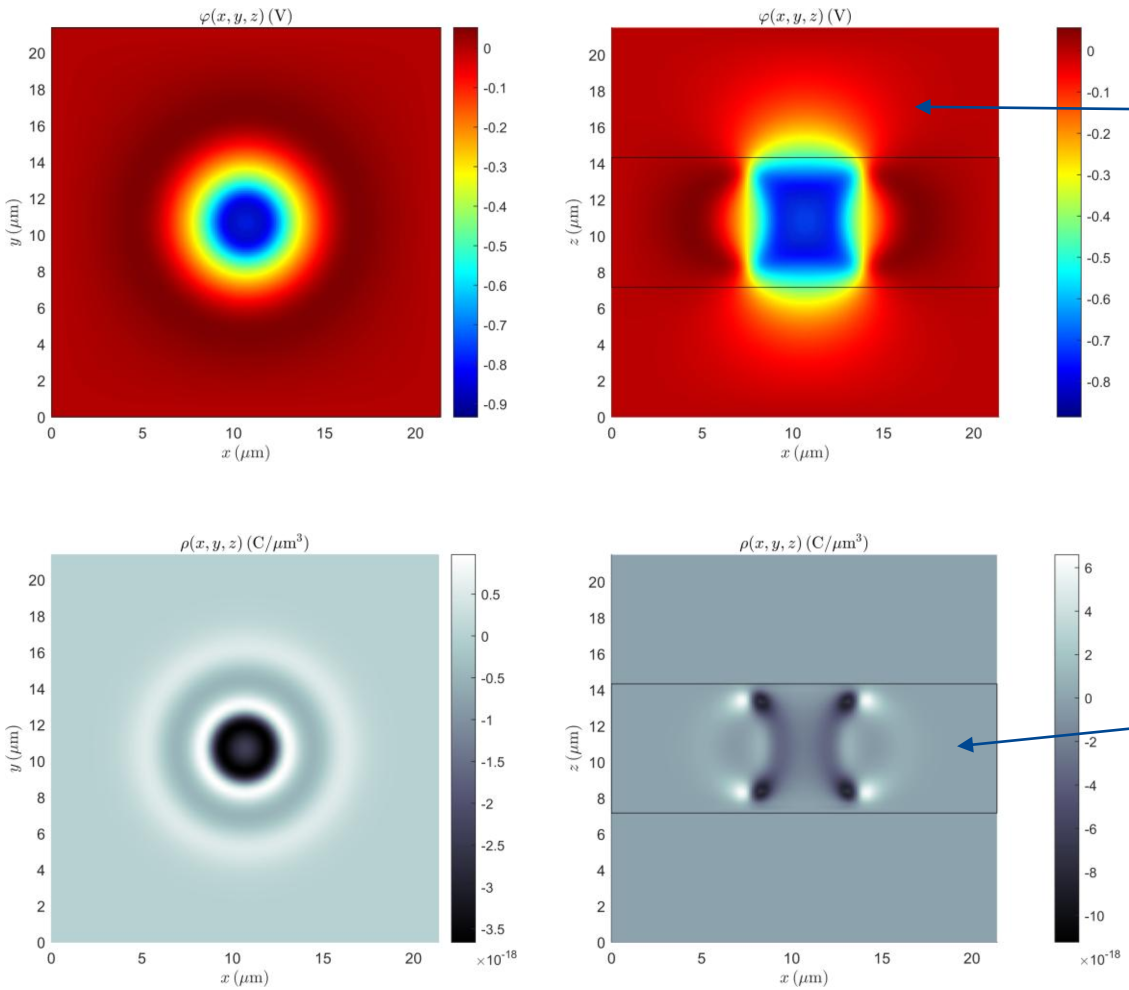
Structure of Bloch skyrmionium or a 2π-vortex[17]

$(Q_{\mathrm{Sk}} = 0)$



[17] A. Bogdanov and A. Hubert, *The stability of vortex-like structures in uniaxial ferromagnets*, J. Magn. Magn. Mater. **195** (1999) 182

Flexoelectric CLC hopfion



Electric scalar potential non-zero in $\mathbb{R}^3/\Omega$

Electric charge density confined within

$$\Omega = \left\{ (x, y, z) \in \mathbb{R}^3 \; : \; |z| \leq \frac{d}{2} \right\}$$

Conclusion

Concluding remarks

- Topological defects induce non-uniform strain
- Flexoelectric polarization response $\longrightarrow$ self-induced internal electric field
- We have shown how to include the electrostatic self-energy and how to compute the back-reaction
- Stray depolarizing field outside thin film included
- Method can be applied 3D skyrmion textures in chiral magnets
- Main differences with chiral magnets (CM):
  - Electric potential depends on divergence of polarization (divergence of magnetization in CM)
  - Electrostatic energy is second order (zeroth order in CM)
  - Bloch skyrmions affected by self-interaction (unaffected in CM)