



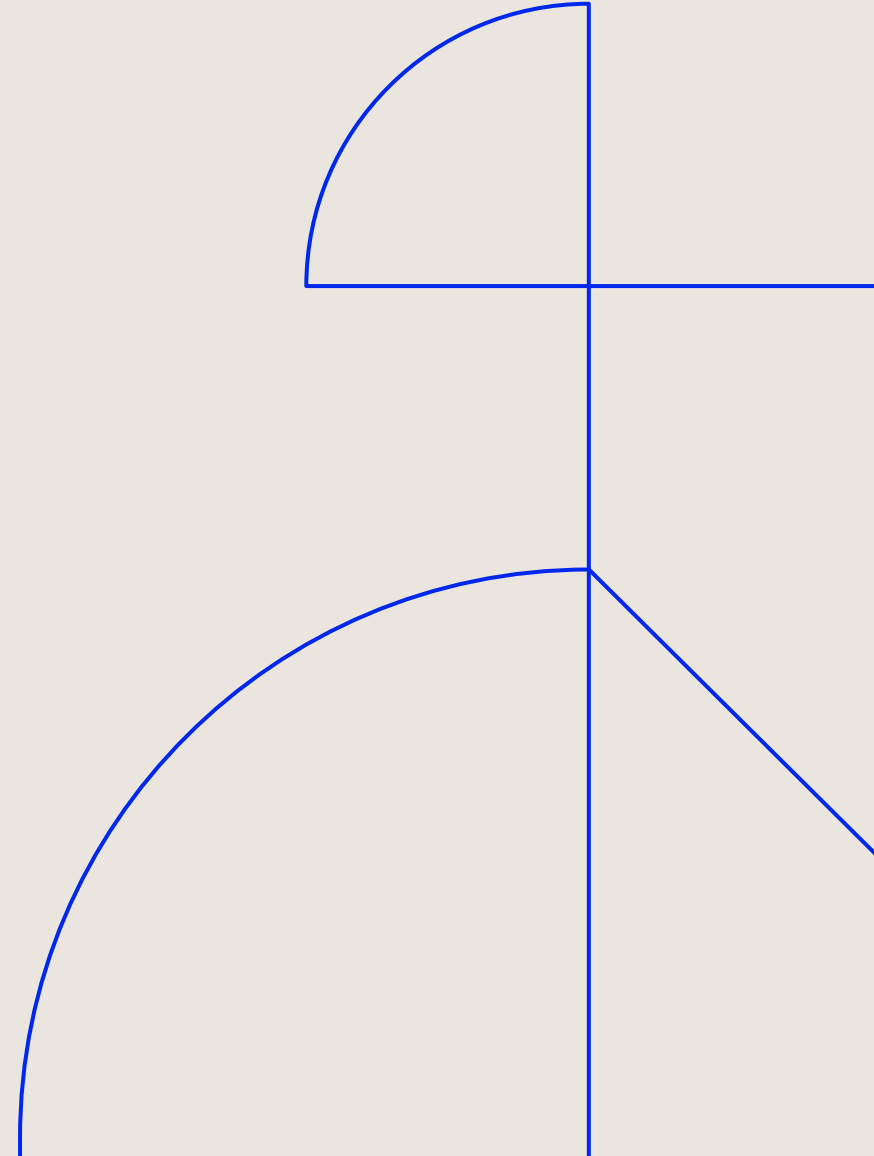
# Electrostatic self-interactions of hopfions and skyrmions in liquid crystals

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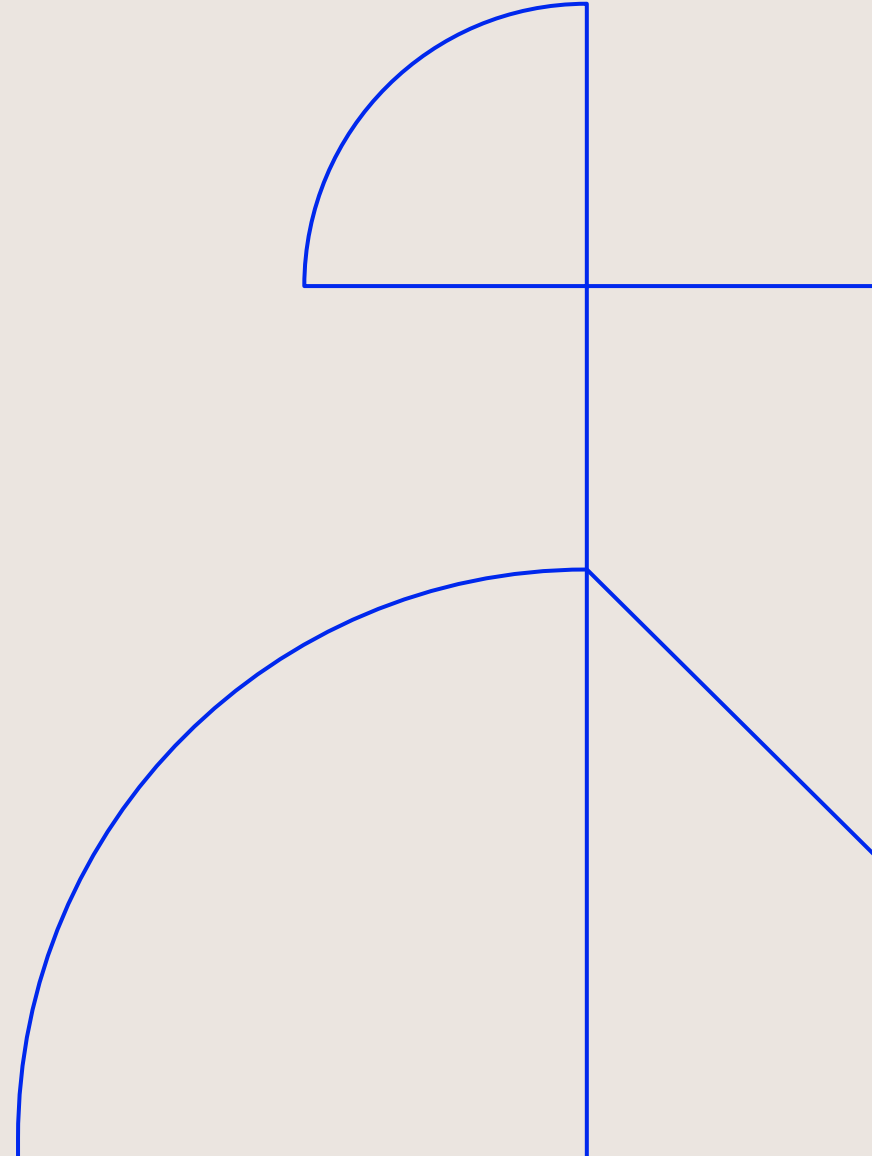
# Motivation



# Motivation

- Non-polar director field  $\vec{n}(\vec{x}) \in \mathbb{RP}^2 \cong S^2/\mathbb{Z}_2$
- Hopfions  $\vec{n} : S^3 \rightarrow \mathbb{RP}^2$  and skyrmions  $\vec{n} : S^2 \rightarrow \mathbb{RP}^2$
- 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

$$E_{\text{FO}} = \frac{1}{2} K \int_{\mathbb{R}^3} d^3 x |\nabla \vec{n}|^2$$

- Energy minimizers are solutions of Laplace equation  $\Delta \vec{n} = \vec{0}$
- Metastable inhomogeneous solutions found by Belavin and Polyakov<sup>[1]</sup> in ferromagnets
- More insight can be gained by considering elastic modes
- Decompose director gradient tensor into these normal modes<sup>[2]</sup>  $(\vec{B}, T, S, \Delta)$

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

[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  $\vec{n} \mapsto -\vec{n}$

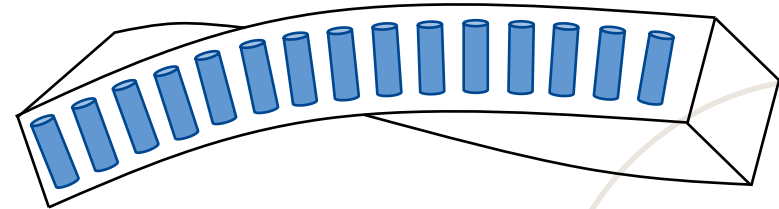
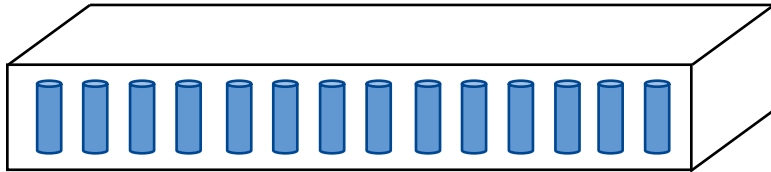


- Elastic bend energy  $|\vec{B}|^2 = [\vec{n} \times (\vec{\nabla} \times \vec{n})]^2$

# 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

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

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

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

- Can introduce enantiomorphy into the system → **chiral** liquid crystals

# Chiral liquid crystal (CLC)

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

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

- Equivalent to **DMI** term in chiral magnets arising from Dresselhaus SOC
  - Mechanism responsible for stabilization of bulk skyrmions
  - Favours Bloch modulations

# Experimental realization

- CLCs placed between parallel plates with separation  $d$
- System restricted to confined geometry<sup>[4]</sup>


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

- Apply potential difference  $U \rightarrow$  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<sup>[5]</sup>

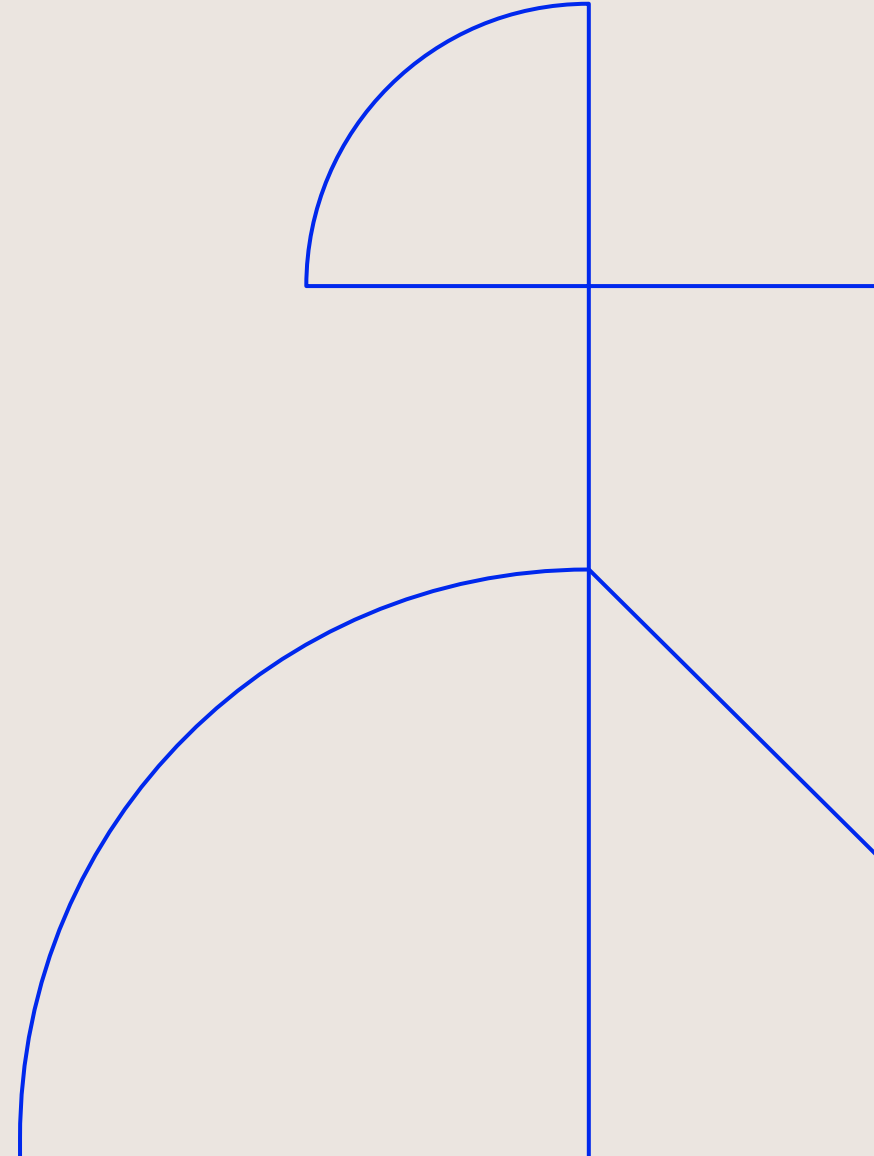
$$\mathcal{E}_{\text{anch}} = -\frac{1}{2} W_0 n_z^2$$


 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 non-uniform strain
- Orientational distortions  $\rightarrow$  macroscopic electric polarization  $\vec{P}_f$
- Fix splay, induce polarization:

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

- Fix bend, induce polarization:

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

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

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

[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

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

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

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

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

- Electrostatic potential** satisfies the **Poisson equation**<sup>[8]</sup>

$$\Delta\varphi = -\nabla^2\varphi = -\frac{1}{\epsilon_0} \vec{\nabla} \cdot \vec{P}_f$$

- Gauss' law  $\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}$

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

# Flexoelectric self-energy

- Energy of a continuous dipole density distribution<sup>[9]</sup>

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

- More useful to express the flexoelectric energy as

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

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

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

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

# Rescaling $F_{\text{flexo}}$

- 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

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

$$\hat{F}_{\text{flexo}} = \frac{1}{2} \frac{L_0 \lambda^2 \epsilon_0}{E_0} \int_{\Omega} d^3 \hat{x} \hat{\varphi} \Delta_{\hat{x}} \hat{\varphi}$$

$$\Delta_{\hat{x}} \hat{\varphi} = - \frac{e_1}{\epsilon_0 \lambda} \vec{\nabla}_{\hat{x}} \cdot \vec{P}$$

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

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

# Scale invariance of $F_{\text{flexo}}$

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

→ 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 $F_{\text{flexo}}$

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

- Potential does not have compact support

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

- Does have  $1/r$  localization

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

- First variation reduces to

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

Need to  
compute



# First variation of $F_{\text{flexo}}$

- First variation is  $\left. \frac{d}{dt} \right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = \epsilon \int_{\Omega} d^3x \varphi \Delta \dot{\varphi}$

- Poisson equation variation

$$\Delta \dot{\varphi} = -\frac{1}{\epsilon} \vec{\nabla} \cdot \left( \left. \frac{d}{dt} \right|_{t=0} \vec{P}(\vec{n}_t) \right)$$

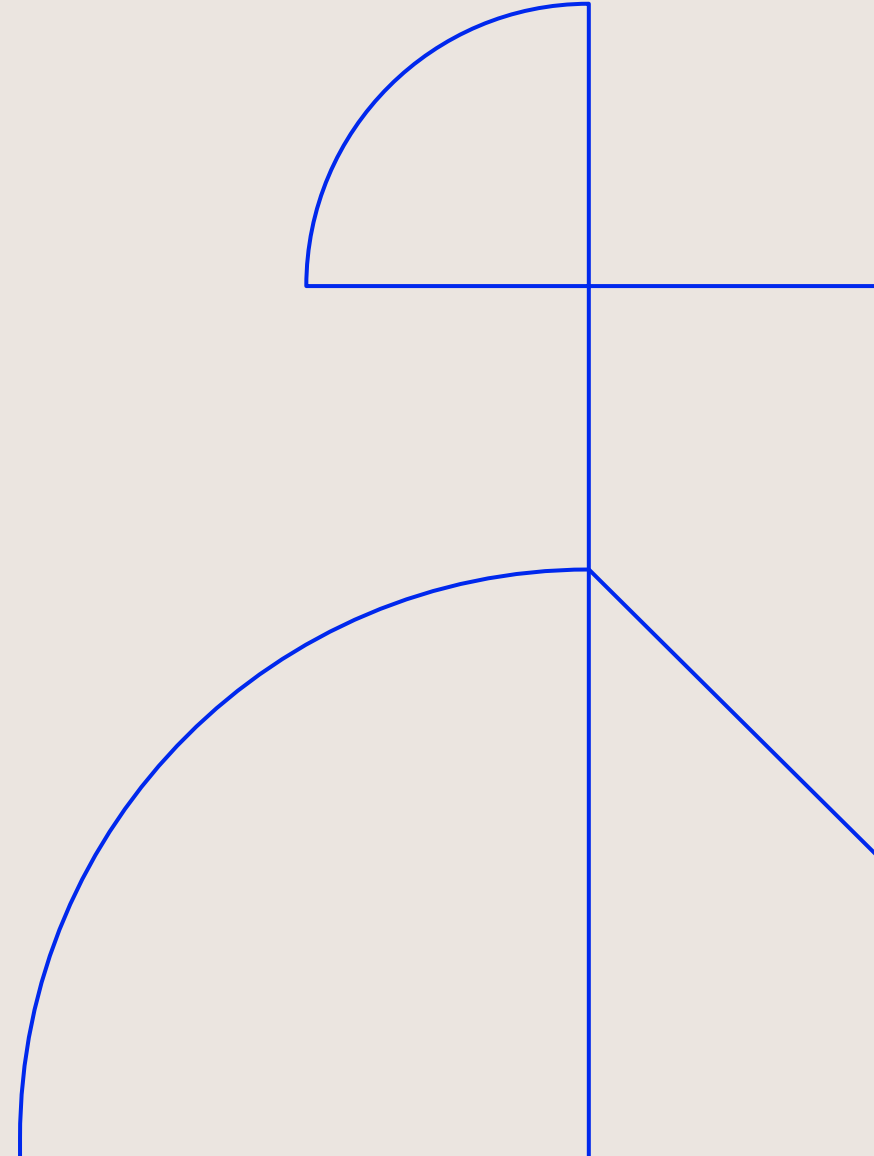
- Flexoelectric variation becomes

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} F_{\text{flexo}}(\vec{n}_t) &= - \int_{\mathbb{R}^2} d^2x \varphi \vec{\nabla} \cdot \left( \left. \frac{d}{dt} \right|_{t=0} \vec{P}(\vec{n}_t) \right) = \int_{\mathbb{R}^2} d^2x \vec{\nabla} \varphi \cdot \left( \left. \frac{d}{dt} \right|_{t=0} \vec{P}(\vec{n}_t) \right) \\ &= \int_{\mathbb{R}^2} d^2x (\text{grad}_{\vec{n}} F_{\text{flexo}}) \cdot \vec{\epsilon} \end{aligned}$$

$$\vec{\epsilon} = \partial_t \vec{n}_t|_{t=0}$$

$$\text{grad}_{\vec{n}} F_{\text{flexo}} = \frac{\epsilon_3}{e_1} \left[ \left( (\vec{\nabla} \times \vec{n}) \times \vec{\nabla} \varphi \right) + \left( \vec{\nabla} \times (\vec{\nabla} \varphi \times \vec{n}) \right) \right] - \vec{\nabla} (\vec{\nabla} \varphi \cdot \vec{n}) + (\vec{\nabla} \cdot \vec{n}) \vec{\nabla} \varphi$$

# 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<sup>[10]</sup>
- One constant approximation  $K_i = K$
- Vector identity for unit vector  $\vec{n}$ <sup>[11]</sup>:

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

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

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

[10] A.O. Leonov, I.E. Dragunov, U.K. Röbler 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

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

- Electrostatic potential subject to constraint

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

- 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<sup>[12]</sup>: minimize the functional

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

- 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<sup>[13]</sup>
- 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  $\omega$ -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  $F_{\text{FFO}}$

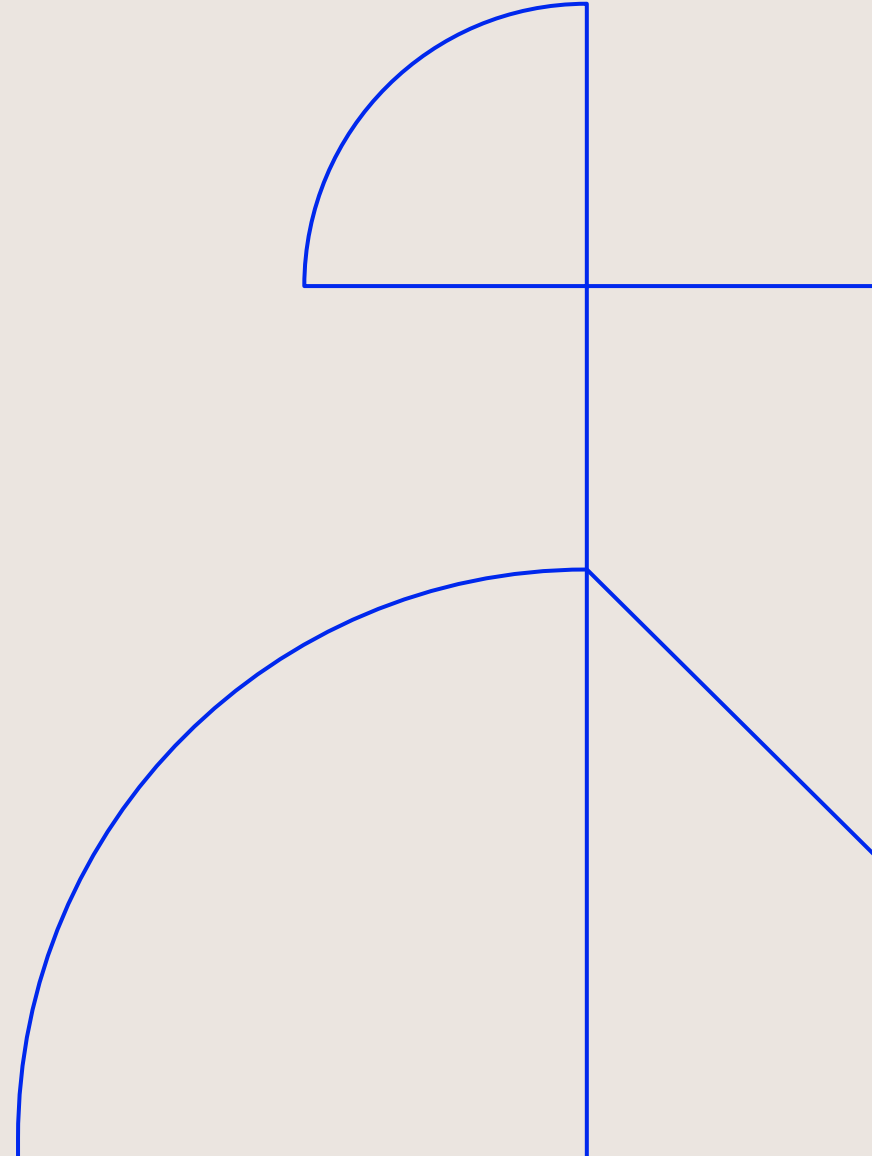
$$\frac{d^2}{dt^2} \vec{n}_t = -\text{grad}_{\vec{n}} (F_{\text{FO}} + F_{\text{flexo}}) [\vec{n}_t]$$

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

# Algorithm summary

1. Perform step of ANF method for director field  $\vec{n}$  using 4<sup>th</sup> order Runge-Kutta method
2. Solve Poisson's equation for electric potential  $\varphi$  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:  $\|F_{\text{FFO}}(\vec{n})\|_{\infty} < 10^{-6}$ . If the convergence criteria has been satisfied, then stop the algorithm
5. Repeat the process (return to step 1)

# Liquid crystal skyrmions



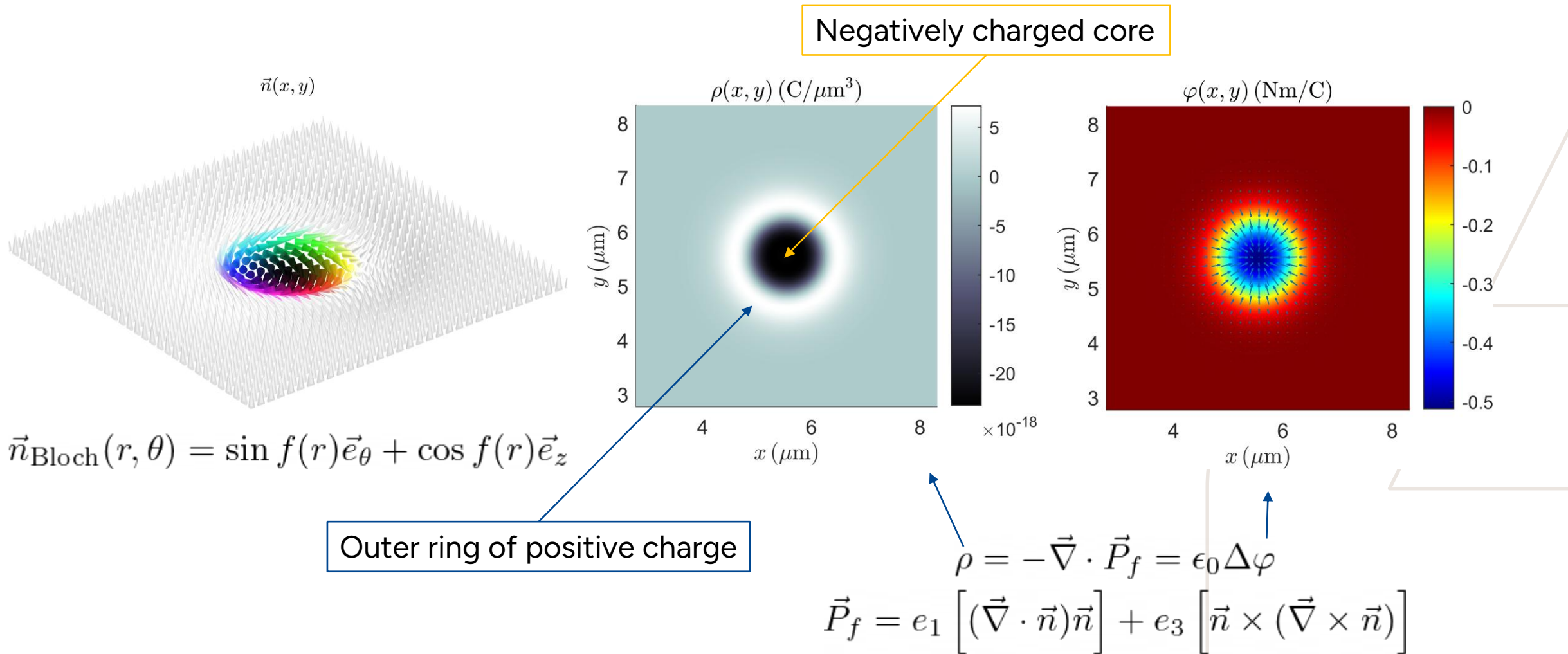
# Twist favoured Bloch skyrmions

- In chiral magnets, demagnetizing magnetic potential satisfies  $\Delta\psi = -\mu_0 M_s \vec{\nabla} \cdot \vec{n}$
- Dresselhaus DMI favours Bloch skyrmions  $\rightarrow \vec{n}_{\text{Bloch}}(r, \theta) = \sin f(r) \vec{e}_\theta + \cos f(r) \vec{e}_z$
- Bloch skyrmions in chiral magnets are solenoidal  $\vec{\nabla} \cdot \vec{n}_{\text{Bloch}} = 0$
- $\rightarrow$  **Unaffected** by magnetostatic self-interaction
- Chiral liquid crystals: Bloch ansatz is solenoidal, associated polarization is not

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

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

# Twist favoured Bloch skyrmions ( $e_1 = e_3$ )





# Splay and bend favoured liquid crystals

- Nematic liquid crystal  $F_{FO} = \frac{1}{2}K \int_{\Omega} d^3x \left\{ |\vec{S}|^2 + T^2 + |\vec{B}|^2 \right\}$   
 $\vec{S} = \vec{n}(\vec{\nabla} \cdot \vec{n})$  Splay vector

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

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

- What about splay and bend favoured liquid crystals?

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

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

$$\rightarrow F = \int_{\mathbb{R}^3} d^3x \left\{ \frac{K}{2} (\nabla \vec{n})^2 + K q_0 [n_z (\vec{\nabla} \cdot \vec{n}) - \vec{n} \cdot \vec{\nabla} n_z] + V(\vec{n}) \right\}$$

DMI from  
Rashba SOC

# Splay and bend favoured Néel skyrmions

- Adimensional splay and bend favoured liquid crystals

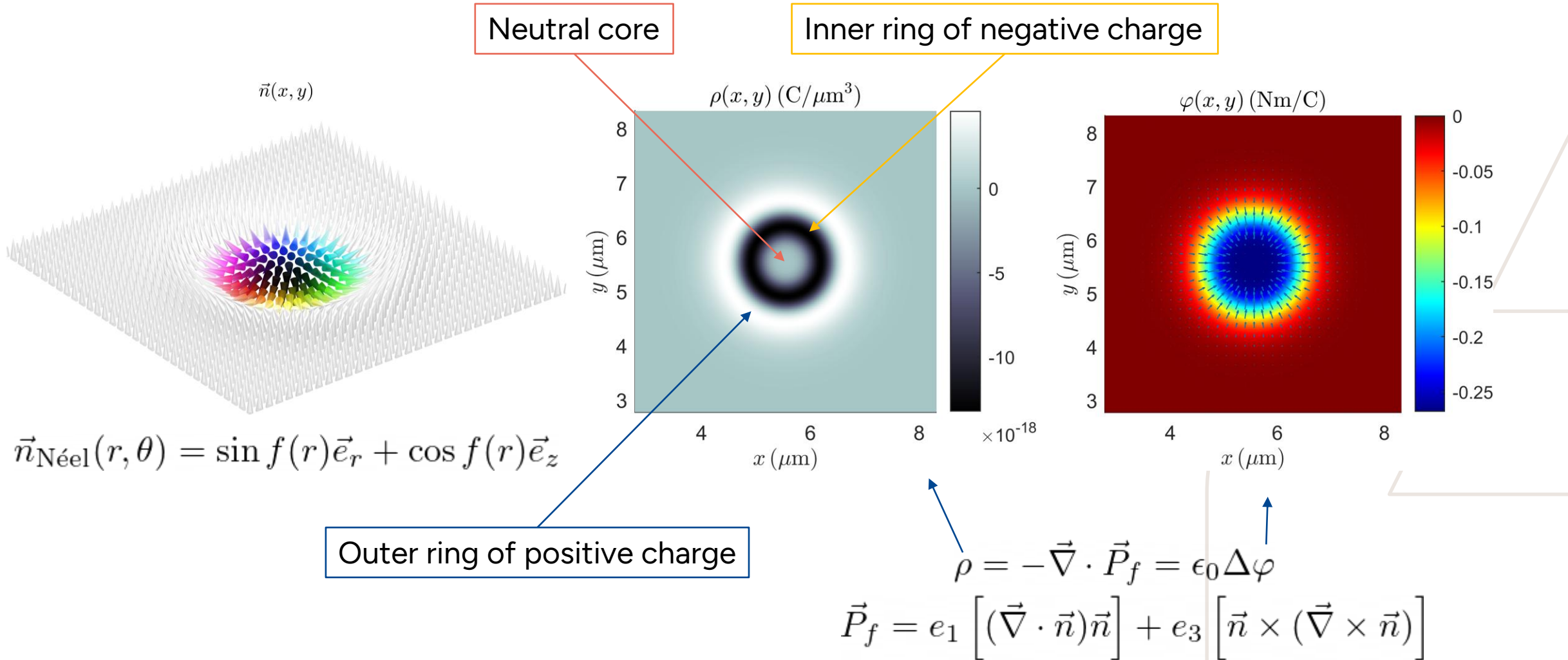
$$F = \int_{\mathbb{R}^2} d^2x \left\{ \frac{1}{2} (\nabla \vec{n})^2 + \boxed{n_z (\vec{\nabla} \cdot \vec{n}) - \vec{n} \cdot \vec{\nabla} n_z} + \frac{1}{q_0^2} \frac{1}{K} V(\vec{n}) + \frac{\epsilon}{2} \varphi \Delta \varphi \right\}$$

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

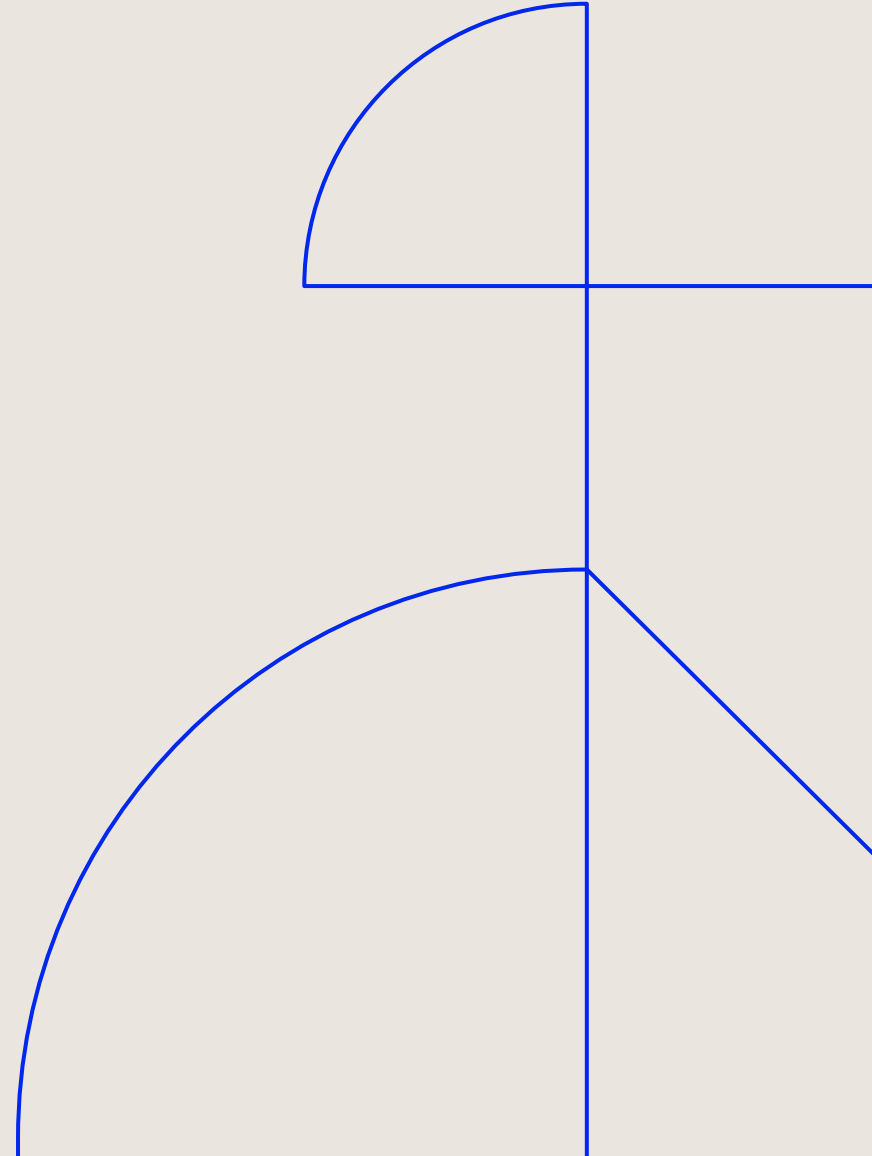
$$\vec{P}_{\text{Néel}} = \left[ \frac{1}{r} \sin^2 f(r) + \left( 1 - \frac{e_3}{e_1} \right) \frac{1}{2} \sin 2f(r) \frac{df}{dr} \right] \vec{e}_r + \left[ \frac{1}{2r} \sin 2f(r) + \left( \cos^2 f(r) + \frac{e_3}{e_1} \sin^2 f(r) \right) \frac{df}{dr} \right] \vec{e}_z$$

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

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

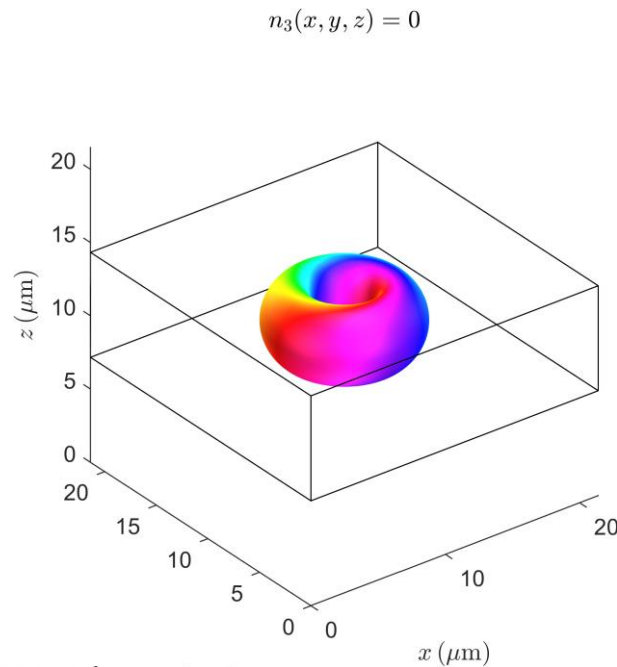
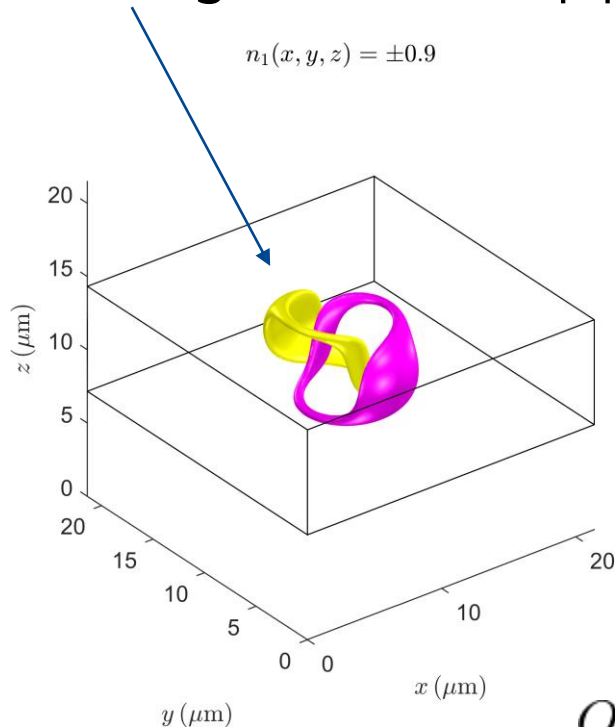


# Liquid crystal hopfions



# 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



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

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

# Hopfions

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

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

- The three functions introduced are<sup>[15]</sup>

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

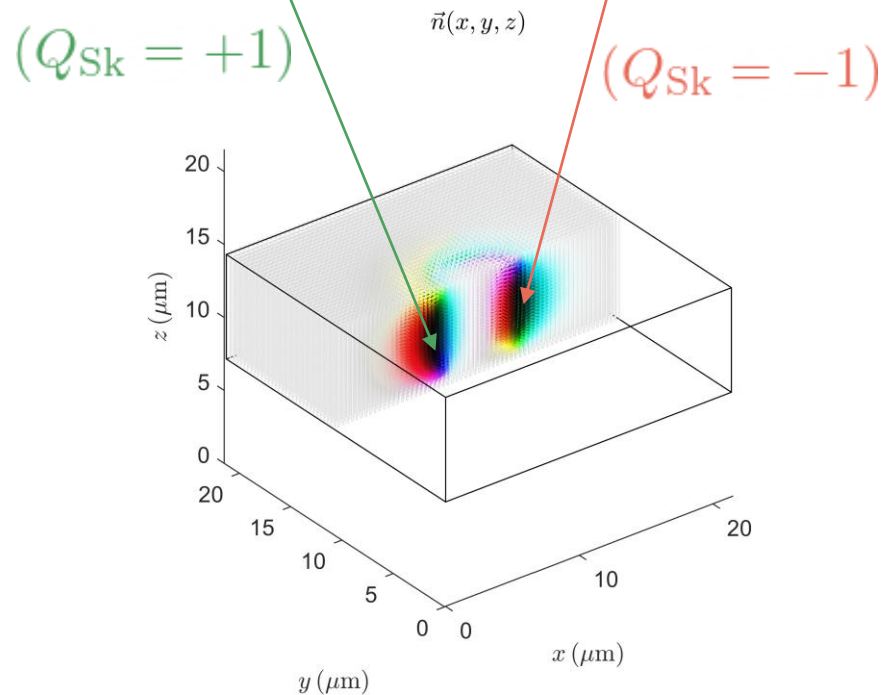
[14] J. Hietarinta, J. Palmu, J. Jäykkä and P. Pakkanen, *Scattering of knotted vortices (Hopfions) in the Faddeev–Skyrme model*, New J. Phys. **14** (2012) 013013

[15] P. Sutcliffe, *Hopfions in chiral magnets*, J. Phys. A: Math. Theor. **51** (2018) 375401

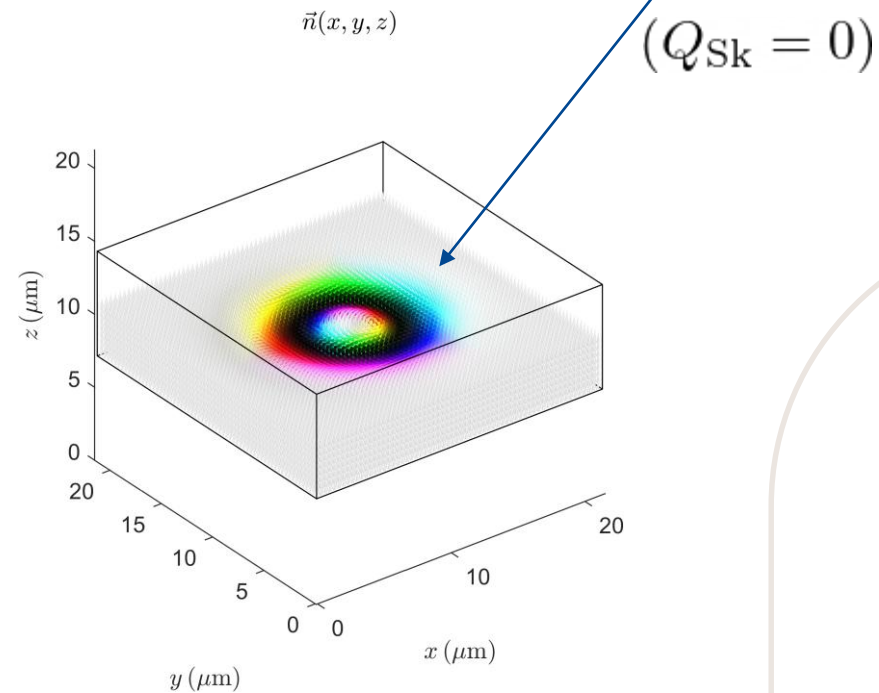
[16] J. Hietarinta and P. Salo, *Faddeev–Hopf knots: dynamics of linked un-knots*, Phys. Lett. B **451** (1999) 60

# Hopfion structure ( $e_1 = e_3 = 4 \text{ pCm}^{-1}$ )

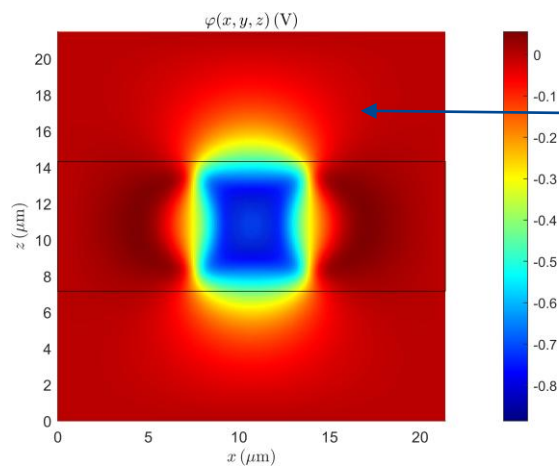
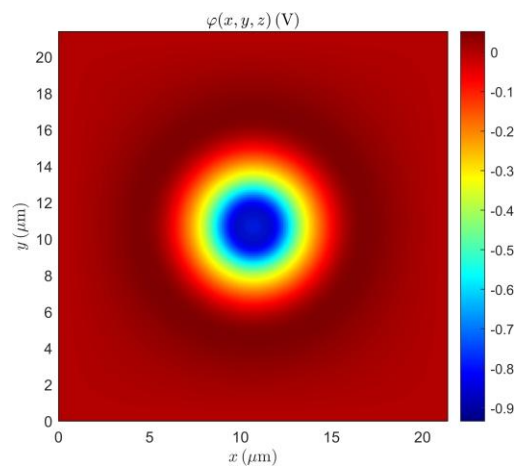
Skyrmion twisting as it winds around the hopfion core, changing from an in-plane **skyrmion** to an out-of-plane **antiskyrmion**



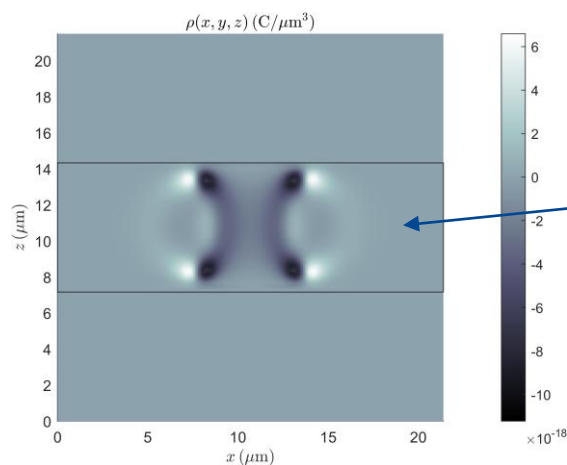
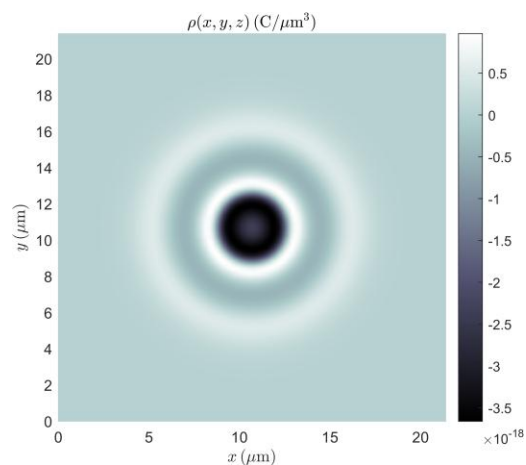
Structure of Bloch skyrmionium or a  $2\pi$ -vortex<sup>[17]</sup>



# Flexoelectric CLC hopfion ( $e_1 = e_3 = 4 \text{ pCm}^{-1}$ )



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

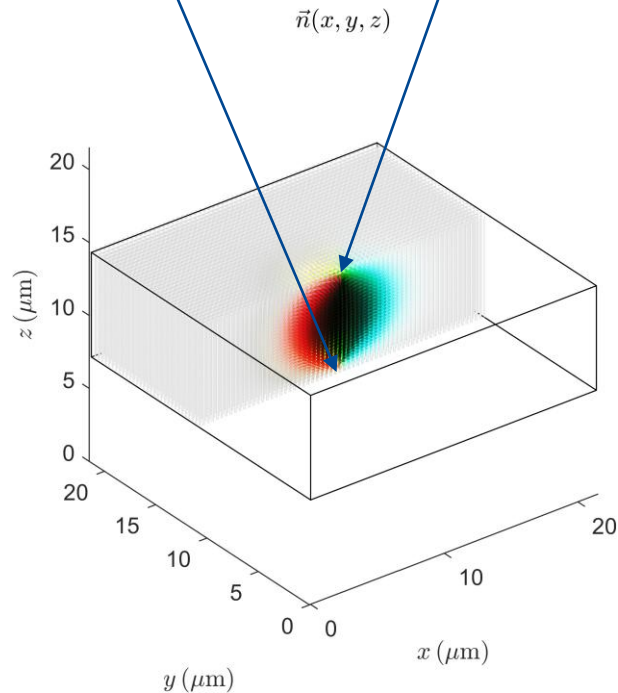


Electric charge density confined within  
 $\Omega = \left\{ (x, y, z) \in \mathbb{R}^3 : |z| \leq \frac{d}{2} \right\}$

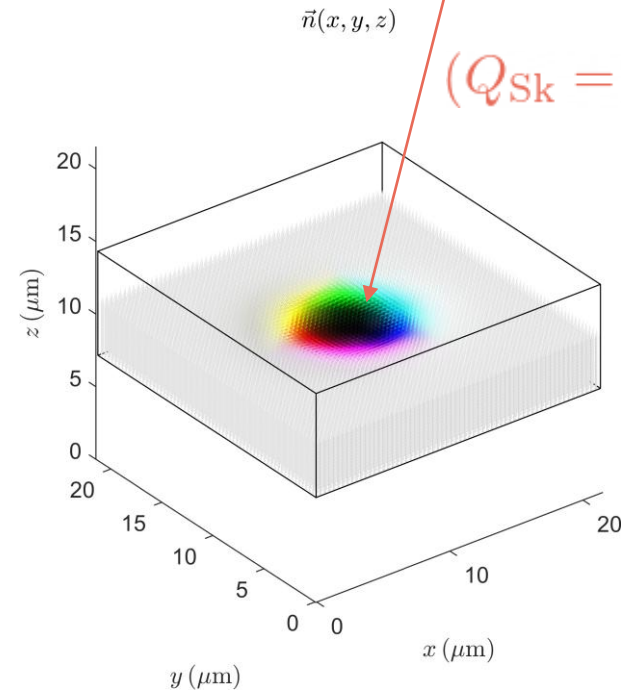


# Hopfion $\longrightarrow$ Skyrmion ( $e_1 = e_3 = 8 \text{ pCm}^{-1}$ )

Skyrmion terminating at point defects due to boundary conditions<sup>[18]</sup>

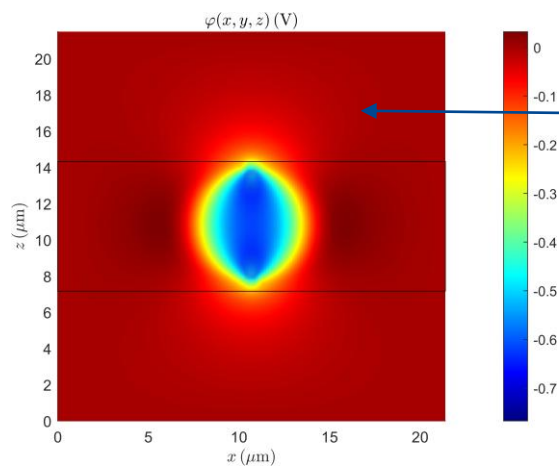
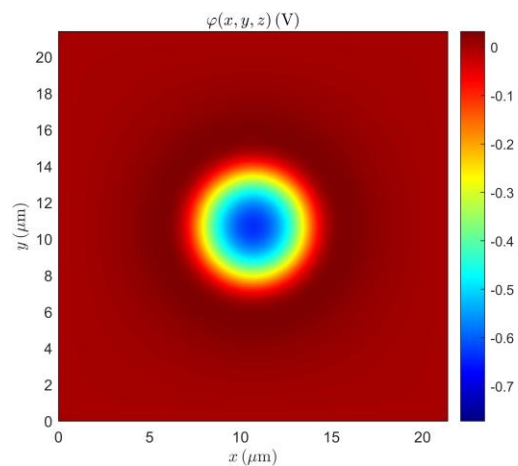


Structure of a Bloch skyrmion

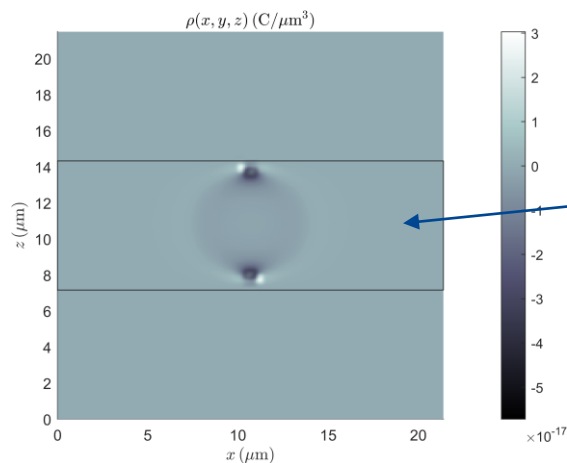
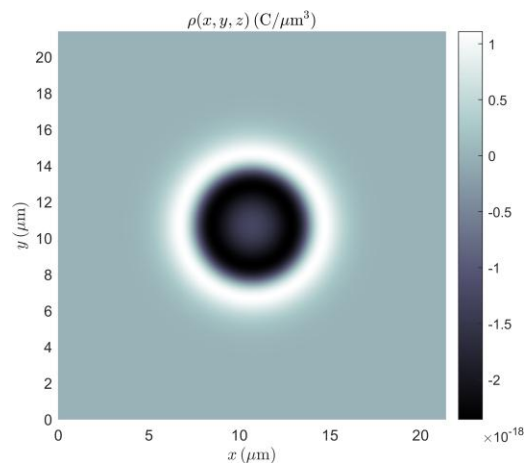


[18] J. B. Tai and I. I. Smalyukh, Surface anchoring as a control parameter for stabilizing torons, skyrmions, twisted walls, fingers, and their hybrids in chiral nematics, Phys. Rev. E **101** (2020) 042702

# Flexoelectric CLC skyrmion ( $e_1 = e_3 = 8 \text{ pCm}^{-1}$ )

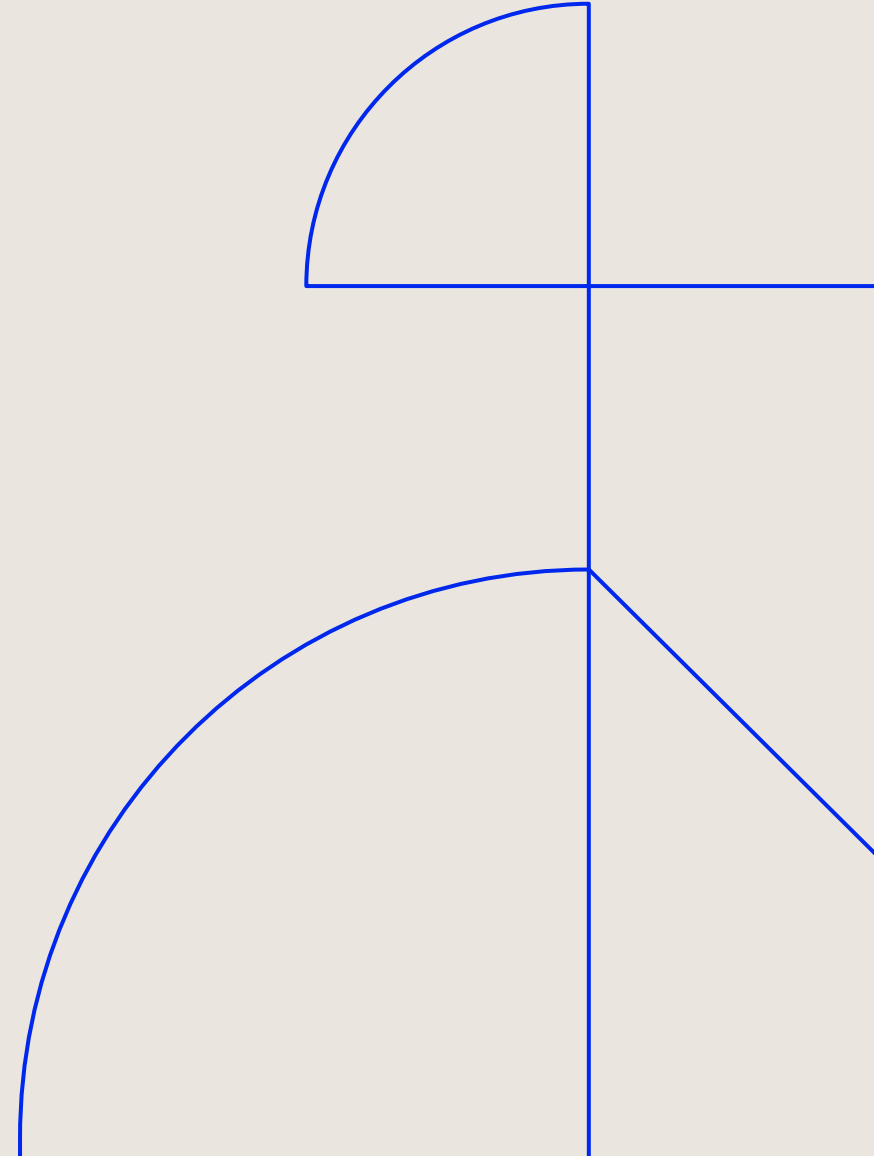


Electric scalar potential  
non-zero in  $\mathbb{R}^3/\Omega$



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 → 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)
- Flexoelectric self-interaction can destabilize hopfion into skyrmion