



# Flexoelectric self-polarization effect on topological defects in liquid crystals

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Joint work with Martin Speight

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# Outline

- 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**)
- 
- Based on works [arXiv:**2504.17772**] and [arXiv:**2504.17778**]
  - Slides available online at [paulnleask.github.io/talks/](https://paulnleask.github.io/talks/)

# Nematic liquid crystal

- Frank-Oseen free energy for an anisotropic NLC is

$$F_{\text{FO}} = \int_{\Omega} d^3x \left\{ \frac{1}{2} K_1 |\vec{S}|^2 + \frac{1}{2} K_2 T^2 + \frac{1}{2} K_3 |\vec{B}|^2 + V(\vec{n}) \right\}$$

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

Standard splay vector

$$T = \vec{n} \cdot (\vec{\nabla} \times \vec{n})$$

Pseudoscalar twist

$$\vec{B} = -(\vec{n} \cdot \vec{\nabla})\vec{n} = \vec{n} \times (\vec{\nabla} \times \vec{n})$$

Standard bend vector

- No 1<sup>st</sup> order terms (in derivatives of the director) are present:

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

→ Nothing to stabilize topological solitons

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

# Twist favoured (chiral) liquid crystal

- Molecular chirality characterized by cholesteric twist  $q_0 = \frac{2\pi}{p}$
- Enantiomorphy introduced via twist  $T \mapsto T + q_0$  [1]
- 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** skyrmions



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

# Relation to chiral magnets

- Stability of skyrmions in chiral liquid crystals arises from **same mechanism** responsible for existence of skyrmions in **chiral magnetic** systems
- One constant approximation  $K_i = K$
- Vector identity for unit vector  $\vec{n}$ <sup>[2]</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<sup>[3]</sup>

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

[2] A. Hubert and R. Schäfer, *Magnetic Domains*, Springer Berlin, Heidelberg (2014)

[3] A.O. Leonov, I.E. Dragunov, U.K. Röbner and A.N. Bogdanov, *Theory of skyrmion states in liquid crystals*, Phys. Rev. E **90** (2014) 042502

# Splay and bend favoured liquid crystal

- Nematic liquid crystal  $F_{\text{FO}} = \frac{1}{2}K \int_{\Omega} d^3x \left\{ |\vec{S}|^2 + T^2 + |\vec{B}|^2 \right\}$
- We have considered **twist** favoured (chiral) liquid crystals,  $T \mapsto T + q_0$
- What about **splay** and **bend** favoured liquid crystals?

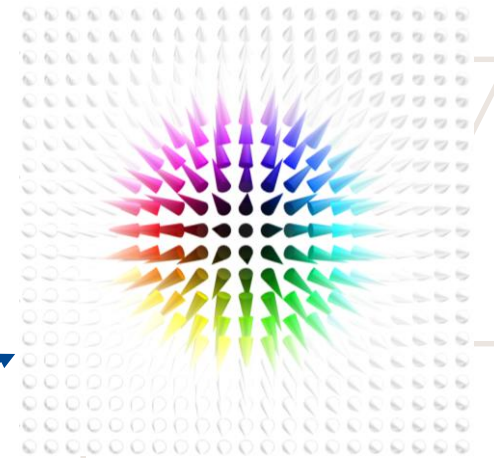
$$F_{\text{FO}} = \frac{1}{2}K \int_{\Omega} d^3x \left\{ |\vec{S} + \vec{S}_0|^2 + T^2 + |\vec{B} + \vec{B}_0|^2 \right\}$$

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

$$F_{\text{FO}} = \int_{\Omega} d^3x \left\{ \frac{K}{2} (\nabla \vec{n})^2 + Kq_0 \left[ n_z (\vec{\nabla} \cdot \vec{n}) - \vec{n} \cdot \vec{\nabla} n_z \right] + V(\vec{n}) \right\}$$

DMI from  
Rashba SOC

Favours **Néel** hedgehog skyrmions



# Experimental realization

- LCs 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  $\vec{E}_{\text{ext}} = \left( 0, 0, \frac{U}{d} \right)$
- LCs 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)

# Flexoelectric self-polarization

- Flexoelectricity: coupling between **electrical polarization** and **non-uniform strain**
- Orientational distortions  $\rightarrow$  macroscopic electric polarization  $\vec{P}_f$
- Polarization caused by mechanical curvature (flexion) of director (flexoelectric)<sup>[6,7]</sup>:

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

- Associated **electrostatic potential** satisfies the **Poisson equation**:

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

- Gauss' law

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

- Flexoelectric energy = electrostatic self-energy of **electric charge density**

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

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

[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



# Back-reaction 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

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} F_{\text{flexo}}(\vec{n}_t) &= - \int_{\Omega} d^3x \varphi \vec{\nabla} \cdot \left( \left. \frac{d}{dt} \right|_{t=0} \vec{P}(\vec{n}_t) \right) = \int_{\Omega} d^3x \vec{\nabla} \varphi \cdot \left( \left. \frac{d}{dt} \right|_{t=0} \vec{P}(\vec{n}_t) \right) \\ &= \int_{\Omega} d^3x (\text{grad}_{\vec{n}} F_{\text{flexo}}) \cdot \vec{\epsilon} \end{aligned}$$

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

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

# Numerical 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>[8,9]</sup>: minimize the functional

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

- 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>[10]</sup>
- Conjugate stepsize determined using Polak-Ribiere-Polyak method

[8] P. Leask and M. Speight, *Demagnetization in micromagnetics: magnetostatic self-interactions of bulk chiral magnetic skyrmions* [arXiv:2504.17772]

[9] P. Leask, *Flexoelectric polarization in chiral liquid crystals: electrostatic self-interactions of topological defects* [arXiv:2504.17778]

[10] D. Harland, P. Leask and M. Speight, *Skyrmion crystals stabilized by  $\omega$ -mesons*, J. High Energ. Phys. **06** (2024) 116

# Algorithm summary

1. Perform step of accelerated gradient descent method for director field  $\vec{n}$
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)



# Skyrmions in liquid crystals

## TWIST FAVOURED

- Dresselhaus DMI favours Bloch skyrmions

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

- Bloch ansatz is solenoidal

$$\vec{\nabla} \cdot \vec{n}_{\text{Bloch}} = 0$$

- Associated polarization is not

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

## SPLAY-BEND FAVOURED

- Rashba DMI prefers Néel skyrmions

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

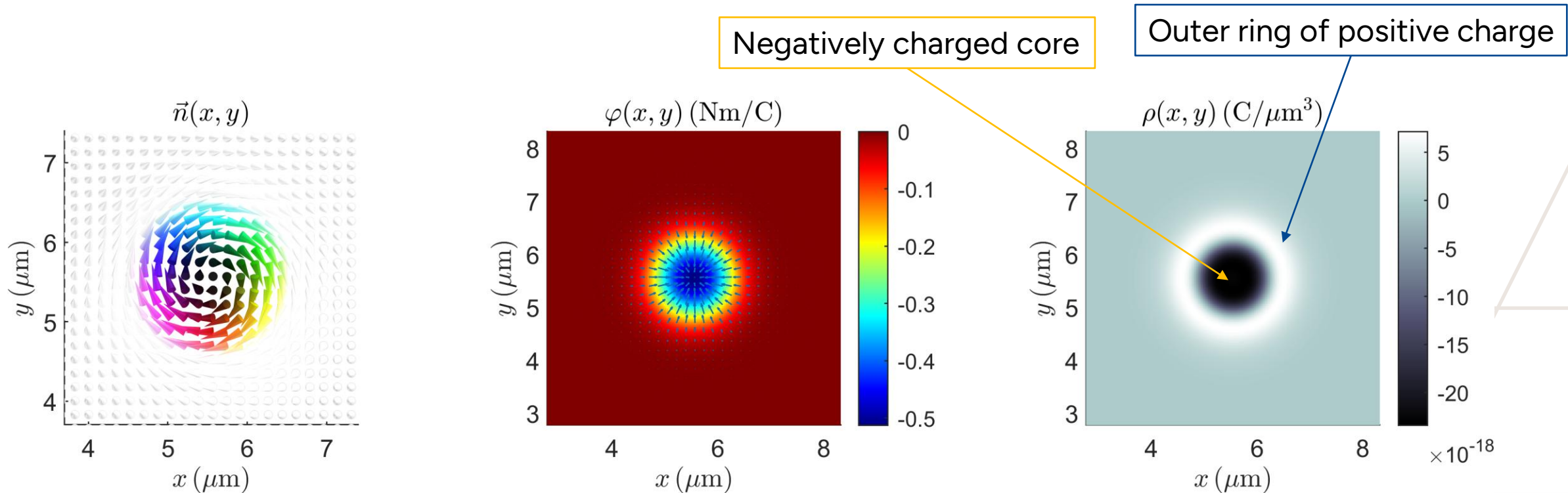
- Néel ansatz is not solenoidal

$$\vec{\nabla} \cdot \vec{n}_{\text{Néel}} = -\frac{df}{dr} \cos f(r) \neq 0$$

- Associated polarization is also not solenoidal

- 
- 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  $e_1 = e_3$

# Twist favoured Bloch skyrmions

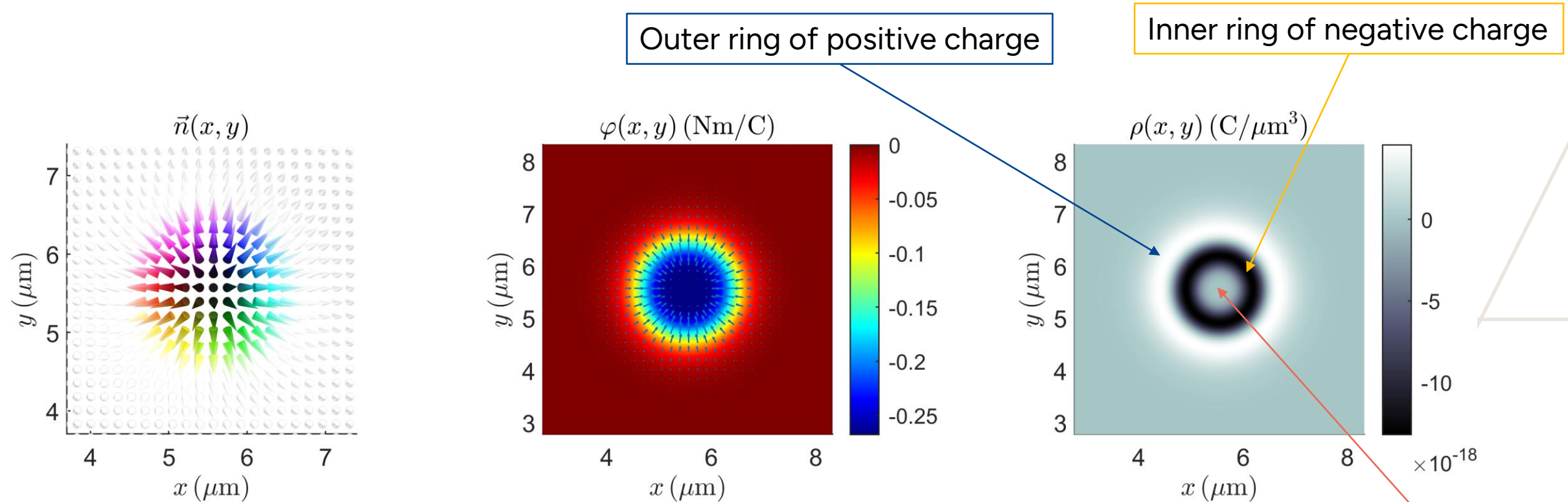


$$\vec{n}_{\text{Bloch}}(r, \theta) = \sin f(r) \vec{e}_\theta + \cos f(r) \vec{e}_z$$

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

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

# Splay-bend favoured Néel skyrmions



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

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

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

# Electrostatic self-interaction of skyrmions

## CHIRAL MAGNETS

- Demagnetizing field  $\vec{B} = -\vec{\nabla}\psi$
- Associated magnetic potential  $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$   

$$\Delta\psi = -\nabla^2\psi = \mu_0\rho, \quad \rho = -M_s(\vec{\nabla} \cdot \vec{n})$$
- Magnetostatic self-energy

$$E_{\text{demag}} = \frac{1}{2\mu_0} \int_{\mathbb{R}^2} d^2x \psi \Delta\psi$$

- Behaves like potential term in 2D

$$E_{\text{demag}}(\vec{n}_\lambda) = \frac{1}{\lambda^2} E_{\text{demag}}(\vec{n})$$

- Bloch skyrmions **unaffected** by demagnetization  

$$\vec{\nabla} \cdot \vec{n}_{\text{Bloch}} = 0$$

## LIQUID CRYSTALS

- Depolarizing field  $\vec{E} = -\vec{\nabla}\varphi$
- Associated electric potential  $\varphi : \mathbb{R}^3 \rightarrow \mathbb{R}$   

$$\Delta\varphi = -\nabla^2\varphi = \frac{\rho}{\epsilon_0}, \quad \rho = -\vec{\nabla} \cdot \vec{P}(\vec{n})$$
- Electrostatic self-energy

$$E_{\text{depol}} = \frac{\epsilon_0}{2} \int_{\mathbb{R}^2} d^2x \varphi \Delta\varphi$$

- Scale invariant in 2D

$$E_{\text{depol}}(\vec{n}_\lambda) = E_{\text{depol}}(\vec{n})$$

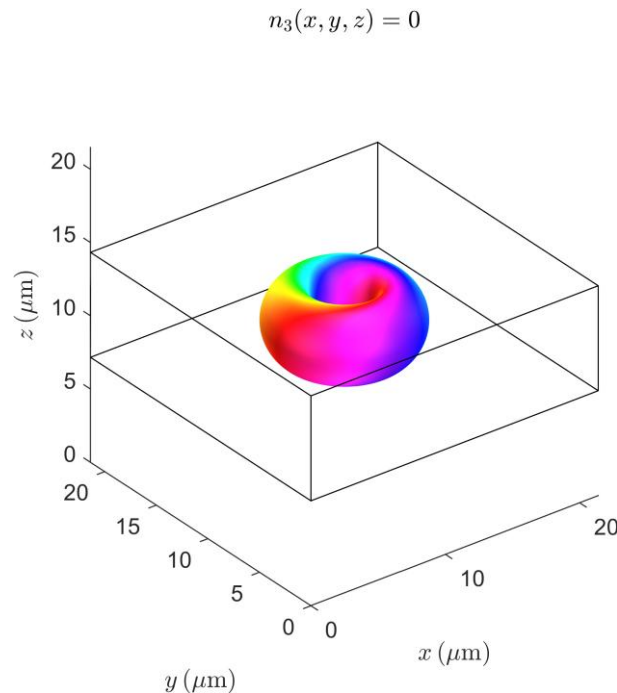
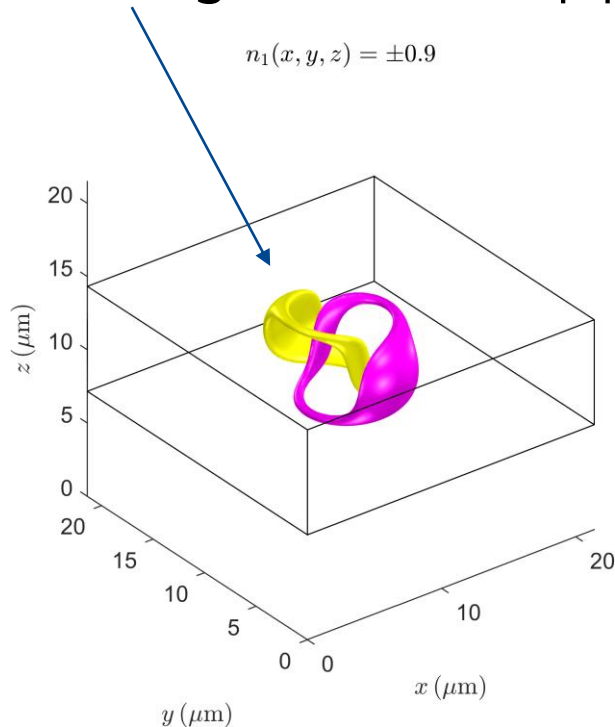
- Bloch skyrmions **affected** by depolarization  

$$\vec{\nabla} \cdot \vec{P}_{\text{Bloch}} = \frac{e_3}{r} \frac{df}{dr} \sin 2f(r) \neq 0$$



# 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

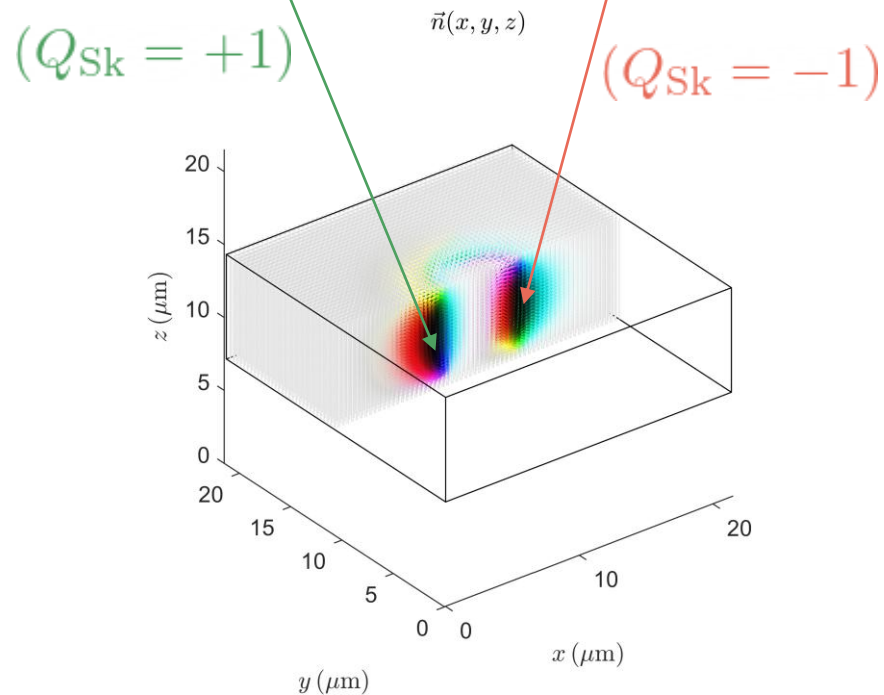


$$Q_{\text{Hopf}} \in \pi_3(\mathbb{RP}^2) = \pi_3(S^2) = \mathbb{Z}$$

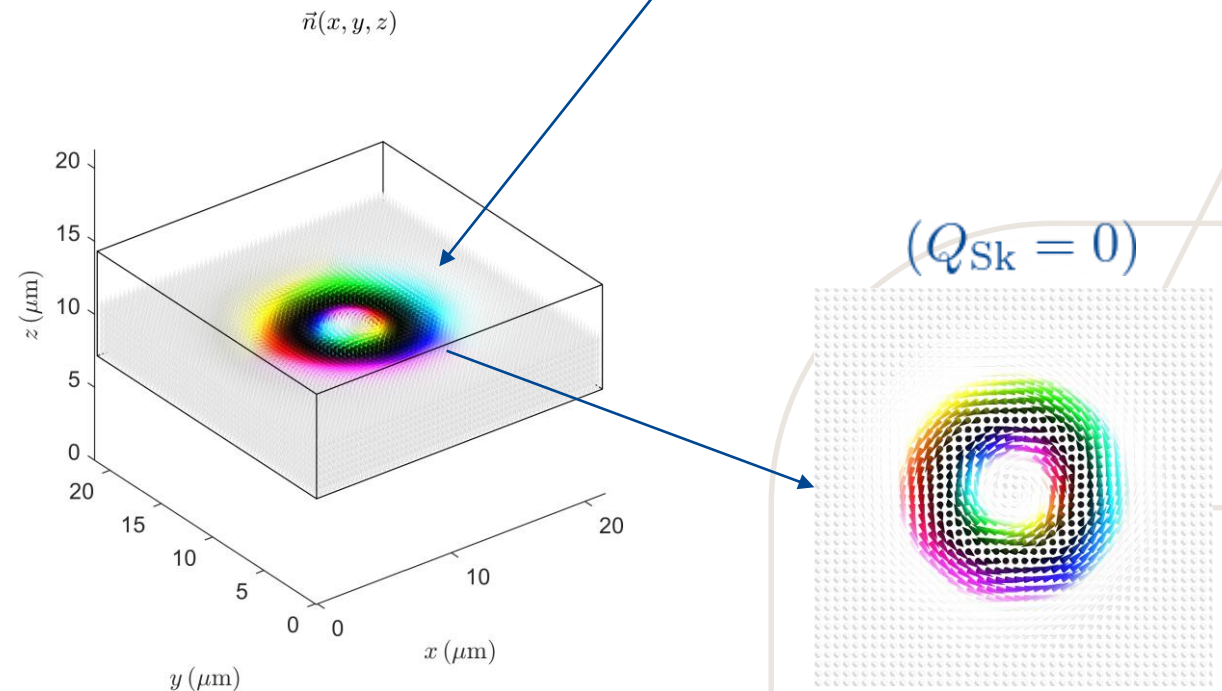
$Q_{\text{Hopf}} = 1$  Hopfion ansatz<sup>[11]</sup>

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

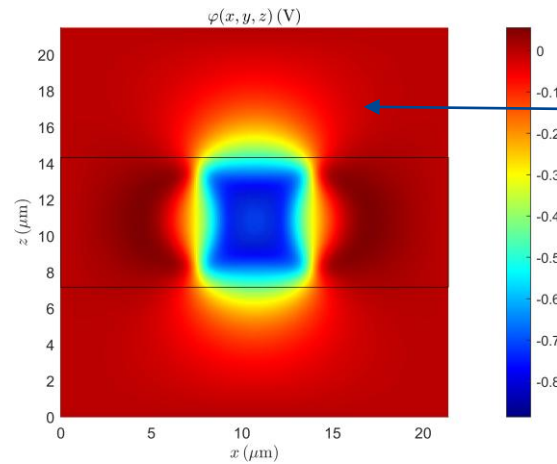
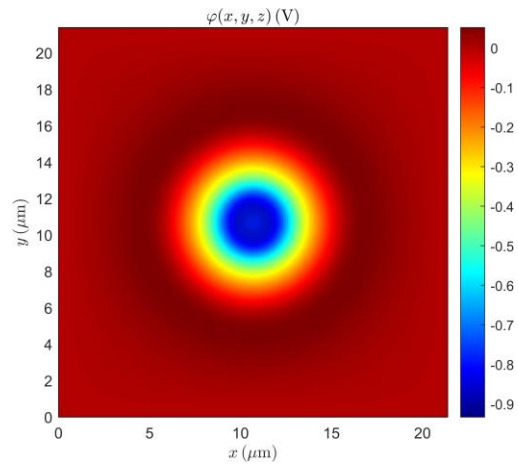
Skyrmion twisting as it winds around the hopfion core, changing from an in-plane **skyrmion** to an out-of-plane **antiskyrmion**



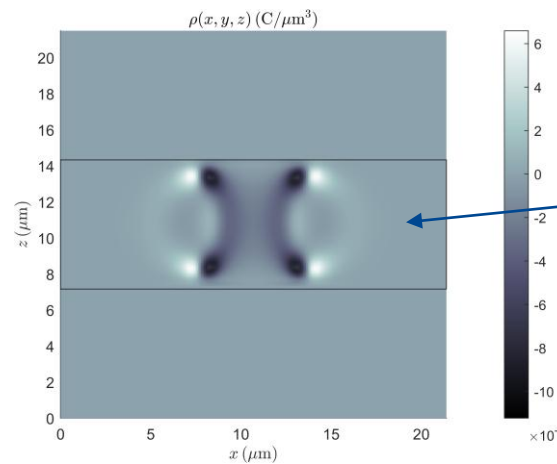
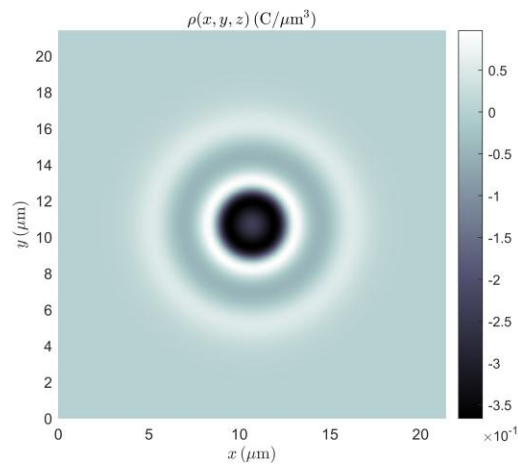
Structure of Bloch skyrmionium or a  $2\pi$ -vortex<sup>[12]</sup>



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



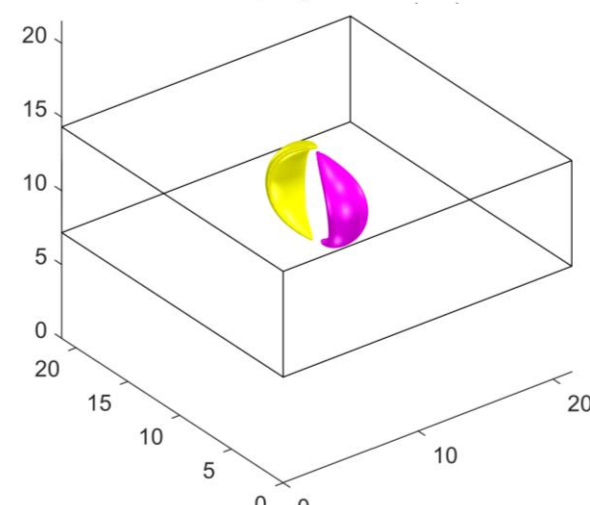
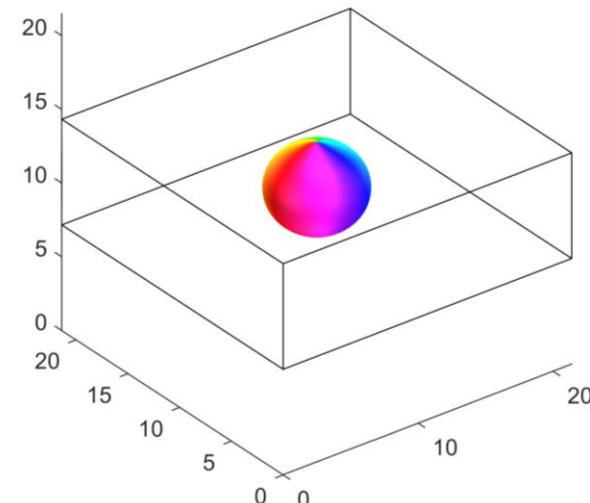
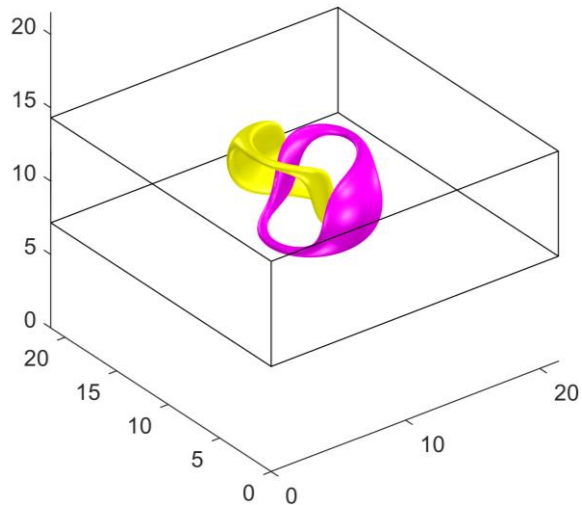
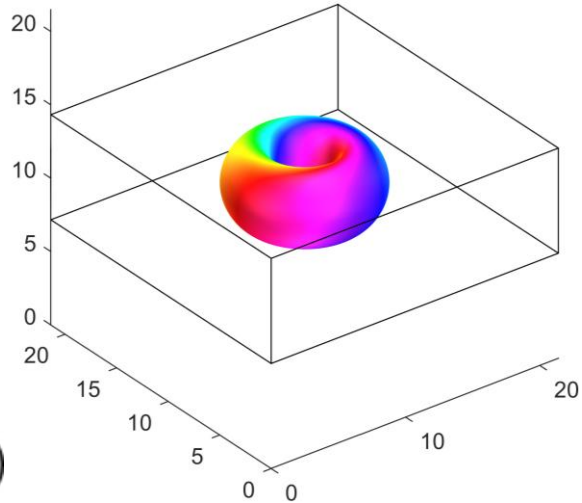
Electric scalar potential  
non-zero in  $\mathbb{R}^3/\Omega$



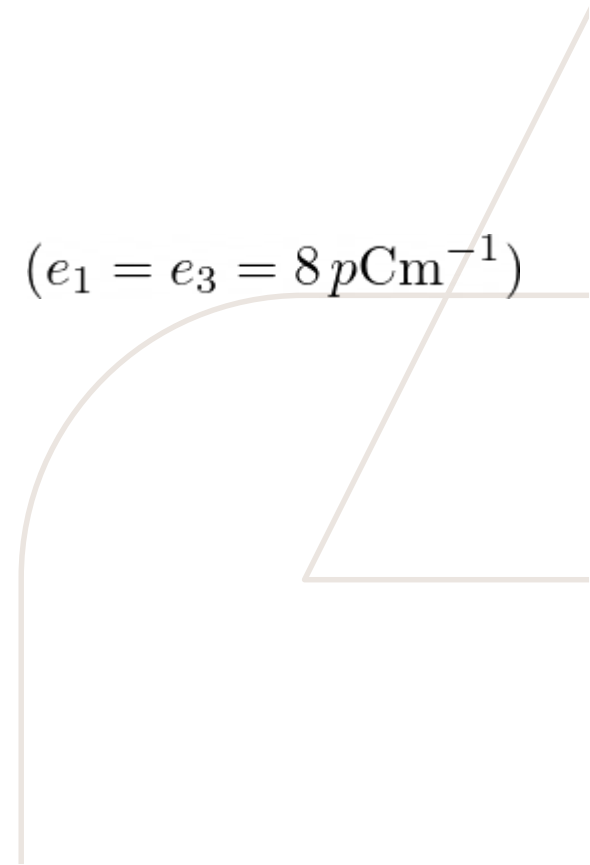
Electric charge density confined within  
 $\Omega = \left\{ (x, y, z) \in \mathbb{R}^3 : |z| \leq \frac{d}{2} \right\}$

# Hopfion to skyrmion transition

$$(e_1 = e_3 = 4 p\text{Cm}^{-1})$$



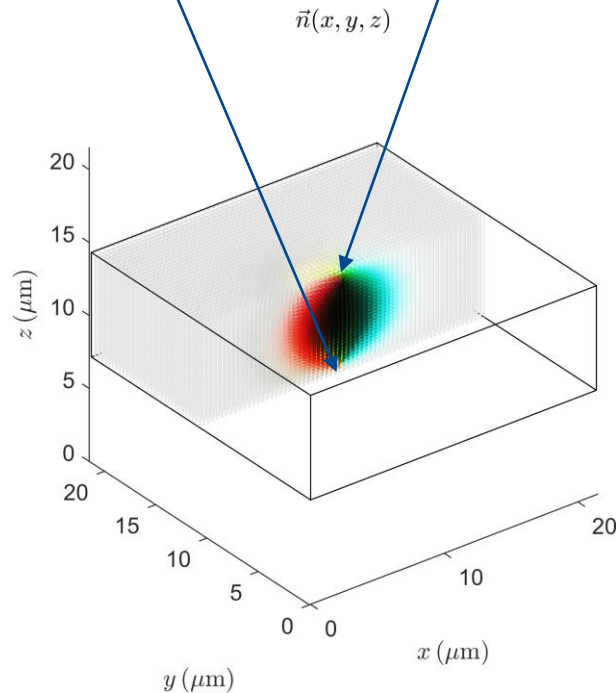
$$(e_1 = e_3 = 8 p\text{Cm}^{-1})$$



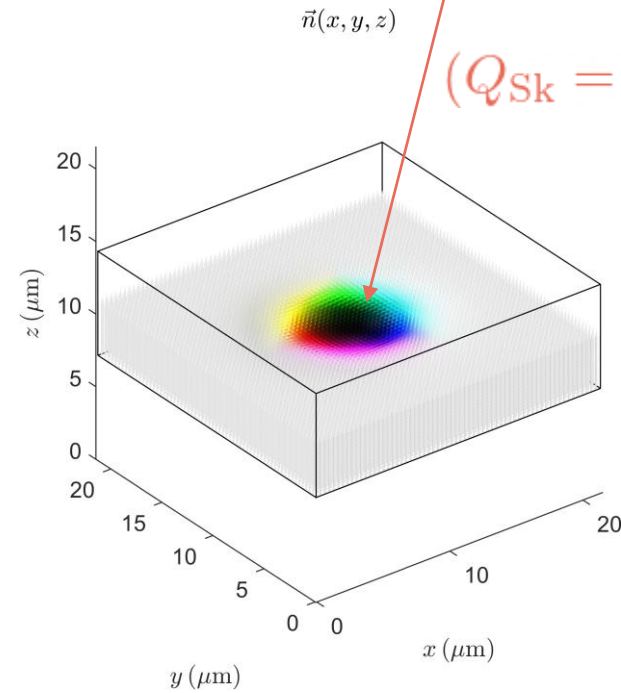


# Hopfion $\longrightarrow$ Skyrmion ( $e_i = 8 \text{ pCm}^{-1}$ )

Skyrmion terminating at point defects due to boundary conditions<sup>[13]</sup>

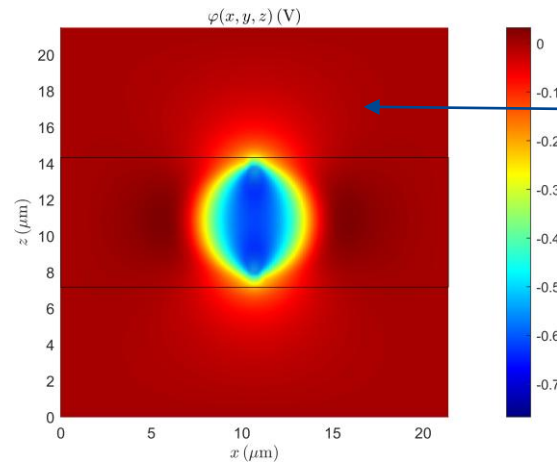
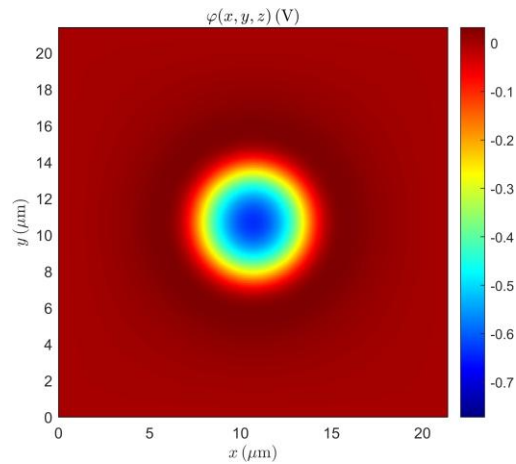


Structure of a Bloch skyrmion

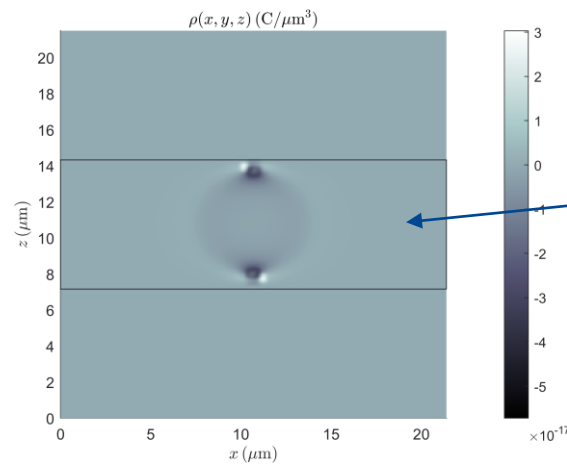
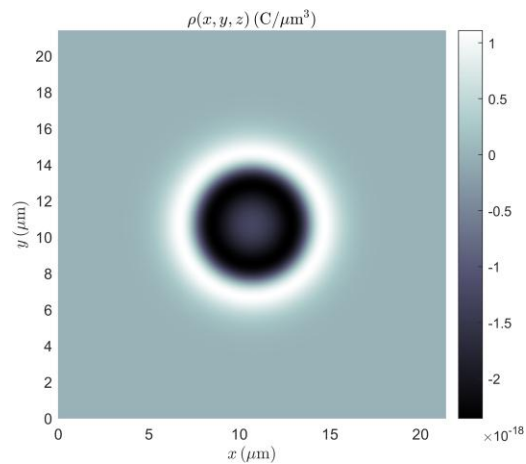


[13] J. B. Tai and I. I. Smalyukh, *Surface anchoring as a control parameter for stabilizing torons, skyrmions, twisted walls, fingers, and their hybrids in chiral nematics*, Phys. Rev. E **101** (2020) 042702

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



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



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

# 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 cell included
- Flexoelectric self-interaction can destabilize hopfion into skyrmion
- Method can be applied 3D spin textures in chiral magnets