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Flexoelectric self-polarization effect on topological defects in liquid crystals

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Outline

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

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

Nematic liquid crystal

- Frank-Oseen free energy for an anisotropic NLC is

$$F_{\mathrm{FO}} = \int_\Omega \mathrm{d}^3x \left\{ \frac{1}{2}K_1|\vec{S}|^2 + \frac{1}{2}K_2T^2 + \frac{1}{2}K_3|\vec{B}|^2 + V(\vec{n}) \right\}$$

$\vec{S} = S\vec{n} = \vec{n}(\vec{\nabla}\cdot\vec{n})$ 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 1st order terms (in derivatives of the director) are present:

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

→ 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 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** 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 $\vec{n}$[2]:

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

- Frank-Oseen energy reduces to chiral magnet energy with Dresselhaus DMI[3]

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

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

Splay and bend favoured liquid crystal

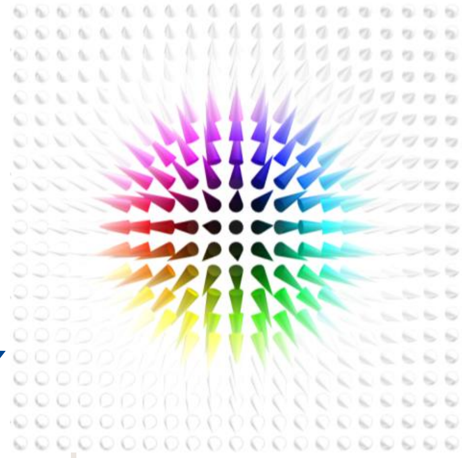
- Nematic liquid crystal $F_{\mathrm{FO}} = \frac{1}{2}K\int_\Omega \mathrm{d}^3x \left\{|\vec{S}|^2 + T^2 + |\vec{B}|^2\right\}$
- We have considered **twist** favoured (chiral) liquid crystals, $T \mapsto T + q_0$
- What about **splay** and **bend** favoured liquid crystals?

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

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

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

DMI from Rashba SOC



Favours **Néel** hedgehog skyrmions

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Experimental realization

- LCs 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 $\vec{E}_{\text{ext}} = \left(0, 0, \frac{U}{d}\right)$
- 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[5]

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

W_0: 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**
- Polarization caused by mechanical curvature (flexion) of director (flexoelectric)[6,7]:

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

- 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

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

[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_{flexo}

- First variation is

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = \epsilon_0 \int_\Omega \mathrm{d}^3x\, \varphi \boxed{\Delta\dot{\varphi}}$$

- Poisson equation variation

$$\boxed{\Delta\dot{\varphi} = -\frac{1}{\epsilon_0}\vec{\nabla}\cdot\left(\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\vec{P}_f(\vec{n}_t)\right)}$$

- Flexoelectric variation becomes

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F_{\text{flexo}}(\vec{n}_t) = -\int_\Omega \mathrm{d}^3x\, \varphi\vec{\nabla}\cdot\left(\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\vec{P}_f(\vec{n}_t)\right) = \int_\Omega \mathrm{d}^3x\, \vec{\nabla}\varphi\cdot\left(\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\vec{P}_f(\vec{n}_t)\right)$$

$$= \int_\Omega \mathrm{d}^3x\, \left(\boxed{\mathrm{grad}_{\vec{n}}\, F_{\text{flexo}}}\right)\cdot\boxed{\vec{\varepsilon}}$$

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

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

Numerical problem

- Topological solitons are **minimizers** of the flexoelectric Frank-Oseen energy

$$F_{\mathrm{FFO}}(\vec{n}) = \int_\Omega \mathrm{d}^3x \left\{ \frac{K}{2}(\nabla\vec{n})^2 + Kq_0 \left[\vec{n}\cdot(\vec{\nabla}\times\vec{n})\right] + V(\vec{n}) + \frac{\epsilon_0}{2}\varphi\Delta\varphi \right\}$$

- Electrostatic potential subject to constraint

$$\begin{cases} \Delta\varphi = -\frac{1}{\epsilon_0}\vec{\nabla}\cdot\vec{P}_f & \mathrm{in}\,\Omega, \\ \Delta\varphi = 0 & \mathrm{in}\,\mathbb{R}^3/\Omega. \end{cases} \qquad \Omega = \left\{ (x,y,z)\in\mathbb{R}^3 \;:\; |z| \leq \frac{d}{2} \right\}$$

- Reformulate problem as unconstrained optimization problem[8,9]: minimize the functional for fixed $\vec{n}$, $\vec{P}_f(\vec{n})$

$$F(\varphi) = \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}^3x\, |\vec{\nabla}\varphi|^2 + \frac{1}{\epsilon_0}\int_\Omega \mathrm{d}^3x\, \varphi\left(\vec{\nabla}\cdot\vec{P}_f\right)$$

- Approach: non-linear conjugate gradient method with line search strategy[10]

[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 ω-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 potential φ using NCGD with Fletcher-Reeves 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)

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 <u>is not</u>

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

SPLAY-BEND FAVOURED

- Rashba DMI prefers Néel skyrmions

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

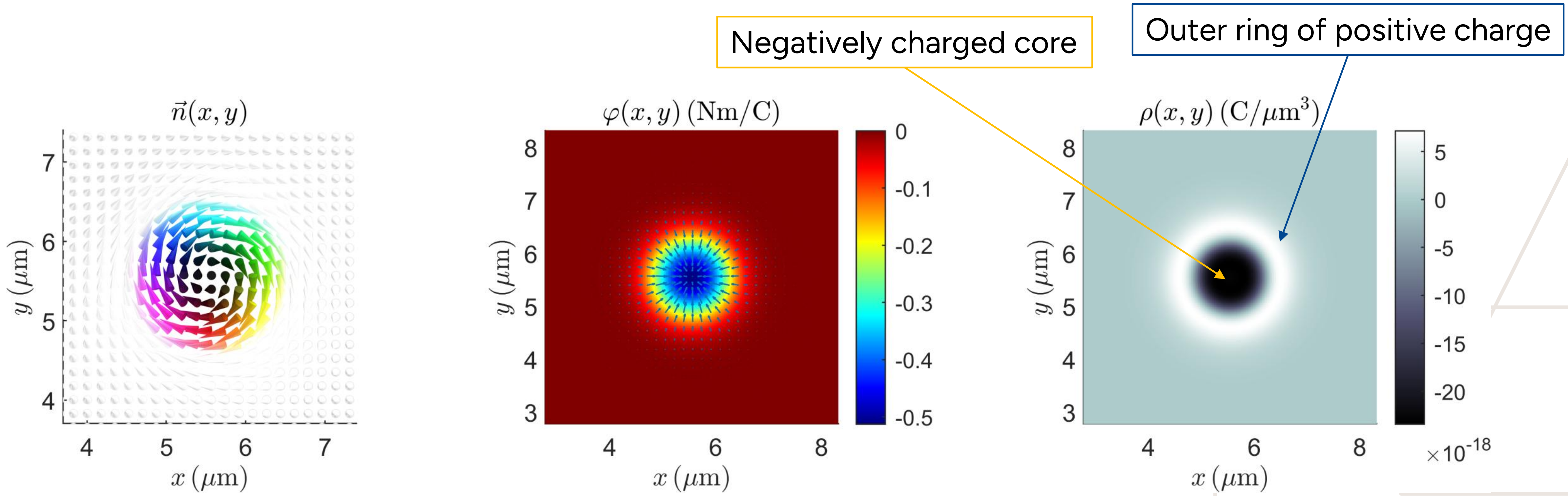
- Néel ansatz is not solenoidal

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

- Associated polarization is also not solenoidal

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

Twist favoured Bloch skyrmions

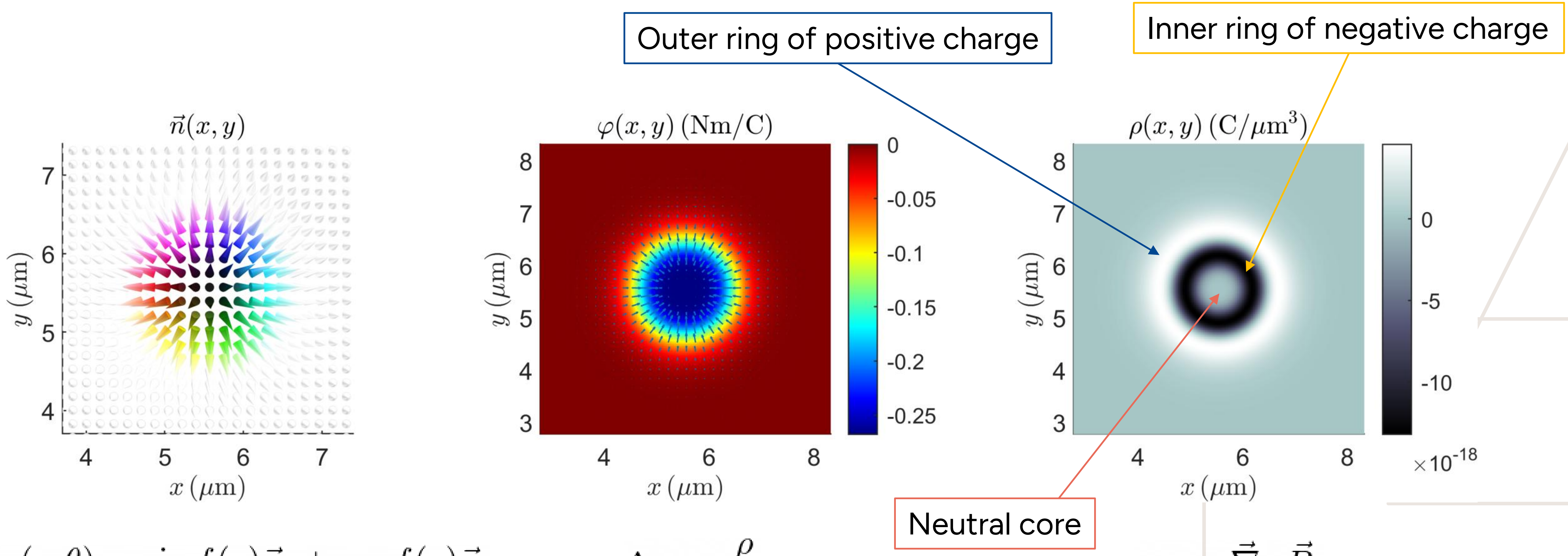


$$\vec{n}_{\text{Bloch}}(r,\theta) = \sin f(r)\vec{e}_\theta + \cos f(r)\vec{e}_z$$

$$\Delta\varphi = \frac{\rho}{\epsilon_0}$$

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

Splay-bend favoured Néel skyrmions



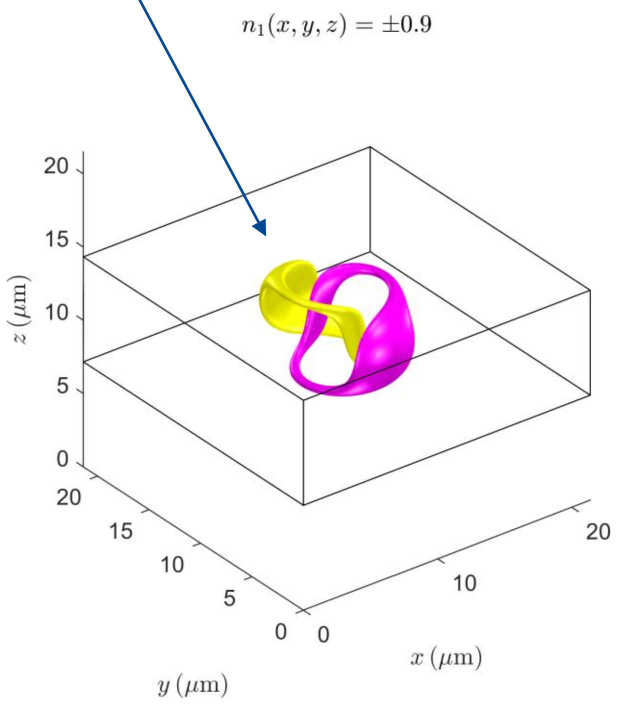
$$\vec{n}_{\text{Néel}}(r,\theta) = \sin f(r)\vec{e}_r + \cos f(r)\vec{e}_z$$

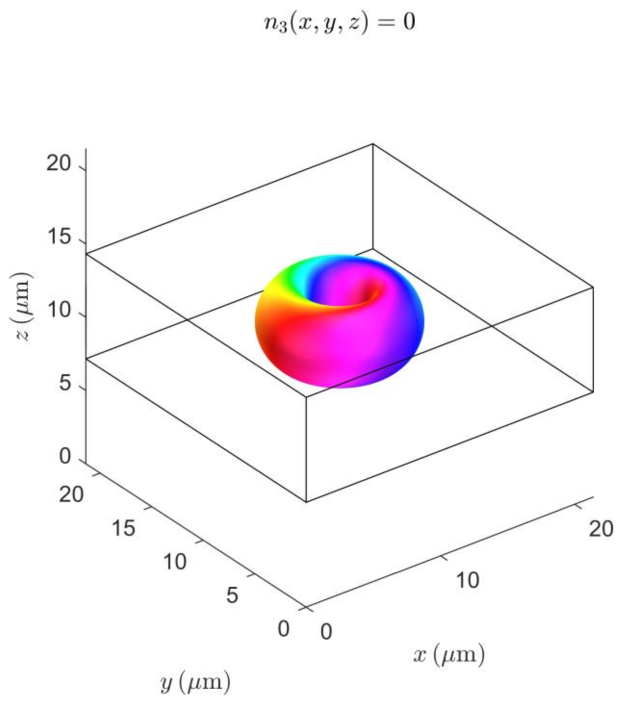
$$\Delta\varphi = \frac{\rho}{\epsilon_0}$$

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

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[11]

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

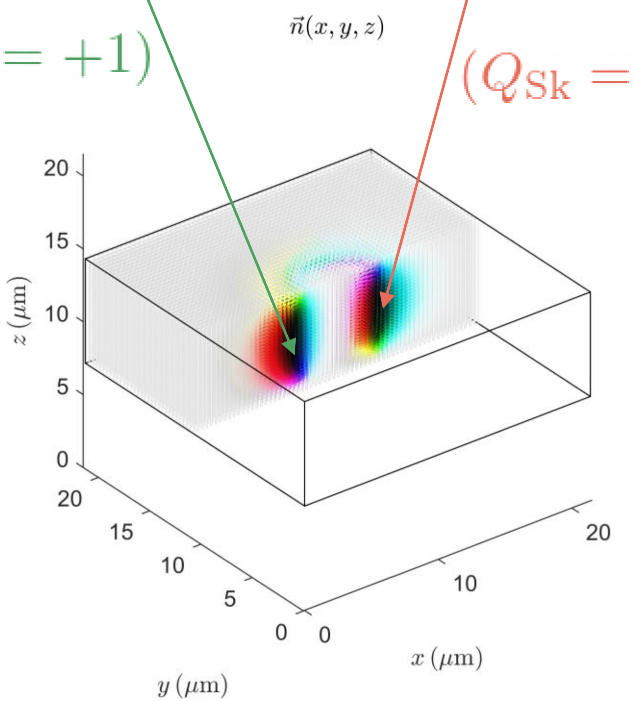
Hopfion structure $(e_i = 4\,\mathrm{pCm}^{-1})$

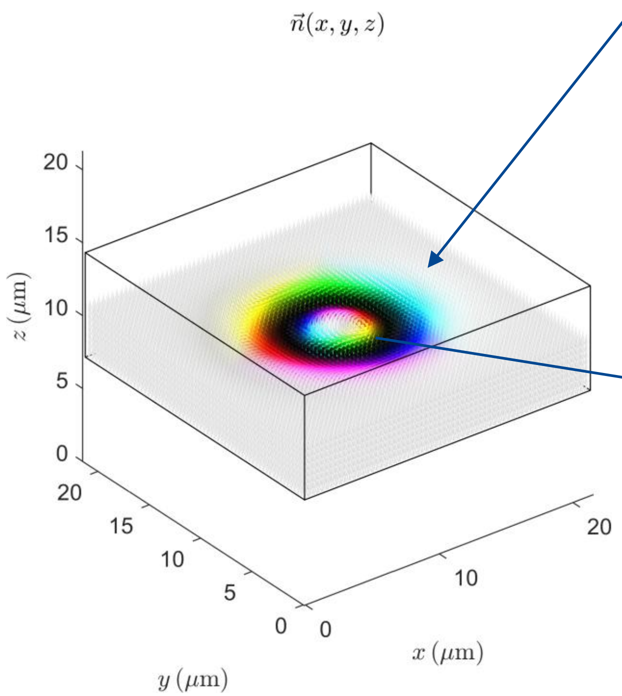
Skyrmion twisting as it winds around the hopfion core, changing from an in-plane skyrmion to an out-of-plane antiskyrmion

Structure of Bloch skyrmionium or a 2π-vortex[12]

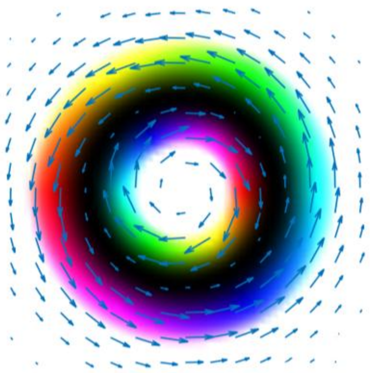
$(Q_{\mathrm{Sk}} = +1)$

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



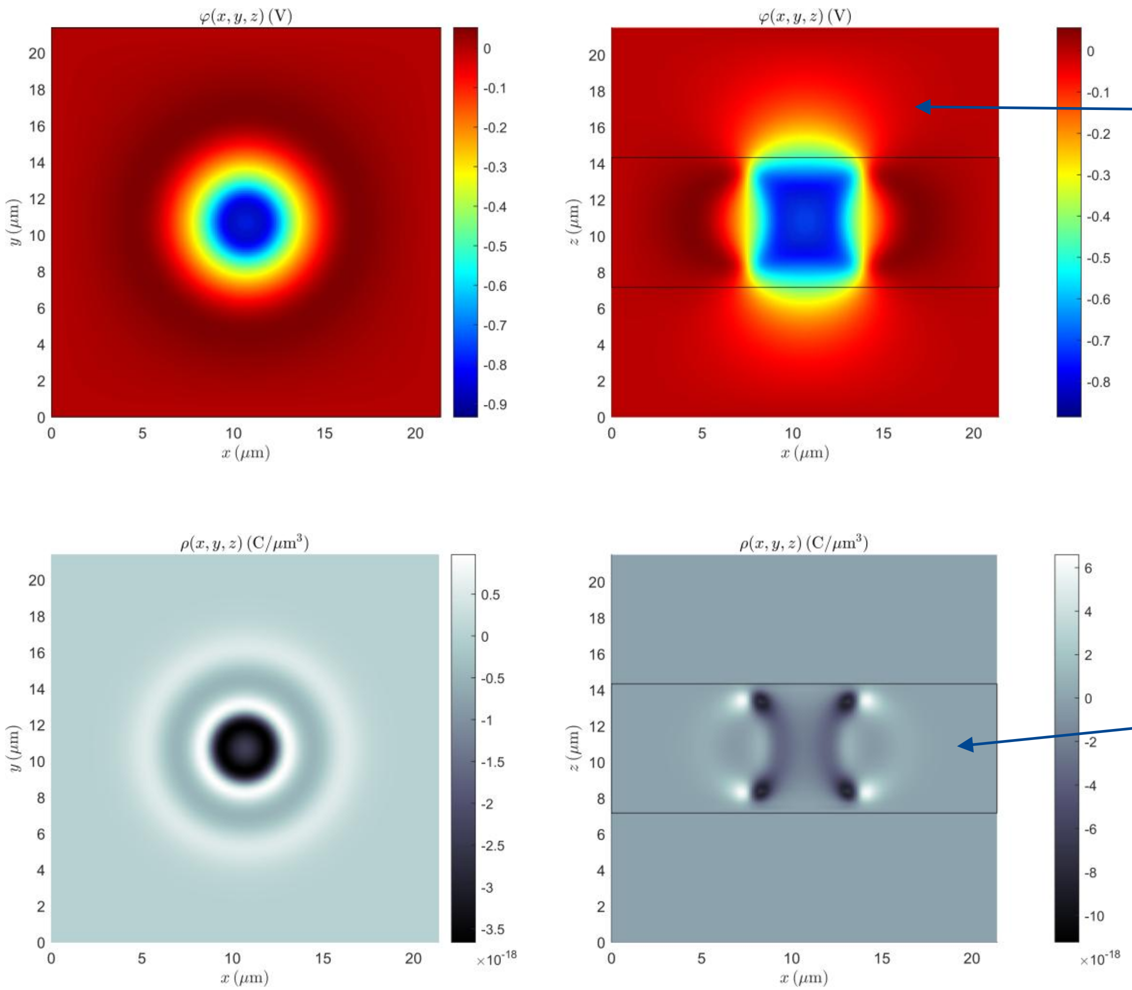


$(Q_{\mathrm{Sk}} = 0)$



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

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



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

Electric charge density confined within

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

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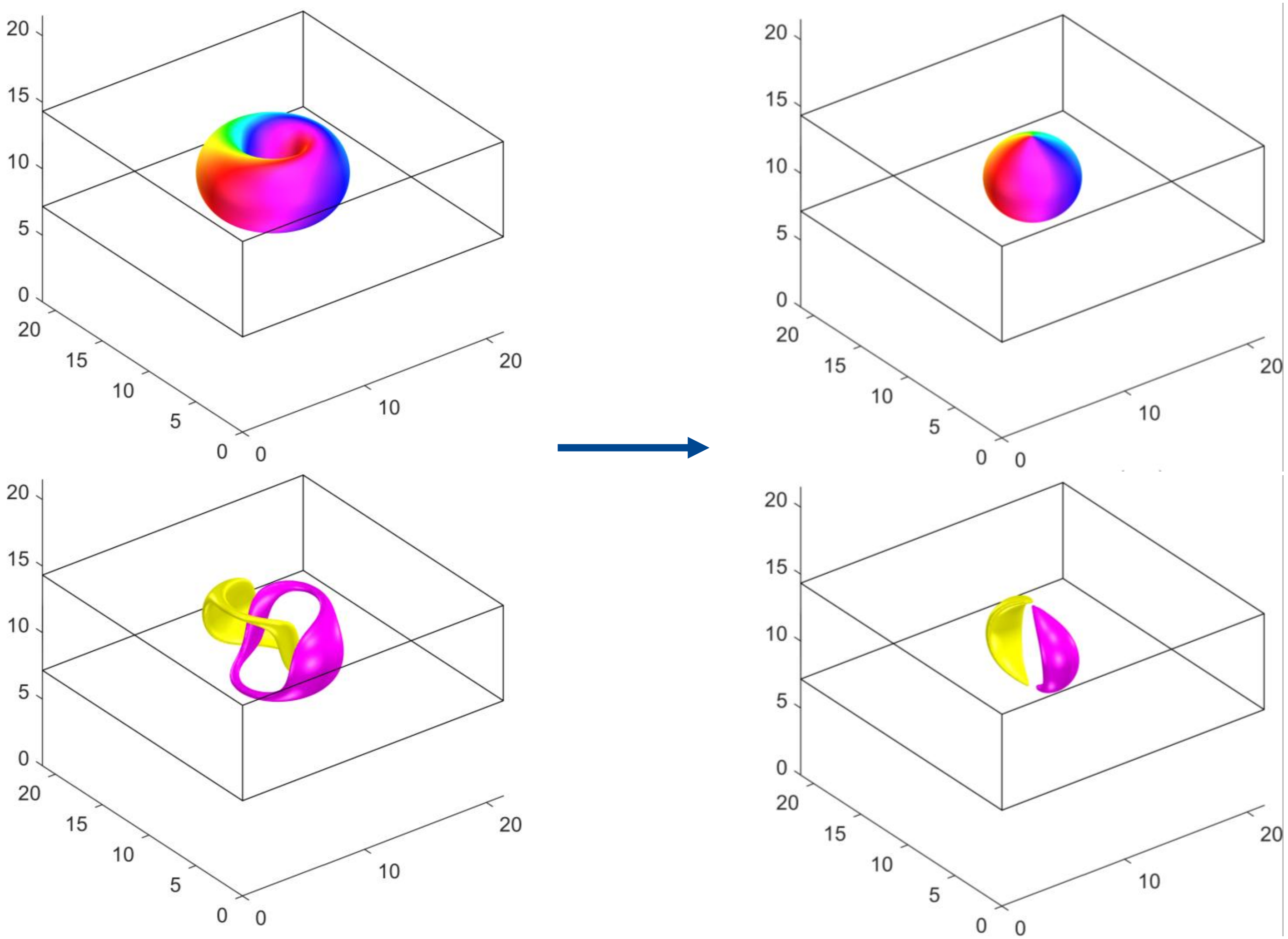
Hopfion to skyrmion transition

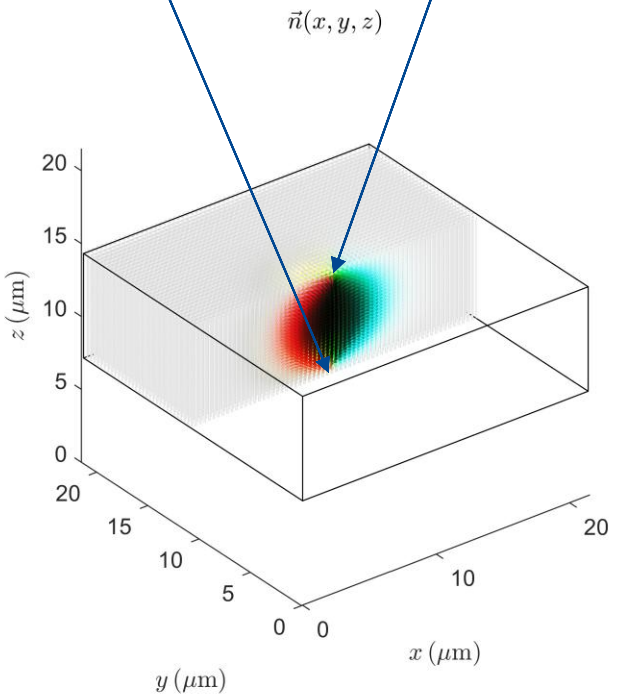
$(e_1 = e_3 = 4\,p\mathrm{Cm}^{-1})$



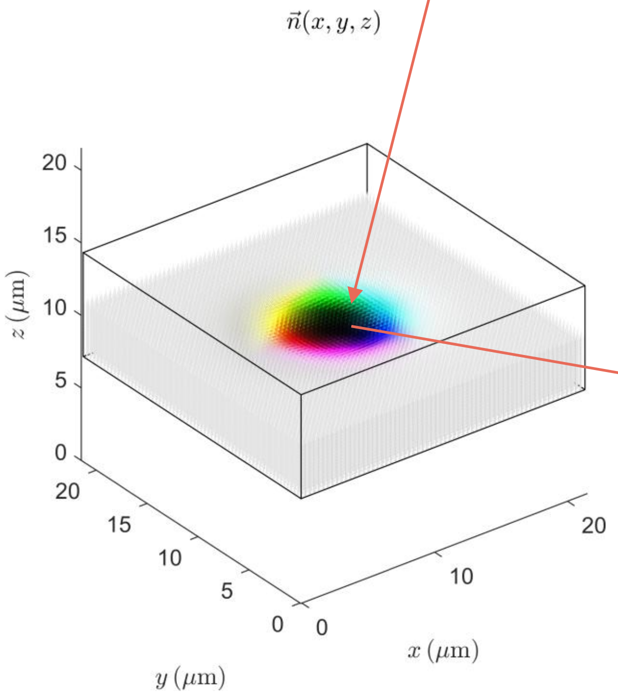
$(e_1 = e_3 = 8\,p\mathrm{Cm}^{-1})$

Hopfion ⟶ Skyrmion $(e_i = 8\,\mathrm{pCm}^{-1})$

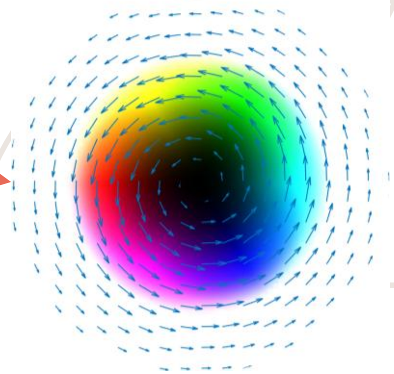
Skyrmion terminating at point defects due to boundary conditions[13]



Structure of a Bloch skyrmion



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



[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

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 confined geometry included
- Flexoelectric self-interaction can **destabilize hopfions into skyrmions**
- We showed how to relate liquid crystals to chiral magnets
- While they are similar, the manifestation of topological defects in each system is unique
- **Electrostatic self-interaction** also **behaves differently** in both systems

Summary: electrostatic self-interactions of skyrmions

CHIRAL MAGNETS

- Demagnetizing field $\vec{B} = -\vec{\nabla}\psi$
- Associated magnetic potential $\psi : \mathbb{R}^2 \to \mathbb{R}$

$$\Delta\psi = \mu_0\rho, \quad \rho = -M_s(\vec{\nabla}\cdot\vec{n})$$

- Magnetostatic self-energy

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

- Behaves like potential term in 2D

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

- Bloch skyrmions **unaffected** by demagnetization $\vec{\nabla}\cdot\vec{n}_{\mathrm{Bloch}} = 0$

LIQUID CRYSTALS

- Depolarizing field $\vec{E} = -\vec{\nabla}\varphi$
- Associated electric potential $\varphi : \mathbb{R}^2 \to \mathbb{R}$

$$\Delta\varphi = \rho/\epsilon_0, \quad \rho = -\vec{\nabla}\cdot\vec{P}_f(\vec{n})$$

- Electrostatic self-energy

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

- Scale invariant in 2D

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

- Bloch skyrmions **affected** by depolarization $\vec{\nabla}\cdot\vec{P}_{\mathrm{Bloch}} = \frac{e_3}{r}\frac{\mathrm{d}f}{\mathrm{d}r}\sin 2f(r) \neq 0$