The surface energy of a baby Skyrme crystal

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Summary

Motivation

- The $(3+1)$-dimensional Skyrme model is a nonlinear field theory of pions.
- Nuclei are modelled as topological solitons (Skyrmions).
- Many Skyrmions look like chunks of the infinite crystal.
- Ultimately, we want to produce correct binding energies for quantised Skyrmions.
- The baby Skyrme model is mainly a $(2+1)$-dimensional analogue of the Skyrme model.
- It does however arise in condensed matter physics in ferromagnetic quantum hall systems.

Baby Skyrme model

- The general baby Skyrme model consists of a single scalar field $\phi : \Sigma \to S^2$ where (Σ, g) is a Riemannian manifold, and (S^2, h, ω) is the 2-sphere with area 2-form ω and h is the induced metric from embedding S^2 in $\mathbb{R}^3$.
- We are interested in baby Skyrmions on:
  - the plane, $\Sigma = \mathbb{R}^2$;
  - the cylinder, $\Sigma = S^1 \times \mathbb{R}$; and
  - the lattice, $\Sigma = \mathbb{R}^2/\Lambda$.
- The static energy functional on Σ is given by

$$E[\phi] = \int_\Sigma \left\{ \frac{1}{2}|\mathrm{d}\phi|^2 + \frac{1}{2}|\phi^*\omega|^2 + V[\phi] \right\} \mathrm{vol}_g,$$

  where we consider the standard $O(2)$ potential $V[\phi] = m^2(1 - \phi_3)$ with $m^2 = 0.1$.
- The baby Skyrme map has an associated degree

$$B = -\frac{1}{4\pi} \int_\Sigma \phi^*\omega \in \mathbb{Z}.$$

Baby Skyrmions on $\mathbb{R}^2$

- Physical space is $\Sigma = \mathbb{R}^2$ with local coordinates $x = (x_1, x_2)$.
- Finite energy solutions require us to impose the boundary conditions $\lim_{|x| \to \infty} \phi(x) \equiv \phi_\infty = (0, 0, 1)$ such that $V[\phi_\infty] = 0$.
- Chains solutions were proposed as a good candidate for the global minima for low charges (Foster, 2010).
- Ring solutions were found to be a better candidate for the global minima for charges $B > B_c \in \mathbb{Z}$, where $B_c = 15$ for $m^2 = 0.1$ (Winyard, 2016).
- We show that crystal chunks become the lower energy solution for $B > B_r$ for some $B_r \in \mathbb{Z}$.

Baby Skyrmion chain on $\mathbb{R}^2$

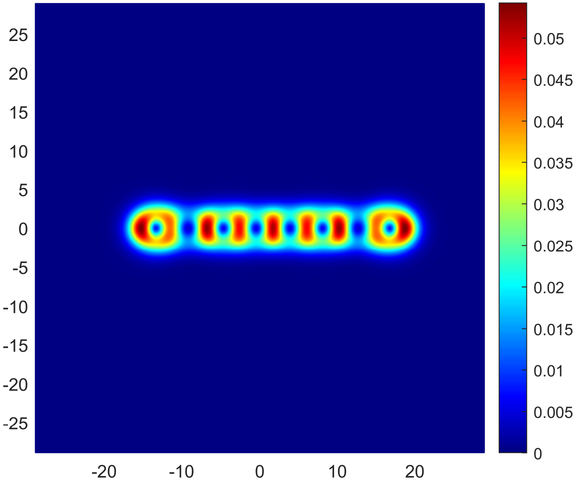

Figure 1: Energy density plot of the $B = 9$ chain solution for $m^2 = 0.1$.

Baby Skyrmion ring on $\mathbb{R}^2$

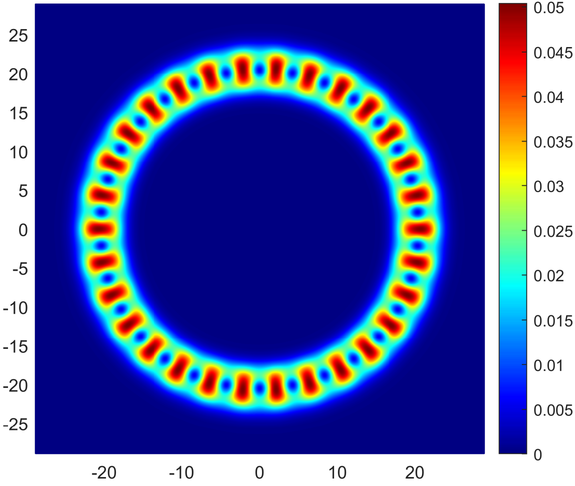

Figure 2: Energy density plot of the $B = 30$ ring solution for $m^2 = 0.1$.

Lattice baby Skyrmions

- The physical space of interest is the 2-torus $\Sigma = \mathbb{R}^2/\Lambda$, where Λ is the set of all 2-dimensional period lattices

$$\Lambda = \left\{ \sum_{i=1}^{2} n_i(\alpha X_i) \mid n_i \in \mathbb{Z}, \alpha \in \mathbb{R}^* \right\}$$

  and $\{X_1, X_2\}$ is a basis for $\mathbb{R}^2$.
- Crystallographic restriction theorem: 5 lattice types in 2-dimensions. Fundamental unit cell is a certain type of a parallelogram.
- To find the optimal crystalline structure, we minimize the static energy over all period lattices.
- Equivalently, we fix our domain of ϕ to be $\mathbb{R}^2/\mathbb{Z}^2$ and identify every other torus $\mathbb{R}^2/\Lambda$ with $\mathbb{R}^2/\mathbb{Z}^2$, but with a nonstandard Riemannian metric g. This metric g is the pullback of the usual metric $\bar{g}$ on $\mathbb{R}^2/\Lambda$ via the diffeomorphism $\mathbb{R}^2/\mathbb{Z}^2 \to \mathbb{R}^2/\Lambda$. As we vary Λ then the metric g varies (Speight, 2014) .

Lattice baby Skyrmions

- Let $F : \mathbb{R}^2/\mathbb{Z}^2 \to \mathbb{R}^2/\Lambda$ be a diffeomorphism with $F \in \mathrm{GL}(2, \mathbb{R})$ and (x_1, x_2) be local coordinates on $\mathbb{T}^2 = \mathbb{R}^2/\mathbb{Z}^2$.
- Identify $\mathrm{GL}(2, \mathbb{R}) = \mathrm{SL}(2, \mathbb{R}) \times \mathbb{R}^*$ and let $A = [X_1\ X_2] \in \mathrm{SL}(2, \mathbb{R})$ and $\alpha \in \mathbb{R}^*$, such that $F = \alpha A$.
- Now identify the Skyrme field as a map $\phi : \mathbb{T}^2 \to S^2$.
- Metric on $\mathbb{T}^2$ is the pullback $g = F^*\bar{g}$, and the volume form is $\mathrm{vol}_g = \sqrt{\det(F^*\bar{g})}\,\mathrm{d}x_1 \wedge \mathrm{d}x_2 = \alpha^2\,\mathrm{d}x_1 \wedge \mathrm{d}x_2$.
- The static energy functional on $\mathbb{T}^2$ is

$$E = \frac{1}{2}\int_{\mathbb{T}^2} \left\{ X_2^2(\partial_1\phi)^2 - 2(X_2 \cdot X_1)(\partial_1\phi \cdot \partial_2\phi) + X_1^2)(\partial_2\phi)^2 \right\} \mathrm{d}x_1\,\mathrm{d}x_2 \\ + \frac{1}{2\alpha^2}\int_{\mathbb{T}^2} (\partial_1\phi \times \partial_2\phi)^2\,\mathrm{d}x_1\,\mathrm{d}x_2 + \alpha^2\int_{\mathbb{T}^2} V[\phi]\,\mathrm{d}x_1\,\mathrm{d}x_2.$$

Lattice baby Skyrmions

- Taking the variation of the static energy functional with respect to α,

$$\frac{\partial E}{\partial \alpha} = -\frac{\kappa^2}{\alpha^3} \int_{\mathbb{T}^2} \left(\partial_1 \phi \times \partial_2 \phi\right)^2 \mathrm{d}x_1 \, \mathrm{d}x_2 + 2\alpha \int_{\mathbb{T}^2} V[\phi] \, \mathrm{d}x_1 \, \mathrm{d}x_2,$$

yields the relation

$$\alpha^2 = \sqrt{\frac{\frac{\kappa^2}{2} \int_{\mathbb{T}^2} \left(\partial_1 \phi \times \partial_2 \phi\right)^2 \mathrm{d}x_1 \, \mathrm{d}x_2}{\int_{\mathbb{T}^2} V[\phi] \, \mathrm{d}x_1 \, \mathrm{d}x_2}} = \sqrt{\frac{E_4}{E_0}}.$$

- Finding the period lattice parameters X_1, X_2 which minimize the Dirichlet energy E_2 is a constrained quadratic optimization problem with the nonlinear constraint $\det([X_1 \; X_2]) = 1$.
- For notational convenience, let us write

$$\mathcal{E}_{ij} = \int_{\mathbb{T}^2} \left(\partial_i \phi \cdot \partial_j \phi\right) \mathrm{d}x_1 \, \mathrm{d}x_2.$$

- Then the Dirichlet energy E_2 can be expressed in the form
$$E_2 = \frac{1}{2}\boldsymbol{x}^T \mathcal{Q}\boldsymbol{x},$$
where $\boldsymbol{x} = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$ is a 4-vector and $\mathcal{Q}$ is the 4×4-symmetric matrix
$$\mathcal{Q} = \begin{bmatrix} \mathcal{E}_{22} & 0 & -\mathcal{E}_{12} & 0 \\ 0 & \mathcal{E}_{22} & 0 & -\mathcal{E}_{12} \\ -\mathcal{E}_{12} & 0 & \mathcal{E}_{11} & 0 \\ 0 & -\mathcal{E}_{12} & 0 & \mathcal{E}_{11} \end{bmatrix}.$$
- Including the Lagrange term $\gamma(\det([X_1\ X_2]) - 1)$ reduces the problem to an eigenvalue problem $\mathcal{B}\boldsymbol{x} = \gamma\boldsymbol{x}$, where
$$\mathcal{B} = \begin{bmatrix} 0 & \mathcal{E}_{12} & 0 & -\mathcal{E}_{11} \\ -\mathcal{E}_{12} & 0 & \mathcal{E}_{11} & 0 \\ 0 & \mathcal{E}_{22} & 0 & -\mathcal{E}_{12} \\ -\mathcal{E}_{22} & 0 & \mathcal{E}_{12} & 0 \end{bmatrix}.$$

Hexagonal crystalline structure

- The optimal lattice is found to be an equianharmonic lattice with a hexagonal crystalline structure.
- Unit cell has sides of equal length $L_H = 9.65$ and angle $\theta = \frac{2\pi}{3}$.
- The infinite crystal has energy $\mathcal{E}_{\text{crystal}} = 1.4543$, which is lower than the infinite chain energy $\mathcal{E}_{\text{chain}} = 1.4548$.
- The energies mentioned above, and throughout, are normalised by the Bogomolny bound, i.e. $\mathcal{E} := E/(4\pi B)$.

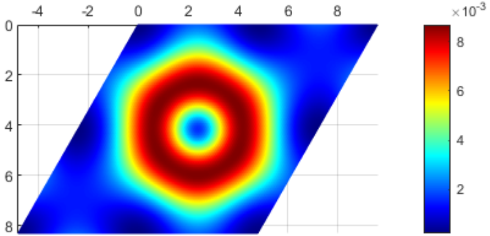

Figure 3: Hexagonal crystalline structure of the infinite crystal.

Crystal slab model on $\mathbb{R} \times S^1$

- Physical space is the cylinder $\Sigma = \mathbb{R} \times S^1$.
- This corresponds to a Dirichlet boundary condition in the x_2-direction, $\lim_{|x_2| \to \infty} = \phi_\infty$, and a periodic boundary condition in the x_1-direction, $\phi(x_1, x_2) = \phi(x_1 + n_1 L, x_2)$, where $n_1 \in \mathbb{Z}$.
- Staggered charge-2 baby Skyrmions are layered on an infinite cylinder of width $L = L_H$ to estimate the surface energy per unit length.
- Applying a least squares fit of the form

$$\mathcal{E}_{\text{slab}} = \mathcal{E}_{\text{crystal}} + 2\frac{L_H}{2n}\mathcal{E}_{\text{surf}},$$

where $\mathcal{E}_{\text{surf}}$ is the surface energy per unit length and number of layers n, we find that $\mathcal{E}_{\text{surf}} = 6.58 \times 10^{-4}$.

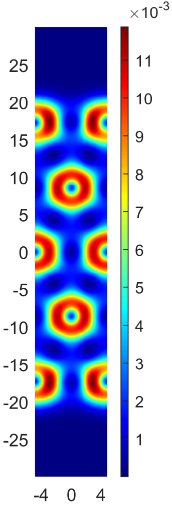

Figure 4: $n = 5$ layer crystal slab solution on infinite cylinder of width L_H.

Crystal chunk approximation

- Isoperimetric inequality in $\mathbb{R}^2$ is $L^2 \geq 4\pi A$, with equality iff the boundary curve is a cirle.
- Minimal crystal surface energy $\Rightarrow$ $L^2 = 4\pi A$ (crystal disks).
- Using this assumption, we can express chunks of the crystal in the form

$$\mathcal{E}_{\text{chunk}} = \mathcal{E}_{\text{crystal}} + 2\mathcal{E}_{\text{surf}}\sqrt{\frac{\pi}{B\rho_B}},$$

  where ρ_B is the charge per unit area.
- Can empirically compare chains, rings and crystal chunks using ring and chain approximations.
- Crystal chunk solutions become global minima for approximately $B > 877$.

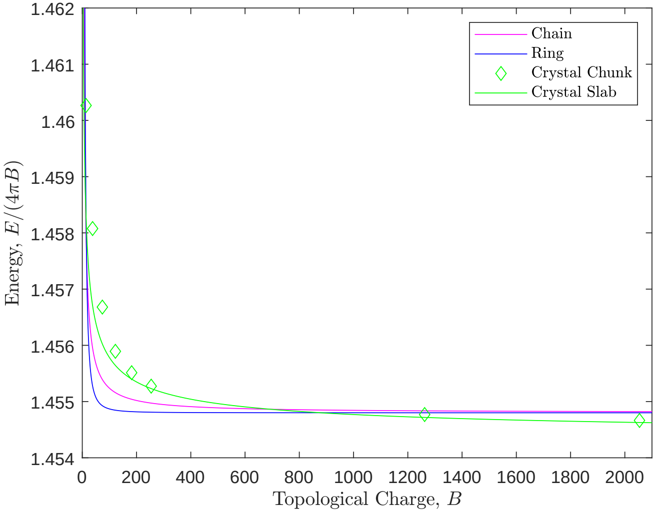

Figure 5: Comparison of ring, chain and crystal chunk approximations.

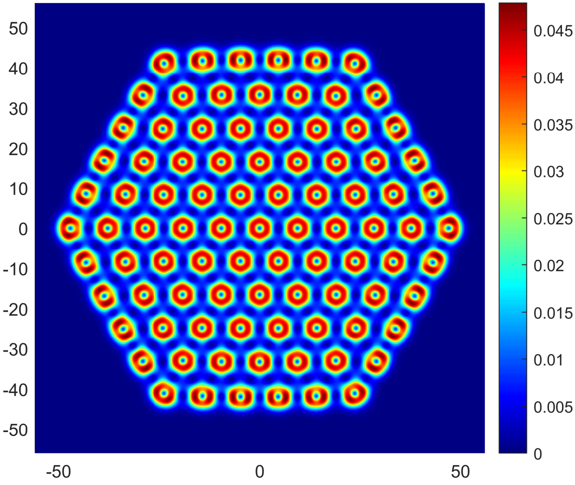

Figure 6: $B = 182$ crystal chunk solution.

$B = 2054$ crystal chunk

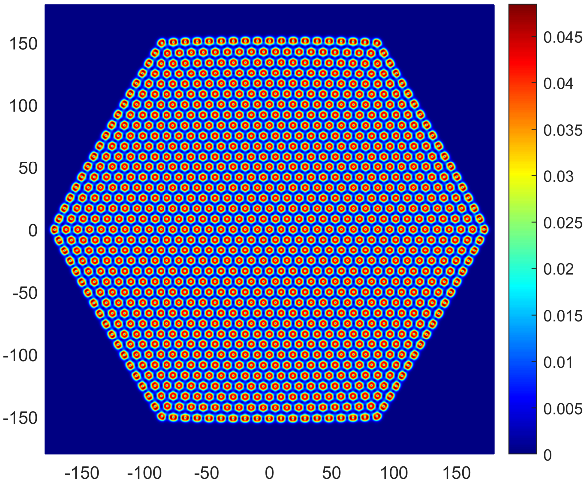

Figure 7: $B = 2054$ crystal chunk solution.

Summary

- Optimal crystal was thought to be a square lattice of half baby Skyrmions.
- Optimal crystalline structure is actually hexagonal.
- Optimal crystal structure in 3D is thought to be cube of half Skyrmions (Kugler & Shtrikman, 1988), see Fig. 8.
- Generalising this method, could a hexagonal structure prevail?

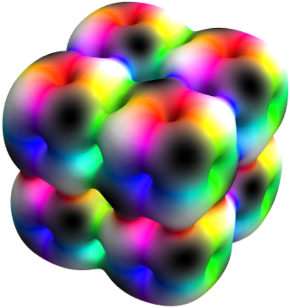

Figure 8: $B = 32$ crystal chunk solution in the Skyrme model.