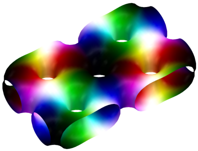
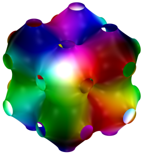
Skyrmion crystals





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Outline

Motivation

- The Skyrme model is a nonlinear field theory of pions (Skyrme, 1961)
- Nuclei are modelled as topological solitons (Skyrmions)
- Want to understand phases, and transitions of phases, of nuclear matter in the Skyrme model
- Ground state of nuclear matter has a crystalline structure in the classical approximation
- Many Skyrmions look like chunks of the infinite crystal (Feist *et al.*, 2013)
- Two candidates proposed:
    - Cubic lattice of half-Skyrmions
    - α-particle lattice
- Which is the lower energy solution (classically)?
- Are the two related?

Skyrme model

- Topological solitons: smooth, spatially localized solutions of non-linear field theories, topologically stable against decay to vacuum.
- Skyrme field $\varphi : (\Sigma, g) \to (G, h)$, e.g. $\mathbb{R}^3/\Lambda \to \mathrm{SU}(2)$
  - Left-invariant Maurer-Cartan form $\theta = \varphi^{-1}\mathrm{d}\varphi \in \Omega^1(G) \otimes \mathfrak{g}$
  - Associated 2-form $\Omega \in \Omega^2(G) \otimes \mathfrak{g}$, $\Omega(X,Y) := [\theta(X), \theta(Y)]$
  - $\mathrm{Ad}(\mathrm{SU}(2))$ invariant inner product, $h(X,Y) = \frac{1}{2}\,\mathrm{Tr}(X^\dagger Y)$
  - Skyrme energy functional

$$E[\varphi] = \int_\Sigma \left\{ c_2 g^{ij} h(L_i, L_j) + \frac{c_4}{2} g^{ia} g^{jb} h(\Omega_{ij}, \Omega_{ab}) + c_0 V(\varphi) \right\} \mathrm{vol}_g$$

  - $V : \mathrm{SU}(2) \to \mathbb{R}$ is the pion mass potential,

$$V(\varphi) = m^2\,\mathrm{Tr}(\mathbb{1} - \varphi)$$

  - Usual coupling constants $c_0 = c_2 = 1$ and $c_4 = 1/4$
  - Derrick's scaling argument $E_4 = E_2 + 3E_0$
- Skyrmions are local minima of E
- Found numerically by discretising E and applying a gradient descent method

Energy bound

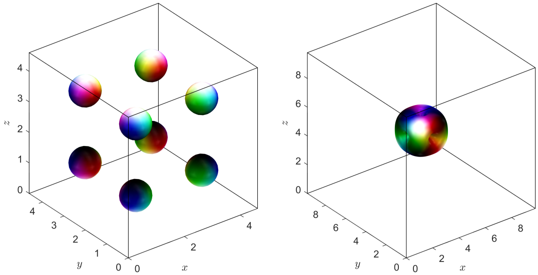
- Pion mass dependent topological energy bound (Harland, 2014)
- Want to find the strongest lower bound attainable
- Faddeev bound: $\alpha_2 E_2 + \alpha_4 E_4 \geq 12\pi^2 \alpha_2^{1/2} \alpha_4^{1/2} |B|$
- Lower bound: $\alpha_0 E_0 + \alpha_4 E_4 \geq \frac{512}{15}\sqrt{\pi}\Gamma^2(3/4)\alpha_0^{1/4}\alpha_4^{3/4}|B|$
- Split E into two terms and use the two above bounds to find a new topological energy bound:

  $$E \geq 12\pi^2 \alpha |B|, \quad \alpha = \sqrt{1-t} + \frac{2}{3\sqrt{\mu}} t^{3/4}$$

  where $\mu = \frac{225\pi^3}{4096 m \Gamma^2(3/4)}$ (Gudnason & Halcrow, 2022)
- $m = 0\,(\mu \to \infty)$ yields the familiar Faddeev bound $E \geq 12\pi^2 |B|$
- $m \to \infty\,(\mu = 0)$ gives the lower bound
- For all other μ the bound is stronger
- Bound maximised by $\frac{\mathrm{d}\alpha}{\mathrm{d}t} = 0 \to t = 1 - \frac{\mu^2}{2}\left(\sqrt{1 + \frac{4}{\mu^2}} - 1\right)$
- Define

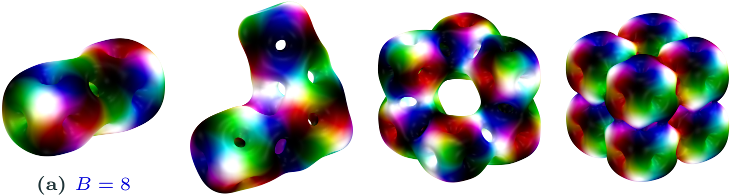
  $$E_{\text{bound}} = \frac{E}{12\pi^2 \alpha |B|}$$

History of Skyrme crystals



(a) Half-Skyrmions lattice **(b)** α-particle

- SC crystal of Skyrmions (Klebanov, 1985)
- BCC crystal of half Skyrmions (Goldhaber & Manton, 1987)
- SC crystal of half Skyrmions (Kugler & Shtrikman, 1988; Castillejo *et al.*, 1989)
- Building Skyrmions from the α-particle (Battye *et al.*, 2007)
- Massless (Silva Lobo, 2010) and massive (Adam *et al.*, 2022) phase transition between α-particle and SC crystal of half Skyrmions
- Constructing Skyrmions from crystal chunks (Feist *et al.*, 2013)
- Phase transitions between different crystals (Perapechka & Shnir, 2017)



(a) $B = 8$ **(b)** $B = 12$ **(c)** $B = 24$ **(d)** $B = 32$

Figure 2: Skyrmions constructed from the α-particle

(a) Constructed from two twisted α-particles (Battye *et al.*, 2007)
(b) Constructed from three twisted α-particles (Battye *et al.*, 2007)
(c) Constructed from six twisted α-particles (Feist *et al.*, 2013)
(b) Constructed from eight α-particles (Battye *et al.*, 2007)

Variational problem

- Skyrme crystals are maps

$$\varphi : \mathbb{R}^3/\Lambda \to \mathrm{SU}(2), \quad \Lambda = \{n_1\mathbf{X}_1 + n_2\mathbf{X}_2 + n_3\mathbf{X}_3 : n_i \in \mathbb{Z}\}$$

- General idea (Speight, 2014): identify $(\mathbb{R}^3/\Lambda, \bar{g}) \longleftrightarrow (\mathbb{R}^3/\mathbb{Z}^3, g)$ via the diffeomorphism $F : \mathbb{T}^3 \to \mathbb{R}^3/\Lambda$ where $\mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$ and $F(\mathbf{x}) = \mathcal{A}\mathbf{x}, \mathcal{A} = [\mathbf{X}_1\, \mathbf{X}_2\, \mathbf{X}_3]$
- Fix Skyrme field to be the map $\varphi : \mathbb{T}^3 \to \mathrm{SU}(2)$
- Metric on $\mathbb{T}^3$ is the pullback $g = F^*\bar{g}$, with $g_{ij} = \mathbf{X}_i \cdot \mathbf{X}_j$
- Vary metric g_s with $g_0 = F^*\bar{g} \iff$ vary lattice Λ_s with $\Lambda_0 = \Lambda$
- Energy minimized over all variations of $g \iff$ optimal period lattice Λ

Variational problem

- Let SPD_n be the space of symmetric positive-definite $n \times n$-matrices.
- For fixed φ, can consider the Skyrme energy to be a map $E : \mathrm{SPD}_3 \to \mathbb{R}$
- E is convex when restricted to geodesics $\Rightarrow$ uniqueness of the lattice
- Simple case: $\Lambda = L\mathbb{Z}^3$, energy scales as $E = LE_2 + \frac{1}{L}E_4 + L^3 E_0$ and

$$\frac{\mathrm{d}E}{\mathrm{d}L} = 0 \quad \Rightarrow \quad L^2 = \frac{1}{2}\left(-\frac{E_2}{3E_0} + \sqrt{\left(\frac{E_2}{3E_0}\right)^2 + \frac{4E_4}{3E_0}}\right)$$

- In general, optimal period lattice Λ:
  - ◇ Massless pions: explicit solution
    - ↬ Matrix square root
  - ◇ Massive pions: numerical solution
    - ↬ Arrested Newton flow or nonlinear conjugate gradient descent

Matrix square root

- Massless case $V(\varphi) = 0$ reduces the problem to
$$\left(\frac{g\mathcal{K}}{\sqrt{\det g}}\right)^2 = \frac{c_2}{c_4}\mathcal{L}\mathcal{K},$$
where, in sigma model notation,
$$\mathcal{L}_{ij} = \int_\Sigma (\partial_i \pi \cdot \partial_j \pi)\,\mathrm{vol}_g$$
and
$$\mathcal{K}^{ij} = \varepsilon^{iab}\varepsilon^{jcd}\int_\Sigma \{(\partial_a\pi\cdot\partial_c\pi)(\partial_b\pi\cdot\partial_d\pi) - (\partial_a\pi\cdot\partial_d\pi)(\partial_b\pi\cdot\partial_c\pi)\}\,\mathrm{vol}_g$$
- Matrix square root:
$$\frac{g\mathcal{K}}{\sqrt{\det g}} = PD^{1/2}P^{-1}, \quad D^{1/2} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & 0 \\ 0 & \sqrt{\lambda_2} & 0 \\ 0 & 0 & \sqrt{\lambda_3} \end{pmatrix}$$
- Setting $\tilde{g} = \frac{g}{\sqrt{\det g}}$ yields $\tilde{g} = PD^{1/2}P^{-1}\mathcal{K}^{-1}$
- Finally, using the fact that $\det g = \frac{1}{(\det \tilde{g})^2}$, we arrive at $g = \frac{\tilde{g}}{\det \tilde{g}}$.

Numerical approach to the lattice

- Aim: solve the unconstrained optimisation problem

$$\min_{g \in \mathrm{SPD}_3} E(g)$$

- Accelerated 2nd order gradient descent with flow arresting
- Solve Newton's equations of motion for a particle on SPD_3 with potential energy $E(g)$ using 4th order Runge–Kutta:

$$\partial_{ss} g_s|_{s=0} = -\left.\frac{\delta E}{\delta g_s}\right|_{s=0}, \quad g_0 = g$$

- Restart flow if $E(t+\delta t) > E(t)$ (arresting)
- Terminate flow when $\left.\frac{\delta E}{\delta g_s}\right|_{s=0} < 10^{-5}$ everywhere

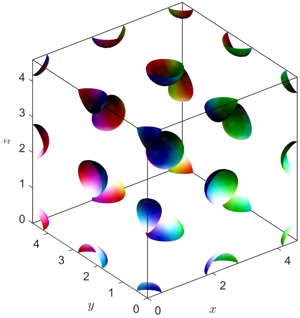


Figure 3: Massless FFC lattice (Kugler & Shtrikman, 1988) and (Castillejo *et al.*, 1989)

- Obtained from Fourier series expansion initial configuration (Castillejo *et al.*, 1989)

$$\sigma = -c_1 c_2 c_3, \quad \pi^1 = s_1 \sqrt{1 - \frac{s_2^2}{2} - \frac{s_3^2}{2} + \frac{s_2^2 s_3^2}{3}}$$

and cyclic, where $c_i = \cos\left(\frac{2\pi x^i}{L}\right)$ and $s_i = \sin\left(\frac{2\pi x^i}{L}\right)$

- Symmetries (Kugler & Shtrikman, 1989):

$$A_1 : (x, y, z) \mapsto (-x, y, z)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (\sigma, -\pi^1, \pi^2, \pi^3)$$
$$A_2 : (x, y, z) \mapsto (y, z, x)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (\sigma, \pi^2, \pi^3, \pi^1)$$
$$C_3 : (x, y, z) \mapsto (x, z, -y)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (\sigma, \pi^1, \pi^3, -\pi^2)$$
$$D_4 : (x, y, z) \mapsto (x + L/2, y, z)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (-\sigma, -\pi^1, \pi^2, \pi^3)$$

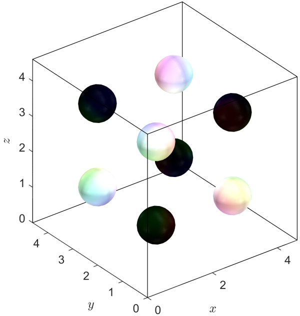


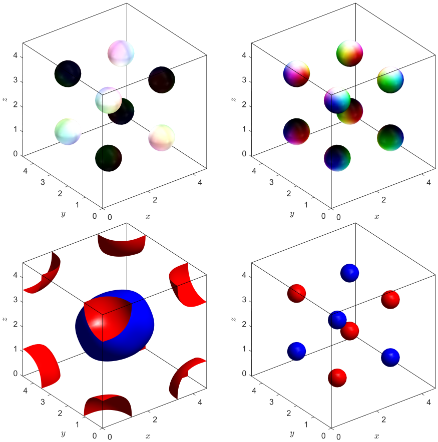
Figure 4: Massless α-particle lattice

- Obtained from $B = 4$ rational map initial configuration (Houghton *et al.*, 1997)

$$R(z) = \frac{z^4 + 2\sqrt{3}iz^2 + 1}{z^4 - 2\sqrt{3}iz^2 + 1}$$

- Symmetries (so far):

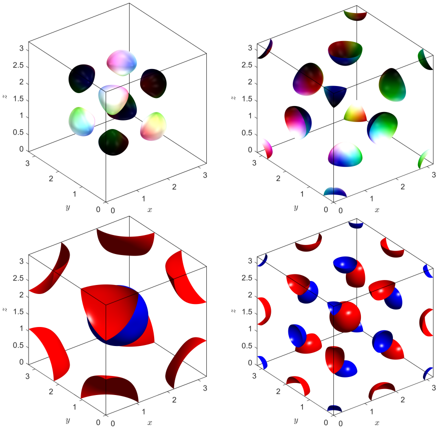
$$E_1 : (x, y, z) \mapsto (-x, y, z)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (\sigma, \pi^1, \pi^2, -\pi^3)$$
$$E_2 : (x, y, z) \mapsto (x + L/2, y + L/2, z + L/2)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (-\sigma, -\pi^1, -\pi^2, -\pi^3)$$
$$E_3 : (x, y, z) \mapsto (-y, x, z)$$
$$(\sigma, \pi^1, \pi^2, \pi^3) \mapsto (\sigma, \pi^1, -\pi^2, -\pi^3)$$



(a) α-lattice **(b)** FCC lattice

Figure 5: Skyrme crystals for $m = 0$. Top row are the isobaryon plots for level set $\mathcal{B} = 0.01$. Bottom row are isosigma plots, where red corresponds to the level set $\sigma = 0.8$ and blue to the level set $\sigma = -0.8$.

Massive Skyrme crystals



(a) α-lattice **(b)** FCC lattice

Figure 6: Skyrme crystals for $m = 1$. Top row are the isobaryon plots for level set $\mathcal{B} = 0.01$. Bottom row are isosigma plots, where red corresponds to the level set $\sigma = 0.8$ and blue to the level set $\sigma = -0.8$.

Isospin quantization

- Collective coordinate quantization of isospin d.o.f. (Adkins *et al.*, 1983)

$$\varphi(x) \mapsto \hat{\varphi}(x,t) = A(t)\varphi(x)A^\dagger(t).$$

  Isorotations are symmetries of E so these configurations are all energy-degenerate.
- Isorotational angular velocity is $\omega_j = -i\,\mathrm{Tr}(\tau^j A^\dagger \dot{A})$
- Maurer-Cartan form transforms as

$$\hat{L}_\mu = \hat{\varphi}^\dagger \partial_\mu \hat{\varphi} = \begin{cases} A\omega_i T_i A^\dagger, & \mu = 0 \\ A L_i A^\dagger, & \mu = i = 1,2,3. \end{cases}$$

- $T_i = \frac{i}{2}\varphi^\dagger[\tau^i, \varphi]$ is also an $\mathfrak{su}(2)$ current
- Effective Lagrangian on restricted space of configurations is $L_{\text{eff}} = L_{\text{rot}} - M_B$, where

$$L_{\text{rot}} = \frac{1}{2}\omega_i U_{ij}\omega_j$$

  and the isospin moment of inertia is

$$U_{ij} = -\int_\Sigma \mathrm{Tr}\left(c_2 T_i T_j + c_4 g^{ab}[L_a, T_i][L_b, T_j]\right)\mathrm{vol}_g$$

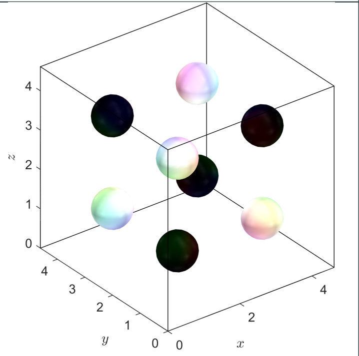
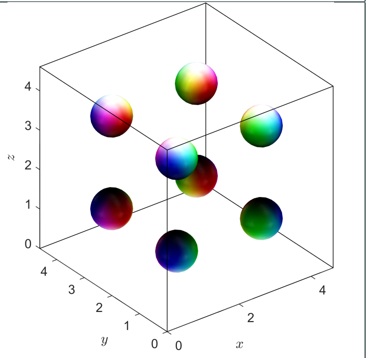
α-lattice	FCC lattice
	
$E^{\alpha} = 1.0378$	$E^{\mathrm{FCC}} = 1.0378$
$U^{\alpha} = \begin{pmatrix} 238.6 & 0 & 0 \\ 0 & 238.6 & 0 \\ 0 & 0 & 297.9 \end{pmatrix}$	$U^{\mathrm{FCC}} = \begin{pmatrix} 297.9 & 0 & 0 \\ 0 & 297.9 & 0 \\ 0 & 0 & 297.9 \end{pmatrix}$

Table 1: Comparison of the massive ($m = 0$) α-lattice and FCC lattice

Massive Skyrme crystals

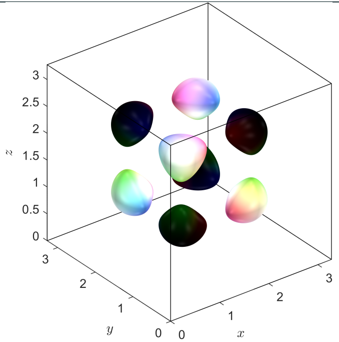
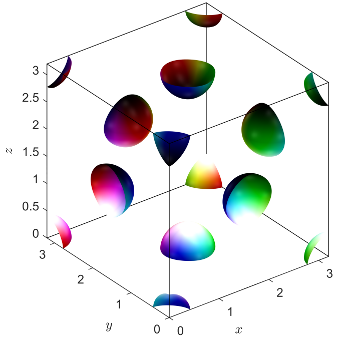
α-lattice	FCC lattice
	
$E^{\alpha} = 1.0631$	$E^{\text{FCC}} = 1.0673$
$U^{\alpha} = \begin{pmatrix} 135.5 & 0 & 0 \\ 0 & 135.5 & 0 \\ 0 & 0 & 167.3 \end{pmatrix}$	$U^{\text{FCC}} = \begin{pmatrix} 165.2 & 0 & 0 \\ 0 & 165.2 & 0 \\ 0 & 0 & 165.2 \end{pmatrix}$

Table 2: Comparison of the massive ($m = 1$) α-lattice and FCC lattice

Comparison of the α-lattice and the FCC lattice

m	E^{α}	E^{FCC}	ΔE
0	1.0378	1.0378	0%
1	1.0631	1.0673	0.4%
3	1.0710	1.0797	0.8%
5	1.0715	1.0816	0.9%
10	1.0710	1.0824	1.1%

Table 3: Comparison of the α-lattice and FCC lattice for various m

- Massless FCC and α-lattice:
  - Energy degenerate
  - Isospin tensor shares common eigenvalue

  $\Rightarrow$ Related by SO(4)-isospin transformation:

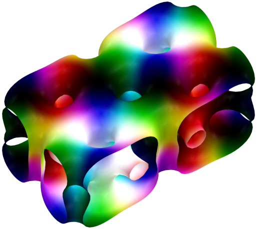
$$Q\pi^{\alpha} = \pi^{\mathrm{FCC}}, \quad Q = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1/\sqrt{3} & -1/\sqrt{6} & 1/\sqrt{2} & 0 \\ 1/\sqrt{3} & -1/\sqrt{6} & -1/\sqrt{2} & 0 \\ 1/\sqrt{3} & 2/\sqrt{6} & 0 & 0 \end{pmatrix}$$

- Massive FCC and α-lattice:
  - Energy is not invariant under SO(4) action

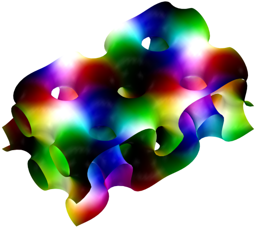
  $\Rightarrow$ α-lattice is the lower energy crystal

Open problems

- What happens when we consider quantum corrections from the isospin d.o.f.? (Adam *et al.*, 2022)
- Crystal energy bound appears to increase with $m \Rightarrow$ lower binding energies for higher m?
- Use lots of random ICs for field and/or lattice to find other (new) crystals, similar to that of (Gudnason & Halcrow, 2022)
- (Gudnason & Halcrow, 2022) find massive Skyrmions with multi-layer graphene structure $\Rightarrow$ stable massive graphene multi-sheets?



(a) In-phase



(b) Out-of-phase

Figure 7: Massive 2-layer graphene sheets