Phase transition threshold and stability of magnetic skyrmions

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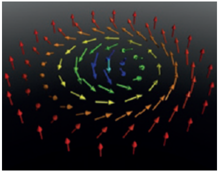
Figure: Ikkei Shimizu

Magnetic skyrmion



Schematic image of Skyrmions. (**From: Melcher, Preceedings of the Royal Society (2014)**)

Nontrivial homotopy class as $\mathbb{R}^2 \to \mathbb{S}^2$.

- **Magnetic skyrmion**: vortex-like structure appearing in magnetic materials ($\sim 100\text{nm}$)
- Stabilization due to non-trivial topology
- Application to future magnetic storage is expected.

Toward understanding the mechanism

- **Micromagnetism** (Landau-Lifshitz 1935):
  Consider the magnetic material as a collection of small magnets, and describe large scale magnetism via interaction of each magnets
- Equilibrium state: (local) minimizer of Landau-Lifshitz energy:

$$E[\mathbf{n}] := (D[\mathbf{n}] + E_{\text{other}}[\mathbf{n}]), \qquad \mathbf{n} : \mathbb{R}^2 \to \mathbb{S}^2.$$

- $\mathbf{n}$: magnetization
- $D[\mathbf{n}] := \frac{1}{2}\int_{\mathbb{R}^2} |\nabla \mathbf{n}|^2 dx$; Exchange interaction energy
- $E_{\text{other}}[\mathbf{n}]$; Other effect (external fields, crystalline structure, etc...)
- Scale: Atomic level $\ll$ Micromagnetics $\ll$ Crystalline lattice
  $\ll 1\text{nm}$ $\sim 100\text{nm}$

Dzyaloshinskii-Moriya interaction

- Skyrmions are observed in the material with Dzyaloshinskii-Moriya interaction:

$$E[\mathbf{n}] := D[\mathbf{n}] + rH[\mathbf{n}] + V[\mathbf{n}], \qquad (r > 0)$$

- Helicity functional (Dzyaloshinskii-Moriya interaction)

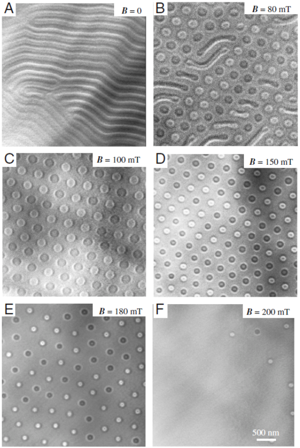
$$H[\mathbf{n}] := \int_{\mathbb{R}^2} (\mathbf{n} - \mathbf{e}_3) \cdot \nabla \times \mathbf{n}\, dx.$$

where

$$\tilde{H}[\mathbf{n}] := \int_{\mathbb{R}^2} \mathbf{n} \cdot \nabla \times \mathbf{n} dx, \qquad \nabla \times \mathbf{n} = \begin{pmatrix} \partial_2 n_3 \\ -\partial_1 n_3 \\ \partial_1 n_2 - \partial_2 n_1 \end{pmatrix}$$

- Potential energy:

$$V[\mathbf{n}] = \frac{1}{2} \int_{\mathbb{R}^2} (1 - n_3)^2 dx, \qquad \mathbf{e}_3 := {}^t(0, 0, 1).$$



The picture of observed magnetization (From: Yu et al., Proc. Natl Acad. Sci. USA 109 (2012))

By experiments, we can observe

- skyrmions when the external field is strong
- helix when the external field is weak

(Occurrence of **phase transition**)

Problem

Can we explain the above phenomena via the Landau-Lifshitz energy?

Setting

$$E[\mathbf{n}] := D[\mathbf{n}] + rH[\mathbf{n}] + V[\mathbf{n}], \qquad (2 \le p \le 4,\ r > 0)$$

- Strong potential energy $\Longleftrightarrow$ Small r.
- Function space:

$$\mathcal{M} := \{\mathbf{n} : \mathbb{R}^2 \to \mathbb{R}^3 \mid |\mathbf{n}|^2 \equiv 1, \quad D[\mathbf{n}] + V[\mathbf{n}] < \infty\}.$$

  ($H[\mathbf{n}]$ is well-defined on $\mathcal{M}$.)
- Topological degree:

$$Q[\mathbf{n}] := \frac{1}{4\pi} \int_{\mathbb{R}^2} \mathbf{n} \cdot \partial_1 \mathbf{n} \times \partial_2 \mathbf{n} dx.$$

  ($\mathbf{n} \in \mathcal{M}_p \Longrightarrow Q[\mathbf{n}]$ is well-defined, $Q[\mathbf{n}] \in \mathbb{Z}$.)
- We restrict ourselves to $Q = -1$. (single skyrmion)

Known results

(Including related energy)

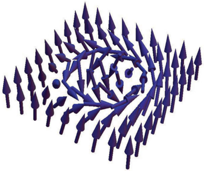
- Existence of minimizer [Melcher 2014], [Döring-Melcher 2017]
- Stability of critical point [Li-Melcher 2018]
- Quantitative analysis of minimizers [Gustafson-Wang 2021]
- Geometric analysis [Barton-Singer-Ross-Schroer 2020]
- Local well-posedness of related dynamical PDEs [Shimizu 2022]

Theorem([DM 2017], [BSRS 2020])

When $r < 1$, then

- $\min\limits_{\substack{\mathbf{n}\in\mathcal{M}_4 \\ Q[\mathbf{n}]=-1}} E_4[\mathbf{n}] = 4\pi(1-2r^2)$
- Minimizing set $\supset \{\mathbf{h}^{2r}(\cdot - a) \mid a \in \mathbb{R}^2\}$, where

$$\mathbf{h}(x) := \left(\frac{-2x_2}{1+|x|^2}, \frac{2x_1}{1+|x|^2}, -\frac{1-|x|^2}{1+|x|^2}\right), \quad \mathbf{h}^{2r}(x) := \mathbf{h}\left(\frac{x}{2r}\right).$$



Schematic graph of $\mathbf{h}$. (**From: Melcher, Preceedings of the Royal Society (2014)**)

- When $r < 1$ (strong potential case), the theorem succeeds in explaining the formation of one Skyrmion under the restriction $Q[\mathbf{n}] = -1$.

The Mechanism behind Theorem

- Key identity:

$$E[\mathbf{n}] = \frac{r^2}{2}\int_{\mathbb{R}^2} |\mathcal{D}_1^r\mathbf{n} + \mathbf{n}\times\mathcal{D}_2^r\mathbf{n}|^2 dx + (1-r^2)D[\mathbf{n}] + 4\pi Q[\mathbf{n}].$$

where

$$\mathcal{D}_j^r\mathbf{n} := \partial_j\mathbf{n} - \frac{1}{r}\mathbf{e}_j\times\mathbf{n}. \qquad \text{(helical derivative)}$$

- When $r < 1$,

$\mathbf{n}$:minimizer

$$\Longleftarrow \quad \mathcal{D}_1^r\mathbf{n} + \mathbf{n}\times\mathcal{D}_2^r\mathbf{n} = 0 \quad \text{and} \quad \min_{\substack{\mathbf{n}\in\mathcal{M}_4\\ Q[\mathbf{n}]=-1}} D[\mathbf{n}] \quad \text{attains}$$

$$\Longleftarrow \quad \{\mathbf{h}^{2r}(\cdot - a) \mid a\in\mathbb{R}\}.$$

Problems

Question.

What happens when $r > 1$?

- No result in this regime.

Premise Proposition

For all $r > 0$, $\mathbf{h}^{2r}$ is a critical point of E_4.

Question

Is $\mathbf{h}^{2r}$ a local minimizer?

- When $r \leq 1$, then the answer is True by [DM 2017], [BSRS 2020] (global minimizer in fact.)
- When $r > 1$, the question has been open.

Main theorem 1 (Linear instability)

Main theorem (Linear instability)

If $r > 1$, then $\mathbf{h}^{2r}$ is linearly unstable; $\forall$ neighborhood of $\mathbf{h}^{2r}$, $\exists \mathbf{n} \in \mathcal{M}$ s.t.

$$E[\mathbf{n}] - E[\mathbf{h}^{2r}] < 0.$$

- This mathematically explains phase transition; the stability of skyrmions breaks down when the external field is weak.
- The threshold is quantified at $r = 1$.

Main theorem 2 (Unboundedness)

We further showed

Main theorem 2 (Unboundedness)

If $r > 1$, then

$$\inf_{\substack{\mathbf{n}\in\mathcal{M}\\ Q=-1}} E[\mathbf{n}] = -\infty.$$

- The counterexample is constructed by 1-helix. (Consistent with experiment)
- The unboundedness of energy is due to the unboundedness of domain.

Outline of proof

Outline of proof of Theorem 1.

- We follow the argument of [Li-Melcher 2018].
- It suffices to show that the Hessian $\mathcal{H}_r$ is not non-negative definite if $r > 1$.
- (ρ, ψ): polar coord. of $x \in \mathbb{R}^2$.
  $\to$ Apply Fourier expansion w.r.t. ψ
  $\to$ The Hessian is decomposed into $\mathcal{H}_k^r$ (k: Fourier mode)
- We can show that $\mathcal{H}_3^r$ is not non-negative definite.
  (We can also show that
  - $\mathcal{H}_k^r$ $(k \geq 2)$ is non-negative definite for large r.
  - $\mathcal{H}_0^r$, $\mathcal{H}_1^r$ is always non-negative definite.)

Hessian

- For $\mathbf{n} \in \mathcal{M}_4$ with $Q[\mathbf{n}] = -1$, we write

$$\mathbf{n} = \mathbf{h}^{2r} + \phi.$$

- Then

$$E_4[\mathbf{n}] - E_4[\mathbf{h}^{2r}] = \frac{1}{2}\langle \mathcal{L}\phi, \phi \rangle_{L^2}$$

where

$$\mathcal{L}\phi := -\Delta\phi + 2r\nabla \times \phi + \phi_3 \mathbf{e}_3 - \Lambda(\mathbf{h}^{2r})\phi,$$

$$\Lambda(\mathbf{h}^{2r}) := |\nabla \mathbf{h}^{2r}|^2 + 2r\mathbf{h}^{2r} \cdot (\nabla \times \mathbf{h}^{2r}) - (1 - h_3^{2r})h_3^{2r} \in \mathbb{R}.$$

- By linearization, we may suppose $\phi(x) \in T_{\mathbf{h}^{2r}(x)}\mathbb{S}^2$ for every $x \in \mathbb{R}^2$.

The Hessian

$$\langle \mathcal{L}\phi, \phi \rangle, \qquad \phi : \mathbb{R}^2 \to \mathbb{R}^3 \qquad \phi(x) \perp \mathbf{h}^{2r}(x).$$

- Several transforms
  - Rescaling: $\phi \to$
  - Orthonormal frame $\{\mathbf{J}_1, \mathbf{J}_2\} \subset T_{\mathbf{h}^{2r}}\mathbb{S}^2$, and write

$$\phi = u_1\mathbf{J}_1 + u_2\mathbf{J}_2, \qquad u_j : \mathbb{R}^2 \to \mathbb{R}$$

  - Let (ρ, ψ): polar coord. of $\mathbb{R}^2$ & Fourier transform w.r.t. ψ:

$$u_j(\rho, \psi) = \alpha_j^{(0)}(\rho) + \sum_{k=1}^{\infty} \left(\alpha_j^{(k)}(\rho)\cos(k\psi) + \beta_j^{(k)}(\rho)\sin(k\psi) \right).$$

$$\langle \mathcal{L}\phi, \phi \rangle_{L^2} = 2\pi \mathcal{H}_0^r(\alpha_1^{(0)}, \alpha_2^{(0)}) + \pi \sum_{k=1}^{\infty} \left(\mathcal{H}_k^r(\alpha_1^{(k)}, \beta_2^{(k)}) + \mathcal{H}_k^r(\beta_1^{(k)}, -\alpha_2^{(k)}) \right).$$

$$\langle \mathcal{L}\phi, \phi\rangle_{L^2} = 2\pi \mathcal{H}_0^r(\alpha_1^{(0)}, \alpha_2^{(0)}) + \pi \sum_{k=1}^{\infty} \left(\mathcal{H}_k^r(\alpha_1^{(k)}, \beta_2^{(k)}) + \mathcal{H}_k^r(\beta_1^{(k)}, -\alpha_2^{(k)}) \right).$$

with

$$\begin{aligned} &\mathcal{H}_k^r[\alpha, \beta] \\ &= \int_0^\infty \Big[(\alpha')^2 + (\beta')^2 + \left(\frac{k^2}{\rho^2} - (\theta'(\rho))^2 + \frac{\cos^2\theta(\rho)}{\rho^2} + \frac{4r^2 \sin\theta(\rho)}{\rho} \right) (\alpha^2 + \beta^2) \\ &\qquad + 4k \left(\frac{\cos\theta(\rho)}{\rho^2} - \frac{2r^2 \sin\theta(\rho)}{\rho} \alpha\beta \right) \Big] \rho d\rho. \end{aligned}$$

where

- $\theta = \theta(\rho) : (0, \infty) \to \mathbb{R}$ is defined by

$$\sin\theta(\rho) = \frac{2\rho}{\rho^2 + 1}, \qquad \theta(0) = \pi, \qquad \theta(\infty) = 0.$$

Key Proposition

Key proposition (Instability at higher mode)

For $k \geq 2$, there exists $r_{k,c} \geq 1$ such that if $r > r_{k,c}$,

$$\exists \alpha, \beta \in C_0^\infty(0,\infty) \quad \text{s.t.} \quad \mathcal{H}_k^r[\alpha,\beta] < 0.$$

Moreover, if $k = 3$, then we can take $r_{3,c} = 1$.

- We can also show that $\mathcal{H}_0^r, \mathcal{H}_1^r \geq 0$ for $\forall \alpha, \beta \in C_0^\infty(0,\infty)$
- The same structure appears in Ginzburg-Landau energy. (cf. [Lamy-Zuniga 2022])

Proof of Key proposition

- Consider scaling limit:

$$\mathcal{I}_k^r[\xi] := \lim_{\lambda \to 0+} \mathcal{H}_k^r\left[\frac{\sin\theta}{\rho}\xi_\lambda, \frac{\sin\theta}{\rho}\xi_\lambda\right], \qquad \xi_\lambda(\rho) = \frac{1}{\lambda^2}\xi(\lambda\rho).$$

Then

$$\mathcal{I}_k^r[\xi] = \int_0^\infty \left[\frac{8}{\rho^3}(\xi')^2 - \frac{8(k-1)(8r^2-k-3)}{\rho^5}\xi^2\right] d\rho.$$

- It is known that:

Fact. (Hardy-Littlewood-Polya 1941)

$$\inf_{\xi \in C_0^\infty(0,\infty)\setminus\{0\}} \frac{\int_0^\infty \frac{(\xi')^2}{\rho^3} d\rho}{\int_0^\infty \frac{\xi^2}{\rho^5} d\rho} = 4.$$

- For all $\varepsilon > 0$, there exists $\xi_\varepsilon \in C_0^\infty(0,\infty)$ s.t.

$$\int_0^\infty \frac{\xi_\varepsilon^2}{\rho^5} d\rho > \frac{1}{4+\varepsilon} \int_0^\infty \frac{(\xi_\varepsilon')^2}{\rho^3} d\rho.$$

Thus

$$\mathcal{I}_k^r[\xi_\varepsilon] < 8[4 + \varepsilon - (k-1)(8r^2 - k - 3)] \int_0^\infty \frac{\xi_\varepsilon^2}{\rho^5} d\rho.$$

- If $k \geq 2$, RHS < 0 for large r.
- If $k = 3$,

$$8[4 + \varepsilon - (k-1)(8r^2 - k - 3)] = 128 \left(1 - r^2 + \frac{\varepsilon}{16}\right).$$

For $r > 1$, we have RHS < 0 if $\varepsilon \ll 1$.

Proof of Theorem 2

If $r > 1$, then
$$\inf_{\substack{\mathbf{n}\in\mathcal{M}\\ Q=-1}} E[\mathbf{n}] = -\infty.$$

- **Key ingredient**: 1-helix

$$\mathbf{b}(x) := \mathbf{h}^{1/r}(x_1, 0) = {}^t\left(0, \frac{2rx_1}{r^2(x_1)^2+1}, \frac{r^2(x_1)^2-1}{r^2(x_1)^2+1}\right).$$

- We have

$$\text{Integrand of E} = \frac{2(1-r^2)}{(r^2x_1^2+1)^2}.$$

In particular, $E[\mathbf{b}] = -\infty$ if $r > 1$.

- To construct counterexample in $\mathcal{M}$, we use $\mathbf{h}^{1/r}$, and stretch the x_1-axis in x_2-direction.

Future study: Critical case: $r = 1$

When $r = 1$,

$$\mathbf{n}: \text{ minimizer} \quad \Longleftrightarrow \quad \mathcal{D}_1^r \mathbf{n} + \mathbf{n} \times \mathcal{D}_2^r \mathbf{n} = 0. \qquad (*)$$

Theorem. [Barton-Singer-Ross-Schroer 2020]

Let

$$v := \frac{1 + n_3}{n_1 + in_2} \qquad \text{(Inverse of stereographic coord.)}.$$

Then,

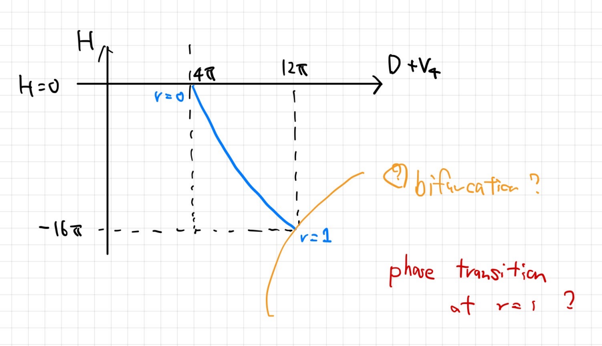
$$(*) \overset{\text{Formally}}{\Longleftrightarrow} \quad \partial_{\overline{z}} v = -\frac{i}{2} r \quad (z := x + iy)$$

$$\Longleftrightarrow \quad v = -\frac{i}{2} r \overline{z} + f(z) \quad (f: \text{holomorphic}).$$

$$\{(*)\} = \{v = -\frac{i}{2} r\bar{z} + f(z)\}$$

Open. (Future work)

- Rigorous argument?
- $\mathcal{M}_4 \cap \{(*)\} = ?$



Thank you for listening