Skyrmions in 2D & 3D Magnets with Broken Bulk & Surface Inversion Symmetry

Mohit Randeria
Ohio State University

Skyrmionics
Santa Fe, August 2017
* Banerjee, Erten & MR,
  Nature Physics 9, 626 (2013)

* Banerjee, Rowland, Erten & MR,

* Rowland, Banerjee & MR,
  Phys. Rev. B 93, 020404(R) (2016)

* Wu, Rowland, Kao & MR [unpublished]

* Ahmed, Rowland, Dunsiger, Esser,
  McComb, MR & Kawakami;
  arXiv:1706.08248
Outline:

- Introduction

- Skyrmions in 2D vs. 3D
  * T=0 phase diagram & role of anisotropy

- Finite temperature Monte Carlo
  * (T,H) phase diagram in 2D

- Rashba & Dresselhaus DMI
  * Broken bulk vs. surface/mirror inversion

- Conclusions
Skyrmions: topological spin textures in chiral magnets

MnSi – SANS
FeCoSi – Lorentz TEM

Mühlbauer et al, Science 323, 915 (2009)


Berry Phase
→ Topological Hall Effect

Pfleiderer & Rosch.

FeGe
Tc = 278K

Z. Yu et. al.,
Nature Mat 10, 106 (2011)

decreasing thickness
Chiral Magnetic Materials

- **Ferromagnetic Exchange**  \(-J \mathbf{S}_i \cdot \mathbf{S}_j\)

- **Chiral DM interaction** (Dzyaloshinskii-Moriya)
  \[ \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \]

**Material constraints for DM:**

1. **Broken Inversion Symmetry** \(\rightarrow\) direction of \(\mathbf{D}\)
2. **Spin-orbit coupling (SOC)** \(\rightarrow\) magnitude of \(\mathbf{D}\)

**Broken Bulk Inversion:** Non-centrosymmetric crystals (MnSi, FeGe, Cu$_2$OSeO$_3$, ...)

**Broken Mirror symmetry:** polar crystals (GaV$_4$S$_8$, ...)

**Broken Surface inversion:** Magnetic multilayers, interfaces & thin films
FM exchange + DMI $\rightarrow$ Spin textures

- **Ferromagnetic Exchange**
  \[-J \mathbf{S}_i \cdot \mathbf{S}_j\]
  \[\sim -J \cos \theta \sim J \theta^2\]

- **DM interaction**
  \[\mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \sim D \sin \theta \sim D \theta\]

\[E(\theta) = J\theta^2/2 - D\theta\]

\[\theta^* = \frac{D}{J}\]

\[E^* \approx D^2/J \sim H_c\]

Spontaneous spin textures
Spirals & Skyrmions

Length scale
\[\sim 1 - 10^3 \text{ nm}\]

Energy scales
\[T_c \sim J\]

Energy scales
\[E^* = D^2/J \sim H_c\]
Skyrmion: Topological spin texture in magnetization \( M(r) = M \hat{m}(r) \)

Skyrmion Crystal (SkX)

“Winding Number” on unit sphere in spin-space

\[
N_{sk} = \frac{1}{4\pi} \int d^2r \ \hat{m} \cdot (\partial_x \hat{m} \times \partial_y \hat{m}) = 0, \pm 1, \pm 2, \ldots
\]

Topological Invariant

\[
\pi_2(S^2) = \mathbb{Z}
\]
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Choosing scales for Length $(J/D)a$ & Energy $D^2/J$

\[ \Rightarrow \text{Two dimensionless parameters} \]
\[ K J / D^2 \text{ and } H J / D^2 \]

Phase Diagram of Chiral Magnets

- $T = 0 \rightarrow$ Minimize Energy
  - $\text{FM} \rightarrow J$
  - $\text{DMI} \rightarrow D$
  - $\text{Anisotropy} \rightarrow + K m_z^2$
  - $\text{Field} \rightarrow - H m_z$

- $3D$ system: Bulk samples

- $2D$ systems: thickness $\ll J/D \ (a = 1)$

Continuum Field Theory (discretized for numerics)
- Analytical Variational calculation at $T=0$
- Numerical Conjugate gradient minimization at $T=0$
- $T > 0$ Monte Carlo (later in talk)
3D Phase Diagram with Broken Bulk Inversion

Hexagonal Crystal of Vortex-like or Bloch skyrmions

Helical or Bloch Spiral

Wilson, Butenko, Bogdanov & Monchesky, PRB 89, 094411 (2014)
2D vs. 3D Phase Diagram

In 2D
* Skyrmion phase greatly enhanced
* Importance of easy-plane anisotropy
* No Cone phase

Banerjee, Rowland, Erten & MR, PRX (2014)
Rowland, Banerjee & MR, PRB (2016)

Square Lattice, see also: Lin, Saxena & Batista, (2015)
All spins up at the u.c. boundary \( \rightarrow \) Skyrmions can exist as isolated excitations in a uniform FM 

\[ KJ/D^2 = 0 \]

\[ HJ/D^2 = 0.7 \]

\[ n_{sk}(r) = \frac{1}{4\pi} \hat{m} \cdot (\partial_x \hat{m} \times \partial_y \hat{m}) \]

\[ N_{sk} = \int d^2r \ n_{sk}(r) = -1 \]

\[ \pi_2(S^2) = \mathbb{Z} \]

Real space \( \rightarrow \) Spin space \( S^2 \)
Evolution of spin-textures in 2D from $H > 2K \rightarrow H < 2K$

$HJ/D^2 = 0.7$

$KJ/D^2 = 0$
Evolution of spin-textures in 2D from $H > 2K \rightarrow H < 2K$

$HJ/D^2 = 0.7$

$KJ/D^2 = 0$

$KJ/D^2 = 0.6$
Evolution of spin-textures in 2D from $H > 2K \rightarrow H < 2K$

- $HJ/D^2 = 0.7$
- $KJ/D^2 = 0$
- $KJ/D^2 = 0.6$
- $KJ/D^2 = 1.2$

Skyrmion Density For $H < 2K$

- Not isolated at center
- Changes sign!
Is the “topological” charge quantized for $H < 2K$?

Spins on u.c. boundary are not all up!
Only p.b.c.’s

Cannot isolate texture in a FM background

Cannot use homotopy to get quantization

Unit cell $T^2 \rightarrow$ Spin space $S^2$

Chern Number
cf. Thouless et al. (TKNN)

$$n_{sk}(\mathbf{r}) = \frac{1}{4\pi} \hat{m} \cdot (\partial_x \hat{m} \times \partial_y \hat{m})$$

$$N_{sk} = \int_{\text{unit cell}} d^2 \mathbf{r} \ n_{sk}(\mathbf{r})$$

$N_{sk} \in \mathbb{Z}$
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**Symmetry → DMI**  \[ D_{ij} \cdot (S_i \times S_j) \]

- **broken bulk inversion**  \[ \vec{r} \not\mapsto - \vec{r} \]
  \[ \hat{D}^D_{ij} = \hat{r}_{ij} \]
  \[ \text{GL Free Energy} = -D_D \hat{m} \cdot (\nabla \times \hat{m}) \]

- **broken surface or mirror inversion**  \[ \vec{z} \not\mapsto - \vec{z} \]
  \[ \hat{D}^R_{ij} = \hat{z} \times \hat{r}_{ij} \]
  \[ \text{GL Free Energy} = -D_R \hat{m} \cdot [(\hat{z} \times \nabla) \times \hat{m}] \]
Systems with both Dresselhaus and Rashba DMI

Energy = FM exchange
+ Dresselhaus DMI + Rashba DMI
+ Anisotropy + Field

T =0 Phase Diagram
Minimize Energy → Variational & Conjugate Gradient

3D system: Bulk or sample with thickness  \( \gg J/D \)

Materials:

• Single crystals with broken bulk inversion and mirror symmetries

• B20 Superlattices (MBE-grown CrGe/MnGe/FeG)

  Ahmed, Esser, Rowland, McComb & Kawakami,
  *J. Crystal Growth* 467, 38 (2017)
Systems with both Dresselhaus and Rashba DMI

\[ D_D = D \cos \beta \]
\[ D_R = D \sin \beta \]
\[ D = \sqrt{D_D^2 + D_R^2} \]

\[ \mathcal{F} [\hat{\mathbf{m}}(\mathbf{r})] = \frac{1}{2} |\nabla \hat{\mathbf{m}}|^2 \]
\[ + \cos \beta \ \hat{\mathbf{m}} \cdot (\nabla \times \hat{\mathbf{m}}) \]
\[ + \sin \beta \ \hat{\mathbf{m}} \cdot [(\mathbf{z} \times \nabla) \times \hat{\mathbf{m}}] \]
\[ + \left( \frac{AJ}{D^2} \right) m_z^2 \]
\[ - \left( \frac{HJ}{D^2} \right) m_z \]

\[ |\hat{\mathbf{m}}(\mathbf{r})| = 1 \]

For simplicity, mirror plane normal, anisotropy axis and Field all chosen in the z-direction
Evolution from Dresselhaus DMI $\rightarrow$ Rashba DMI

Dresselhaus limit

$D_R = D_D$

Rashba limit

Cone: $\mathbf{m}(z) \rightarrow$ gains energy only from $D_D$

Spiral: $\mathbf{m}(x) \rightarrow D = \sqrt{D_D^2 + D_R^2}$

Skyrmion: $\mathbf{m}(x, y)$

KJ/HJD² field

Polarized FM

Hex SkX

Circular cone

Spiral

KJ/D² anisotropy

Polarized FM

mₓ=1

Square SkX

Hex SkX
**Same Phase Diagram for**

* Rashba Limit in 3D and
* 2D Limit

* Rashba limit in 3D
  → No Cone Phase because no DM energy gained by z-axis “twist”

* 2D Chiral Magnet
  → No Cone Phase because spins cannot twist along z-axis

→ Same phase diagram in both cases with spin textures that have no z-dependence, i.e.

\[ \hat{\mathbf{m}} = \hat{\mathbf{m}}(x, y) \]
Evolution from Dresselhaus DMI $\rightarrow$ Rashba DMI

Dresselhaus limit

$D_R = D_D$

$KJ/D^2$

Vortex-like / Bloch

Hedgehog / Neel

Rashba limit
Evolution from Dresselhaus $\rightarrow$ Rashba DMI

Helical / Bloch spiral $\xrightarrow{\tan \beta = D_R / D_D} \rightarrow$ Cycloidal / Neel spiral

$D_R = 0$

$\hat{D}_{ij}^D = \hat{r}_{ij}$

$D_R = 0.5 D_D$

$D_R = 2.0 D_D$

$D_D = 0$

$\hat{D}_{ij}^R = \hat{z} \times \hat{r}_{ij}$

Vortex-like or Bloch

Hedgehog or Neel
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Enhanced stability of Skyrmions and Evolution of their properties

- 2D vs. 3D
- 3D
  * broken surface/mirror inversion
  * importance of Rashba DMI
  * role of easy-plane anisotropy
  * Chern number for skyrmions
- 2D (H,T) phase diagram
  * skyrmion liquid phase

- 2D to 3D crossover with thickness → surface topological textures arXiv:1706.08248
The End