Monte Carlo Simulations of Topological Magnetic Materials

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Introduction

- In the 1970s, experimentalists studying MnSi observed a small region of phase space that they were unable to identify.
- In 2009, a neutron scattering experiment revealed a surprising configuration in momentum space, shown in Fig. 1. This became known as the skyrmion phase.

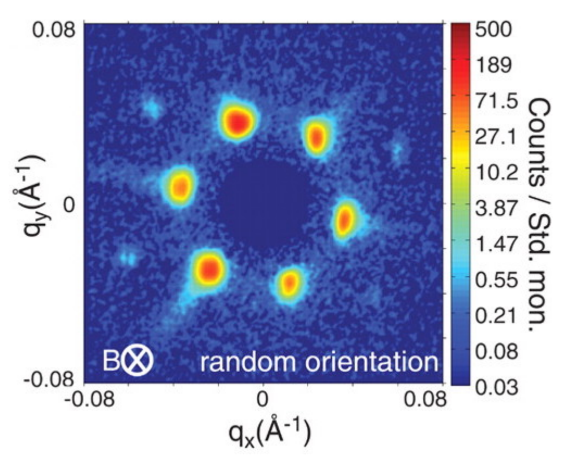


Figure 1: Typical neutron small angle scattering intensities in MnSi. While MnSi is cubic, six Bragg reflections are observed.[1]

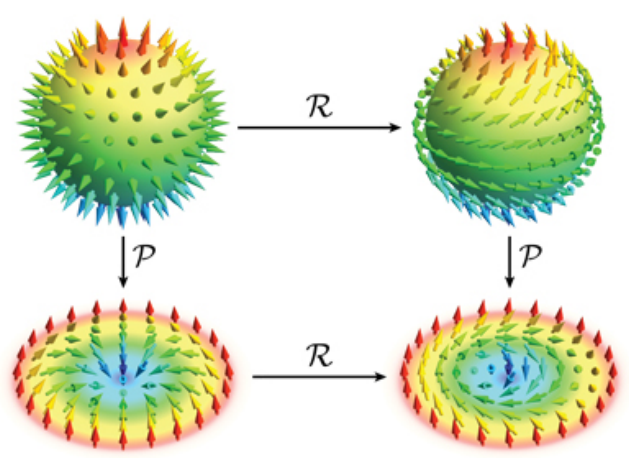


Figure 2: Relationships between various spin configurations. $\mathcal{R}$ denotes a rotation about the z-axis and $\mathcal{P}$ the stereographic projection. Top left is the hedgehog configuration. Bottom are skyrmions.[2]

- The skyrmion is a 2D vortex-like spin configuration (see Fig. 2)
- In the hedgehog configuration, spins point radially outward and wrap around the sphere exactly once, giving it a winding number of 1.
- The skyrmion can be mapped one-to-one with the hedgehog configuration. Thus, it also has a winding number of 1.

$$Q = \frac{1}{4\pi}\int \mathbf{n}\cdot\left(\frac{\partial \mathbf{n}}{\partial x}\times\frac{\partial \mathbf{n}}{\partial y}\right)\mathrm{d}x\mathrm{d}y$$

- The topology of a spin texture is characterized by the topological charge (TC). This is given by the equation for Q above, where **n** is a spin's unit vector.
- The skrymion's nonzero TC implies the unique property of *nontrivial topology*.

Requirements for Skyrmion Phase

- ✓ B20 compound (non-centrosymmetric cubic lattice)
- ✓ Dzyaloshinkii-Moriya (DM) interaction
- ✓ External magnetic field

Objective

Characterize skyrmions using topological charge, not just configuration snapshots.

- ✓ Model lattice with appropriate Hamiltonian
- ✓ Simulate behavior of a 2D lattice over a range of temperatures T
- ✓ Calculate TC of lattice
- ✓ Vary over parameters in Hamiltonian

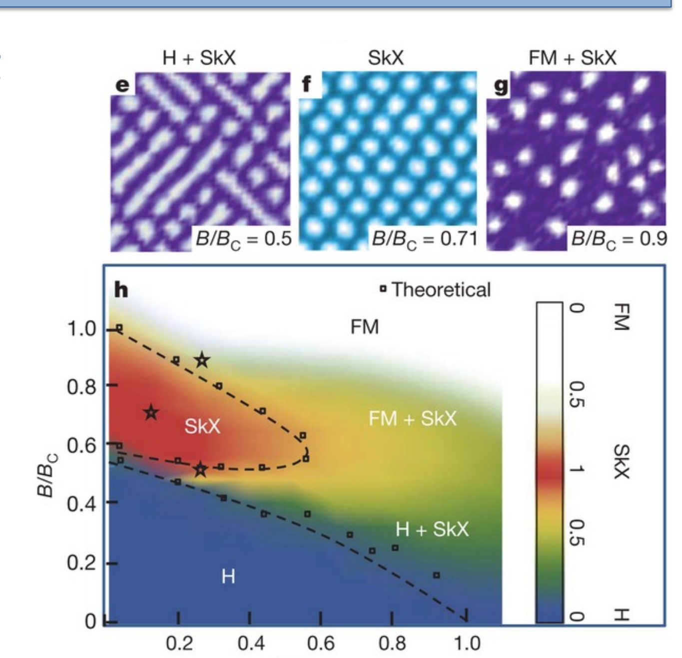


Figure 3: Theoretical phase diagram on 2D square lattice. Here, the skyrmions are visually identified from real space snapshots.[3]

Methodology

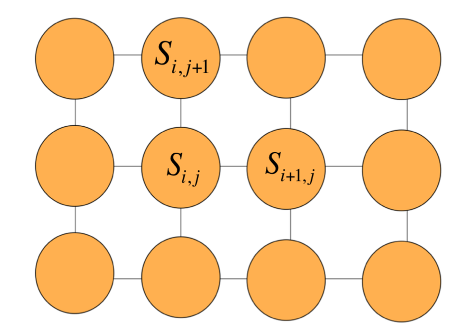
$$H = \sum_{<ij>} \underbrace{-J\mathbf{S}_i\cdot\mathbf{S}_j}_{\text{Heisenberg}} + \underbrace{\mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j)}_{\text{Dzyaloshinkii-Moriya}} - \sum_i \underbrace{\mathbf{H}\cdot\mathbf{S}_i}_{\text{Zeeman}}$$

Hamiltonian

- $\mathbf{S}_i = S\mathbf{n}_i$ is the spin on site i with $\mathbf{n}_i$
- $J > 0$ is the ferromagnetic Heisenberg exchange coupling
- $\mathbf{D}_{ij}$ is the vector of the DM interaction between neighboring sites i and j
- **H** is the applied magnetic field

Spin Lattice

- 2D square lattice replicates MnSi
- Periodic boundary conditions
- Initialize at high temperature random state



Monte Carlo

- Calculate the energy of the lattice E_0
- Make small random adjustment of a spin S and calculate the new lattice energy E_n
- Initialize lattice to high temperature random state
  - If $E_n < E_0$, the new lattice is kept
  - Else, the new lattice is kept with a probability equal to the Boltzmann distribution $e^{(En-Eo)/T}$
- Calculate and record observables
- Repeat 2.4×10^6 times
- Begin again at new lower temperature

Results

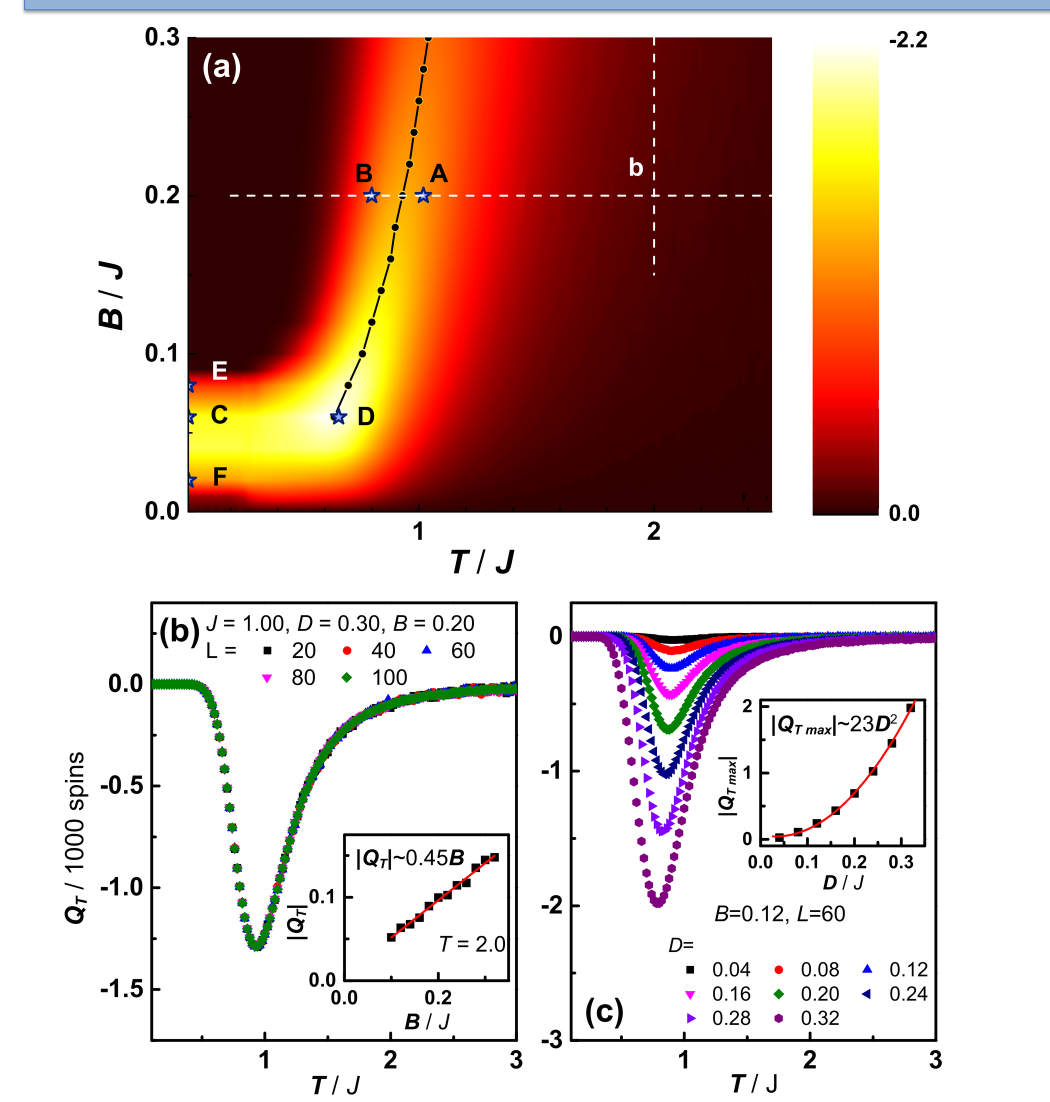


Figure 4: (a) The phase diagram of TC with magnetic field and temperature dependence. $D = 0.30J$. (b) The TC over lattices from 20x20 to 100x100. The inset is the field-dependence of TC. (c) The TC as a function of D. The insert is the square relationship between the peak value of TC and DM interaction.[4]

- Found a dramatic upturn of the TC along a ridge in the B-T phase diagram.
- The skyrmion phase is located at small B and low T, but the nonzero TC extends far beyond this region.
- Fig. 4(b) shows the relation between TC and temperature in this high field region: zero at low and very high T, but elevated around $T = 1.0J$, the Curie temperature of the corresponding Heisenberg model.
- Appears to be immune to finite size effects.

Unexpected Result

Topological charge has dramatic upturn at high field and high temperature.

Looking at snapshots (Fig. 5):

- The emergent topology at finite temperature does not correspond to any ordered phase. This is supported by the lack of spin ordering at points (A) and (B) on either side of the ridge.
- No phase transition occurs from 0 temperature to points (A) or (B). *The emergence of TC is thus a consequence of the thermal fluctuation.*
- The TCs at low field have distinct origins. Point (C) corresponds to the skyrmion phase. Increasing temperature to point (D) results in significant TC without spin ordering. Increasing the field to point (E), results in sparse skyrmions. Decreasing field to point (F), the skyrmion phase begins to transition to the helical phase.
- All of the low-field, low-temperature results are consistent with previous studies.

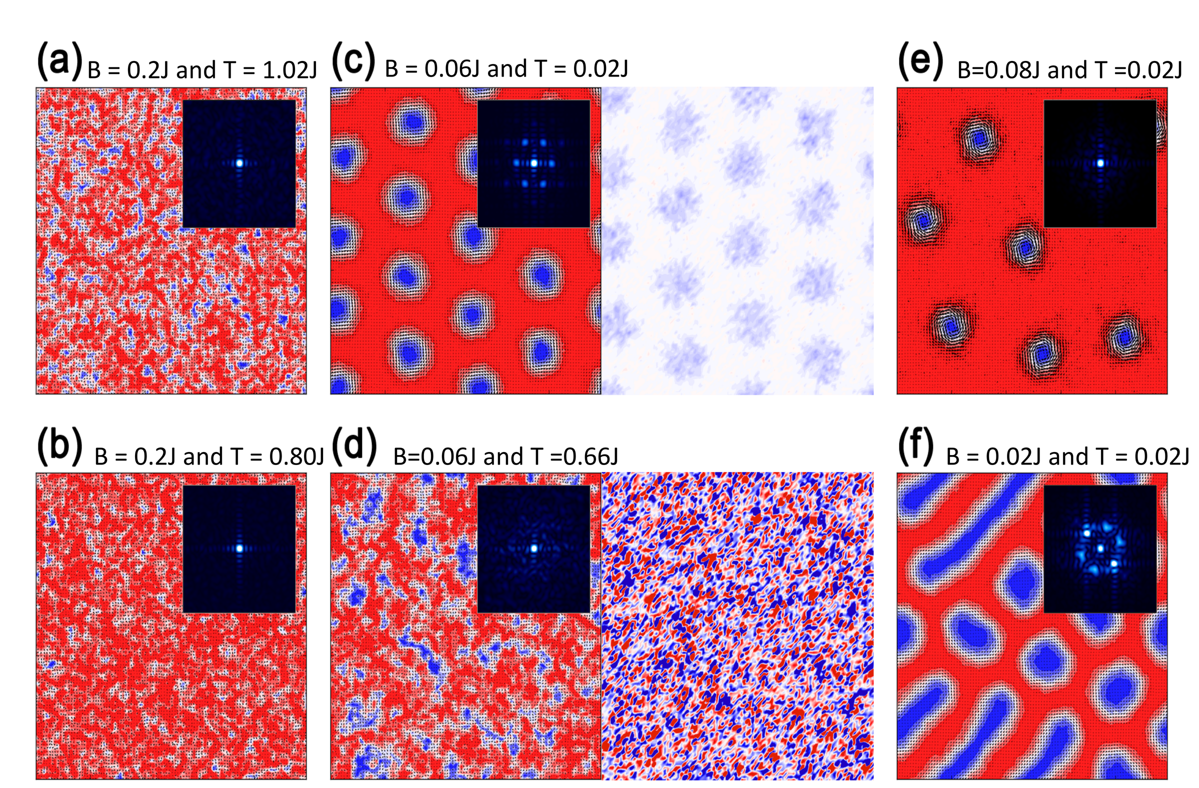


Figure 5: Real space snapshots and corresponding reciprocal space plots by Fast Fourier Transform at points labelled in Fig. 4(a). In the real space snapshots, red contour represents the positive value of S_{iz} while blue represent the negative value. The arrows represent the directions of in-plane components. In (c) and (d), panels to the right show the density of TC.[4]

Conclusion

- Monte Carlo calculations of topological charge successfully characterized the skyrmion phase, producing expected results in the low-field, low-temperature region.
- Discovered a significant upturn of topological charge outside of the skyrmion crystal phase, and without a corresponding ordered phase.
- The topological charge was found to be the result of thermal fluctuation rather than any type of phase transition.
- The upturn was further explained with a field-theoretic analysis.[4]

Applications

Skyrmions' nanometer size and manipulability by small electric currents make them an exciting candidate for next generation memory devices. The development of skyrmion-based topological spintronics is a rapidly growing field.

Future Work

- Similarly characterize the topological charge for a variety of spin lattices.
- Search for spin model with emergent topology that does not host the skyrmion phase.
  - This could extend the topological phenomena to more common materials.
  - Enable further experimental studies and applications.

References

1. Muehlbauer et. al, *Science* **323**, 5916, pp.915-919, (2009).
2. "Skyrmions In Chiral Magnets," *ChristophSchuette*. http://www.christophschuette.com/physics/skyrmions.php.
3. X. Z. Yu et. al, *Nature* **465**, *7300* (2010).
4. W.T. Hou, J.X. Yu, **M. Daly**, J. Zang, Phys. Rev. B **96**, 140403(R), (2017).
5. J.X. Yu, **M. Daly**, J. Zang, submitted to Phys. Rev. B (2018).

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