Simulating Domain Walls in Weyl Semimetals to Study the Effects of Weyl Fermions on Magnetic Behavior

Patrick Chen

Lab: NIST Center for Neutron Research(NCNR)

Mentors: Jonathan Gaudet, Michael Donahue(ITL)

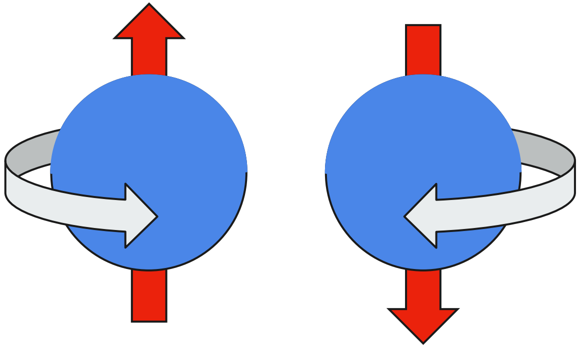
Goal

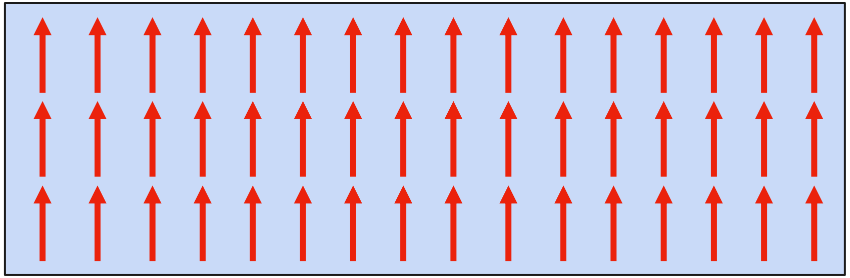
Accurately model the magnetic behavior in Weyl semimetals to explore novel behaviors caused by the influence of Weyl electrons.

Background Information

Spin and Magnetism

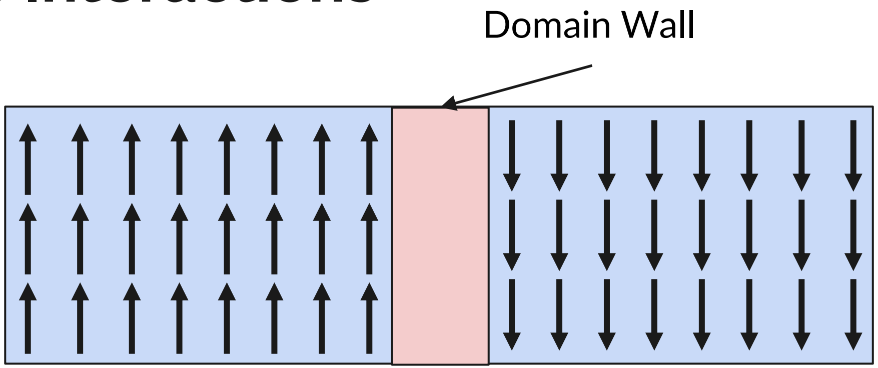
- Spin is an inherent property of elementary particles
  - Can be thought of as a "**tiny magnet**" for the purposes of this presentation
- Large regions of aligned spin are called **ferromagnetic domains** and result in a net magnetization



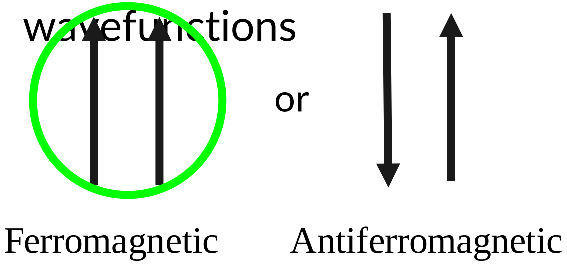


Domain Walls and Magnetic Interactions

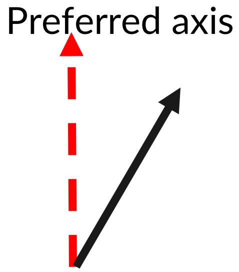
- A single crystal can have multiple domains of differing alignments.
  - Transition region is called a domain wall



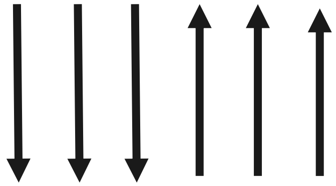
Exchange - Local interaction of neighboring atoms through overlapping wavefunctions



Anisotropy - Preferred axis of alignment

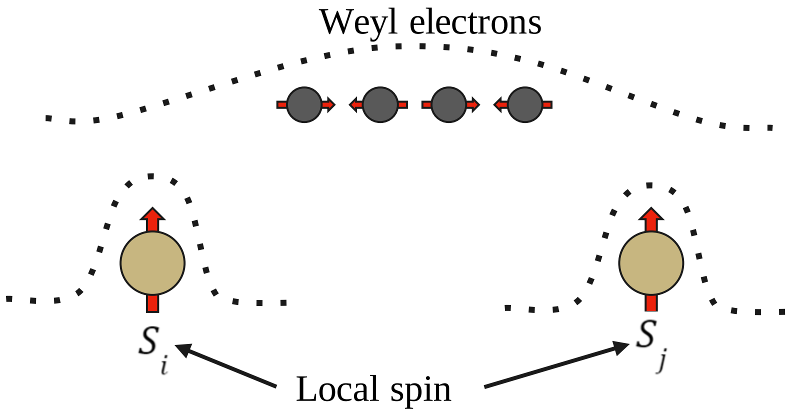


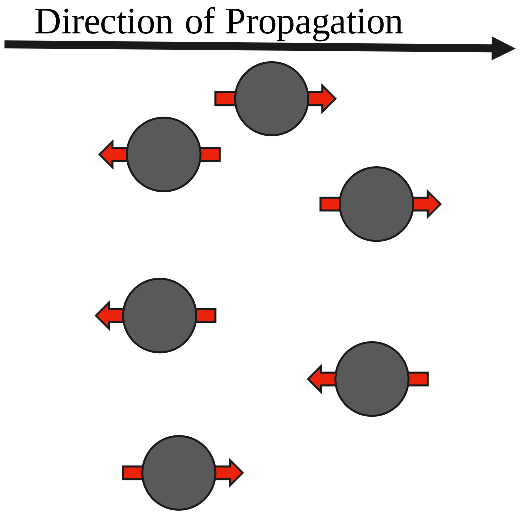
Dipole/Demagnetization - Long range effect due to the net magnetization



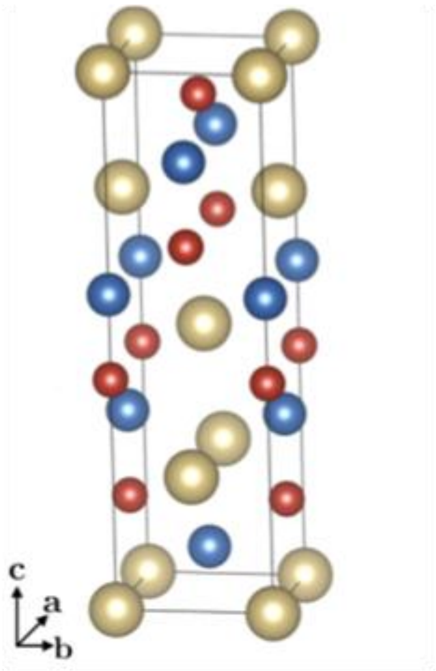
What is special about Weyl semimetals?

- Weyl electrons
  - "**Massless**" - highly mobile
  - **Chiral** - "handedness"
  - Mediates the Dzyaloshinskii-Moriya(DM) interaction that tends to **misalign** neighboring spins



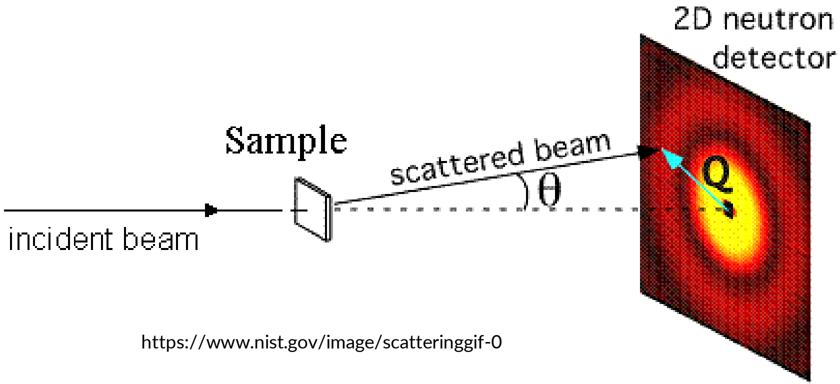


CeAlSi

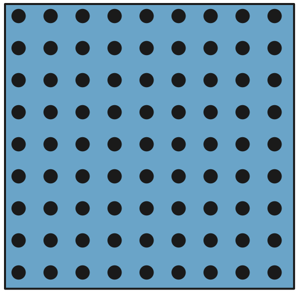


Neutron Scattering

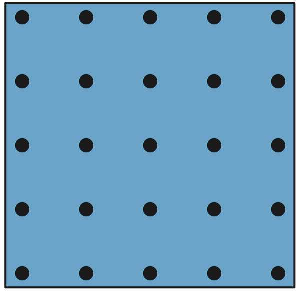
- Why is it useful?
  - Measures **magnetic** and **structural** properties
  - Highly penetrating, so it is able to measure **bulk** properties
  - Sensitive on **nanometer** and **micron** length scales(for Small Angle Neutron Scattering(SANS))



https://www.nist.gov/image/scatteringgif-0



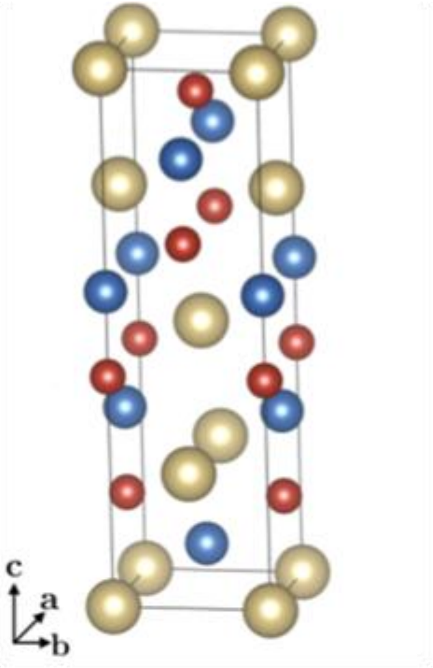
High-q



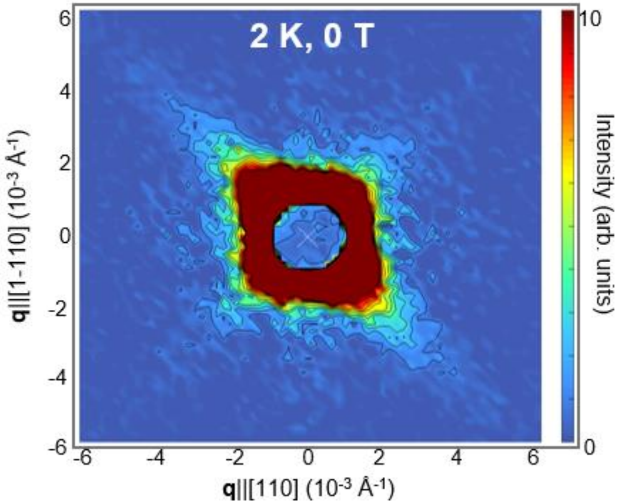
Low-q

Comparison to Neutron Scattering Data

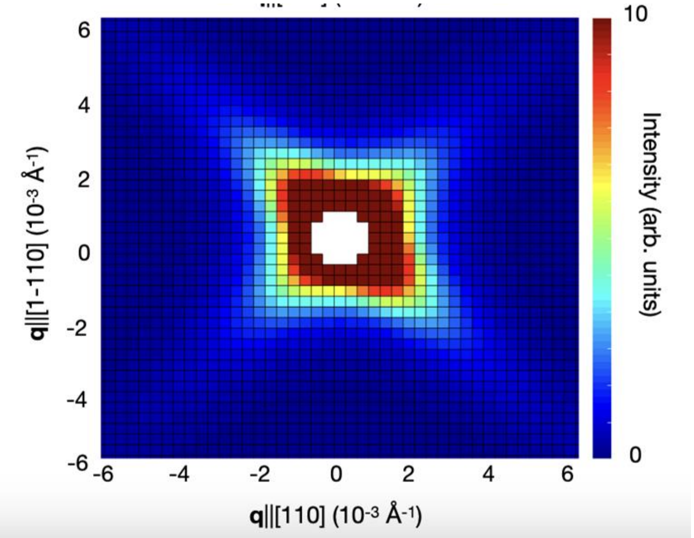
CeAlSi



Measured Scattering Data



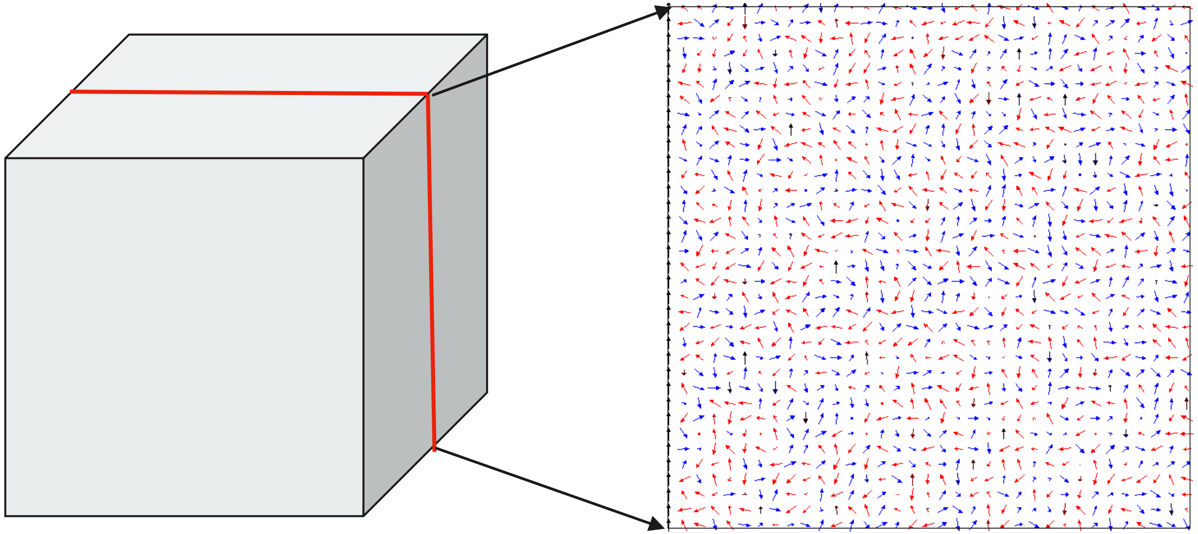
Simulated Scattering of Bilayer Striped Domains



Creating the Model

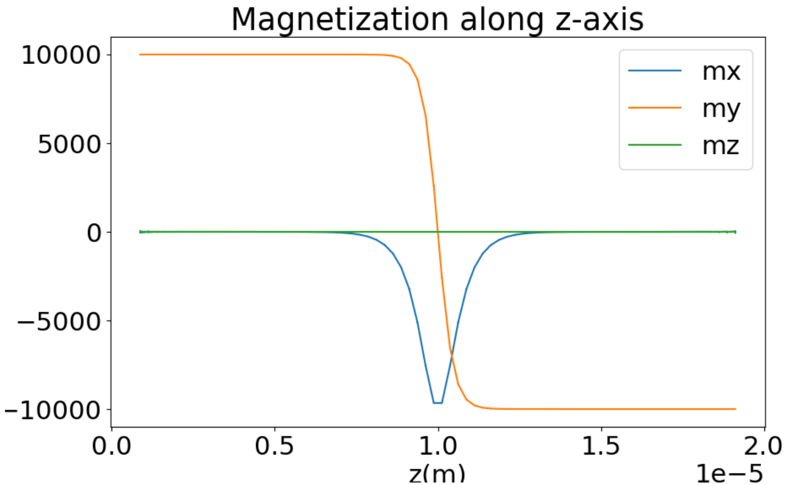
OOMMF Toolkit and Procedures

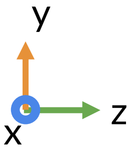
- Initiate from a random configuration of spins
- “Solves” the spin configuration by minimizing energy
- Should be thought of as a small part of a larger crystal

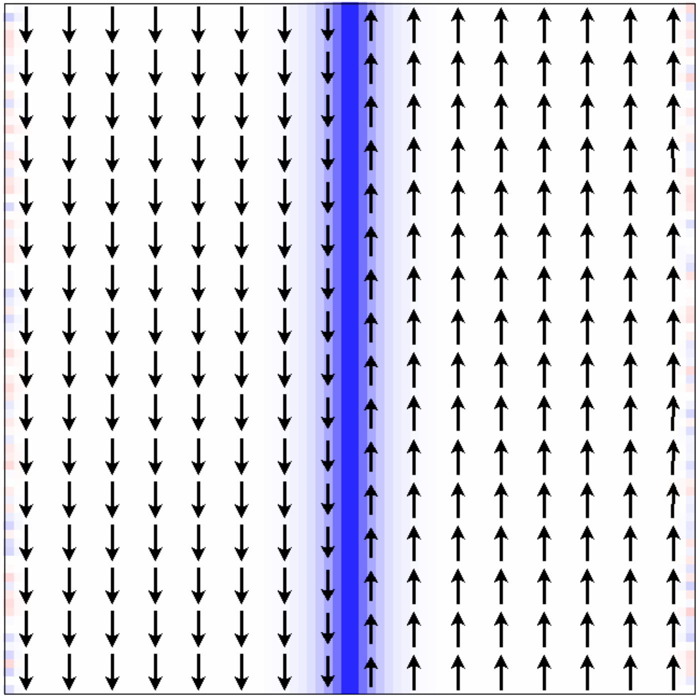


Verification of the OOMMF Simulation

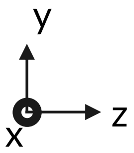
- Includes only the exchange, anisotropy and dipole interactions which are well understood.
    - Expect domain wall to process along the in/out-of-plane direction.







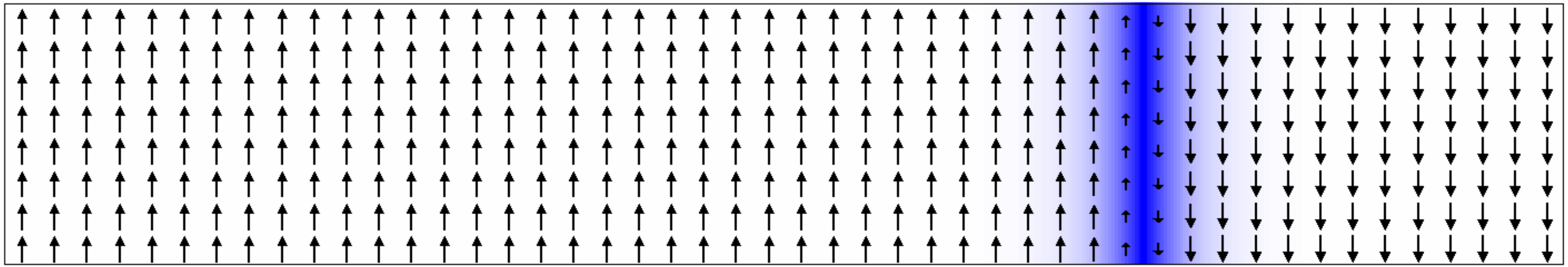
Modeling the DM Interaction



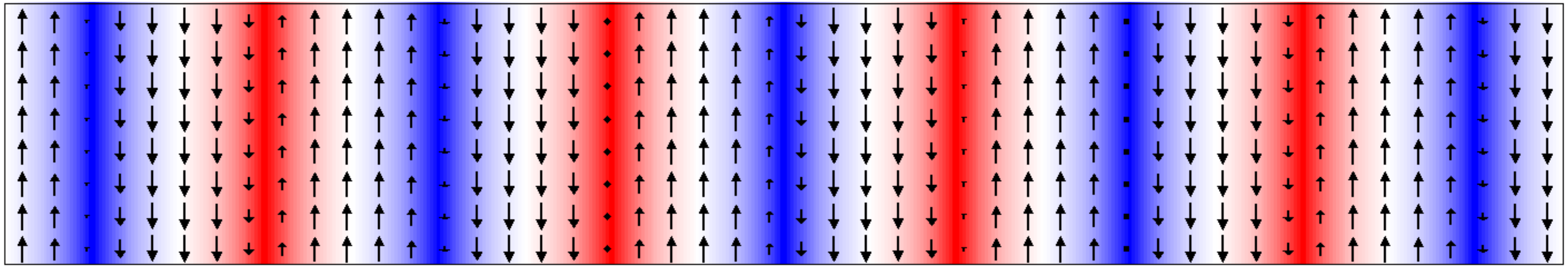
- Expectations
  - More domains, leading to stripes
  - Chiral domain wall transitions

Red - Out of Plane(+x)
Blue - Into Plane(-x)

Without DM



With DM



Conclusion and Future Direction

Results

- Model successfully incorporates the DM interaction
- Observed chiral stripes in simulated Weyl semimetal
  - Connects the theory for DM to observed scattering data

Future Direction

- Tune parameters to correlate more closely with real world measurements
- Generate scattering profiles of these simulations

Acknowledgments

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NIST CENTER FOR NEUTRON RESEARCH

CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING

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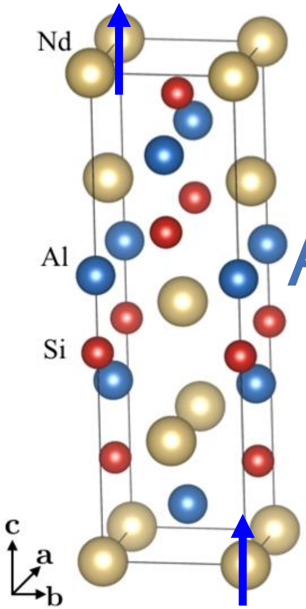
Questions?

<u>RAlX</u>



Al

X=Si or Ge

R = Nd, Sm, or Ce

Exchange

$$E = J[S_i \bullet S_j]$$

DM

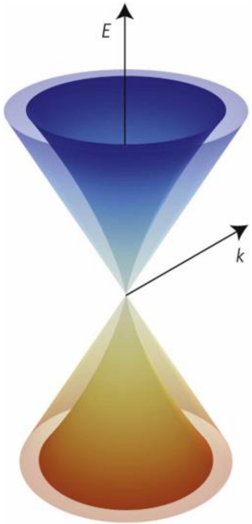
$$E = D \bullet S_i \times S_j$$

$$|A \times B| = |A||B|sin(\theta)$$

$$|A \bullet B| = |A||B|cos(\theta)$$

Break inversion symmetry

$$\vec{r} \neq -\vec{r}$$

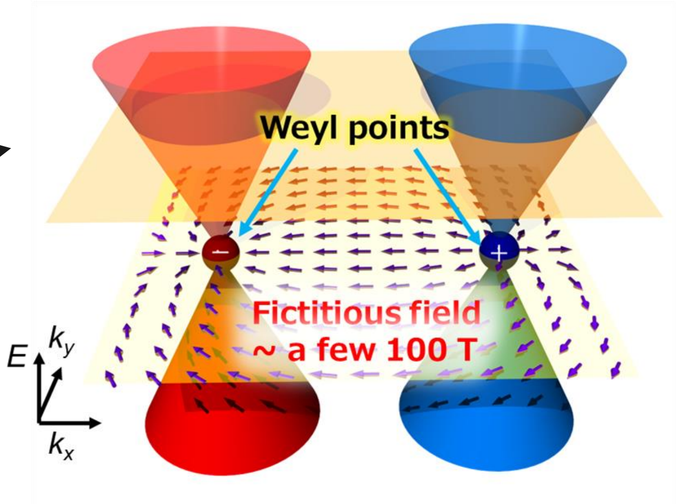


Elias, Nature Physics 7, 701-704 (2011)

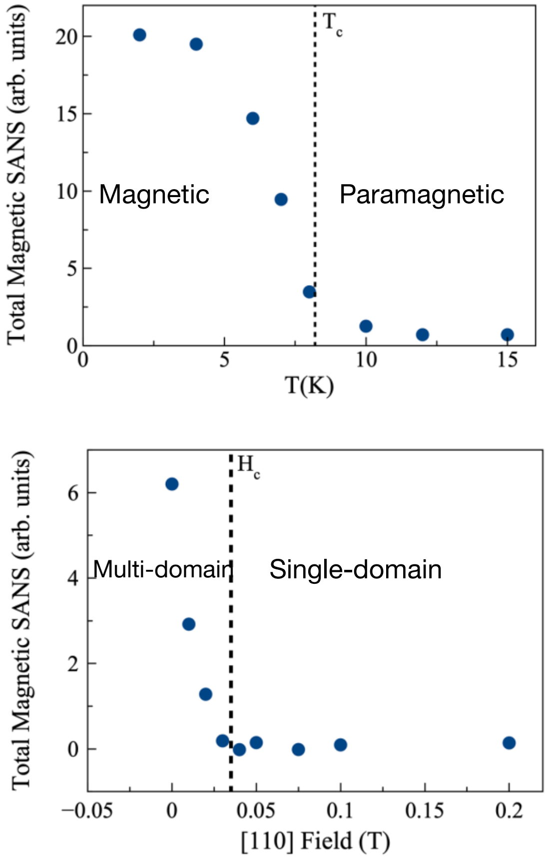
and/or

$$t \neq -t$$

Break time-reversal symmetry(magnetism)



S. Nakatsuji and N. Kiyohara, Nature 527.7577 (2015)


Total Magnetic SANS (arb. units)
T(K)
Tc
Magnetic
Paramagnetic
Total Magnetic SANS (arb. units)
[110] Field (T)
Hc
Multi-domain
Single-domain

2 K