Determination of Magnetic Transitions: Effective Spin Models and Monte Carlo Simulations

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"Magnetic Materials from First Principles", TÜBITAK Workshop
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UNIVERSITY OF NORTH DAKOTA
LEADERS IN ACTION

Scope of magnetic materials in this talk

This talk focuses on **magnetic insulators** with well-localized spins.

3D examples:

Fe_2AlB_2
La_2CuO_4

2D examples:

CrI_3
$Hf_2VC_2O_2$
$Hf_2MnC_2O_2$

What magnetic properties can we calculate?

Quantity	**Requires**
Ground-state magnetization $M(0)$	DFT (VASP)
Magnetization curve $M(T)$	+ Monte Carlo
Curie temperature T_c	+ Monte Carlo
Paramagnetic susceptibility $\chi(T)$	+ Monte Carlo
Magnetic structure factor $M_s(q)$	+ Monte Carlo
Spin wave dispersions $\omega(q)$	+ Monte Carlo
Hysteresis curve $M(H)$	+ micromagnetics
Coercive field H_c	+ micromagnetics

A Multiscale Modeling Approach

First principles (DFT) → Effective spin model → Thermodynamic properties

$$\hat{H} = \hat{H}_{ee} + \hat{H}_{eN} + \hat{H}_{NN} + \hat{H}_{SO} + \ldots$$

eV

$$\hat{H}_{\mathrm{eff}} = -\sum_{\langle ij\rangle} J_{ij}\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + \sum_i H_{\mathrm{MAE}}(\hat{\mathbf{S}}_i) + \ldots$$

$M(0)$
$M(T)$
T_c
…

Energy scales
1 eV – 10 eV

Energy scales
1 μeV – 1 eV

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  by watching other people play the trumpet

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- I supply Jupyter notebooks (Python) and C++ code
- You go through examples hands-on

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- 3D graphics in Python not well integrated with Jupyter notebook
- Examples not 100% portable due to OS-specific details, software dependencies, VASP installation, POTCAR files, etc.

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Therefore:

- I show you Mathematica notebooks and C++ code
- You go through examples later on

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We focus on CrI_3 as a case study!

[Most of this session will be in Mathematica notes]

Summary: Monolayer CrI_3

Attempt 1 (nearest neighbor Ising model): $T_c = 22$ K

Attempt 2 (second-neighbor Ising model) $T_c = 140$ K

Attempt 3 (classical Heisenberg model): $T_c = 0$ K

Attempt 4 (classical Heis + easy-axis aniso): $T_c = 50$ K

Attempt 5 (quantum Heis + easy-axis aniso): ???

Experiment: $T_c = 45$ K

There is a large number of papers on this material, both experimental and theoretical, in case you are interested.

Conclusions (Main Lessons Learned?)

- Magnetism in 2D is subtle and complicated!

- Ferromagnetic order in 2D can exist,
  but it requires two ingredients:
  - exchange coupling *J*
  - easy-axis magnetic anisotropy *K*

- **To make a room-temperature 2D magnetic material, we must optimize both of these properties.**

Beyond ferromagnetism

Classical magnetic order

- Antiferromagnetism
- 120-degree (Y) antiferromagnetism
- Non-commensurate states (spin density wave)
- Non-collinear magnetism, e.g., helimagnets
- Classical geometric & disorder frustration

Quantum magnetism

- Valence bond solid
- Resonating valence bonds
- Valence bond liquid; spin liquid
- Quantum geometric & disorder frustration

Itinerant magnetism ...

Multiferroics ...

Acknowledgments

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E. M. D. Siriwardane, P. Karki, Y. L. Loh, and D. Çakır, "Engineering magnetic anisotropy and exchange couplings in double transition metal MXenes via surface defects," Journal of Physics: Condensed Matter 33, 035801 (2020)

E. M. D. Siriwardane, P. Karki, Y. L. Loh, and D. Çakır, "Strain–Spintronics: Modulating Electronic and Magnetic Properties of Hf2MnC2O2 MXene by Uniaxial Strain," J. Phys. Chem. C 123, 19, 12451-12459 (2019)