Classical Monte Carlo Simulation of α-$RuCl_3$ with Moiré-Induced Modulated Interlayer J (Kitaev–Γ–Heisenberg Model)

Github link:

https://github.com/NepalBanerjee1989/Kitaev_Gamma_Heisenberg_Model_Honeycomb_Lattice/releases/tag/v2.0

This release presents a classical Monte Carlo simulation framework for studying the magnetic phases of the two-dimensional van der Waals magnet α-$RuCl_3$. The simulations are performed on a honeycomb lattice using the **Kitaev–Γ–Heisenberg (KΓH) model** with extended exchange interactions and includes **moire-induced spatially modulated interlayer J** for twisted bilayer α-$RuCl_3$.

Physics Highlights:

- Implemented the **Kitaev–Γ–Heisenberg Hamiltonian** including:
    - Nearest-neighbor (NN) interactions
    - Next-nearest-neighbor (J_2) interactions
    - Third-nearest-neighbor (J_3) interactions
- Introduced **moire-induced modulated interlayer exchange interactions (J)** for twisted bilayer α-$RuCl_3$.
- Predicted a magnetic transition temperature $T_c \approx 6.5K$ for α-$RuCl_3$.
- Observed a **zigzag antiferromagnetic (AFM)** ground state in excellent agreement with experimental reports.
- In the absence of **Kitaev** and **Γ** interactions, the transition temperature increases to approximately **13–14 K**, highlighting the role of anisotropic exchange interactions.

Spin-Liquid Phases:

- **Pure Kitaev limit:**
    - Realization of a **classical Z_2 flux spin-liquid state**.
- **Frustrated Heisenberg limit:**
    - Emergence of a **classical U(1) gauge-like spin-liquid state**.
    - Presence of pinch-point singularities in the static structure factor.

Interpolating Hamiltonian:

An interpolating Hamiltonian with a tuning parameter g is introduced:

$H(g)=(1-g)H\_Heisenberg+gH\_Kitaev$

- g=1 — Classical Z_2 Kitaev spin-liquid phase
- g=0 — Classical U(1) gauge frustrated spin-liquid phase
- g=1/2 — Stabilization of a robust **zigzag-AFM ground state**

This result demonstrates an **order-by-disorder mechanism**, where the interplay between two highly degenerate spin-liquid manifolds leads to long-range magnetic order.

Simulation Methodology:

- Classical **single-spin-flip Metropolis Monte Carlo algorithm**
- Continuous spin update scheme
- Explicit calculation of **Metropolis acceptance probability**
- Simulations performed on a **two-dimensional honeycomb lattice**

Analysis and Outputs:

- **Real-space spin configurations** at low temperatures
- **Static spin structure factor calculations**
- Results show excellent qualitative agreement with experimental **neutron-scattering data**.

Notes:

- This is a purely **classical simulation**; quantum fluctuations are not included.
- The code is designed for **clarity, extensibility, and pedagogical use**.
- Suitable for studies of **frustrated magnetism**, **spin liquids**, and **anisotropic exchange models**.
- Introduces **moire-induced spatially modulated J** for twisted bilayer α-$RuCl_3$, providing a more realistic simulation of these materials.

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