Model Hamiltonian

\[ H = -2J \sum_{(i,j)} S_i^z S_j^z - g \sum_{(i,j)} \frac{S_i^y S_j^y}{|\mathbf{r}_i - \mathbf{r}_j|} - B^y \sum_i S_i^y \]

with \( S^z \in \{-1, +1\} \); \( J > 0 \), \( g < 0 \) on a 2D-lattice in xy-plane

- competition between ferromagnetic exchange and antiferromagnetic dipolar interaction produces magnetic domains and a complex phase diagram
- model Hamiltonian for ultrathin metal films on metal substrates with a strong magnetocrystalline anisotropy favoring out-of-plane alignment; technological applications: electronics, data storage and catalysis

Square lattice results [1-4]

- three phases: striped, tetragonal and paramagnetic
- phase transitions visible as peaks in the specific heat
- calculation of the structure factor

\[ \sigma(k) = \left< \sum_i S_i^z \exp(i \mathbf{k} \cdot \mathbf{r}_i) \right> \]

reveals rotational symmetry of the phases

- additional nematic phase for very specific values of \( J/|g| \) close to stripe

Problem with long-range interactions:

- Calculation of energy difference \( \Delta E \) scales as \( O(N^4)! \)

Monte Carlo methods in statistical physics

- direct numerical evaluation of expectation values is computationally not feasible
- simple (random) sampling gives control over computational effort but may waste time sampling irrelevant configurations
- importance sampling: selects configurations according to the physical probability distribution \( \rho \)

\[ \langle O \rangle \approx \langle O \rangle_{\text{as}} = \frac{\sum_{\mu} O(\mu) \rho(\mu) e^{-\beta H(\mu)}}{\sum_{\mu} e^{-\beta H(\mu)}} \]

Importance sampling implemented as Markov chain. Master equation for \( k \)-th state in chain together with detailed balance condition:

\[ P_{k \rightarrow (k')}(\mu) = P_k(\mu) \sum_{\nu} \left( \frac{P_k(\nu) T(\nu \rightarrow \mu)}{P_k(\mu) T(\mu \rightarrow \nu)} \right) \]

Leads e.g. to the Metropolis algorithm [5] with single spin flip dynamics:

1. start in an arbitrary state
2. randomly select a single spin to flip
3. calculate the resulting energy difference \( \Delta E \)
4. flip it with probability \( \min(1, e^{-\beta \Delta E}) \)
5. measure observables of interest
6. return to step 2

Honeycomb lattice results [6]

- ground state is striped!
- three phases: striped, hexagonal and paramagnetic
- phase transitions visible as peaks in the specific heat
- structure factor calculation reveals 6-fold rotational symmetry of the hexagonal phase

Future work:

- no sign of nematic phase yet; rerun simulations for different values of \( J/|g| \) to determine phase diagram and stripe width transitions
- run simulations with an external magnetic field

References


Free Monte Carlo simulation code for classical spin systems, available at https://github.com/roberttrueger/SSMC

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