Pattern formation in the dipolar Ising model on a two-dimensional honeycomb lattice

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Model Hamiltonian

$$H = -2J\sum_{\langle i,j\rangle} S_i^z S_j^z - g\sum_{\substack{i,j\\ i\neq j}} \frac{S_i^z S_j^z}{|\vec{r}_i - \vec{r}_j|^3} - B^z \sum_i S_i^z$$

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

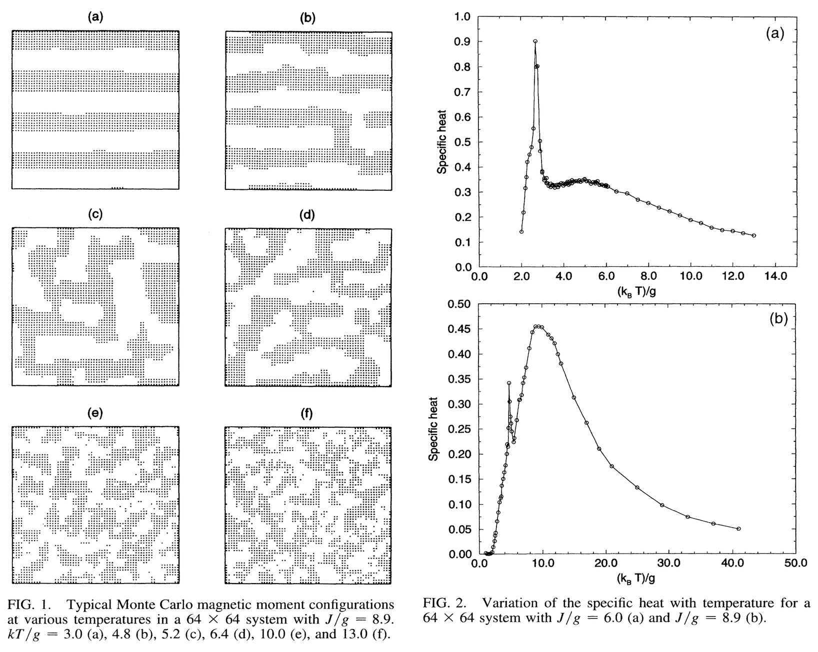
- competition between ferromagnetic exchange and antiferrom. dipolar interaction produces magnetic domains and a complex phase diagram
- model Hamiltonian for ultrathin metal films on metal substrates with a strong magnetocrystalline anisotropy favoring out-of-plane alignment; technological applications: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

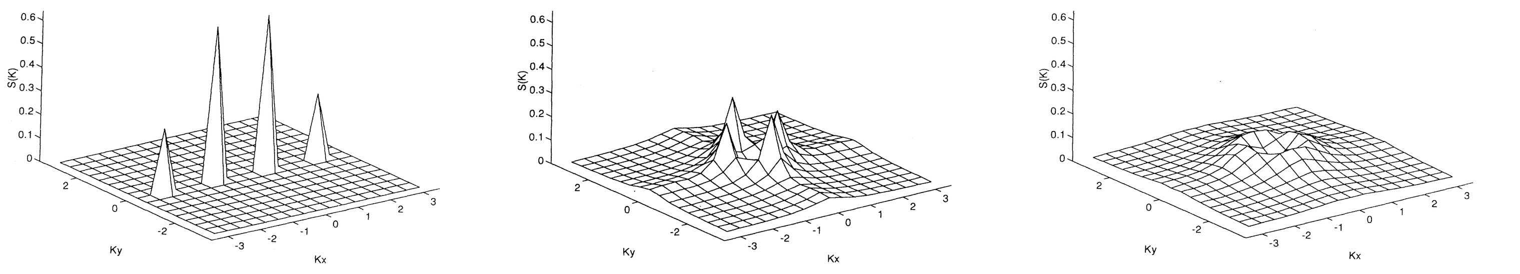
Square lattice results [1-4]

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

$$\sigma(\vec{k}) = \left\langle \left| \sum_j S_j^z \exp\left(\mathrm{i}\,\vec{k}\cdot\vec{r}_j\right)\right|^2 \right\rangle$$

reveals rot. symmetry of the phases





- additional nematic phase for very specific values of $J/|g|$ close to stripe width phase transitions

Question: Influence of the underlying lattice?

Monte Carlo methods in statistical physics

- direct numerical evaluation of expectation values is computationally not feasible

$$\langle O\rangle = \frac{\sum_\mu O(\mu)\,\mathrm{e}^{-\beta H(\mu)}}{\sum_\mu \mathrm{e}^{-\beta H(\mu)}}$$

- simple (random) sampling gives control over computational effort but may waste time sampling irrelevant configurations

$$\langle O\rangle \approx \langle O\rangle_{ss} = \frac{\sum_{\mu_{i=1}}^{\mu_N} O(\mu_i)\,\mathrm{e}^{-\beta H(\mu_i)}}{\sum_{\mu_{i=1}}^{\mu_N} \mathrm{e}^{-\beta H(\mu_i)}}$$

- importance sampling: selects configurations according to the physical probability distribution ρ

$$\langle O\rangle \approx \langle O\rangle_{is} = \frac{1}{N}\sum_{\mu_{i=1}^{(\rho)}}^{\mu_N^{(\rho)}} O\left(\mu_i^{(\rho)}\right)$$

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

$$P_{k+1}(\mu) = P_k(\mu) + \sum_\nu \Big(P_k(\nu)\,T(\nu\to\mu) - P_k(\mu)\,T(\mu\to\nu)\Big)$$

$$P_k(\nu)\,T(\nu\to\mu) = P_k(\mu)\,T(\mu\to\nu)$$

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 ΔE
4. flip it with probability min $\left(1,\ \mathrm{e}^{-\beta\,\Delta E}\right)$
5. measure observables of interest
6. return to step 2

Problem with long-range interactions:
Calculation of energy difference ΔE scales as $\mathcal{O}(N)$!

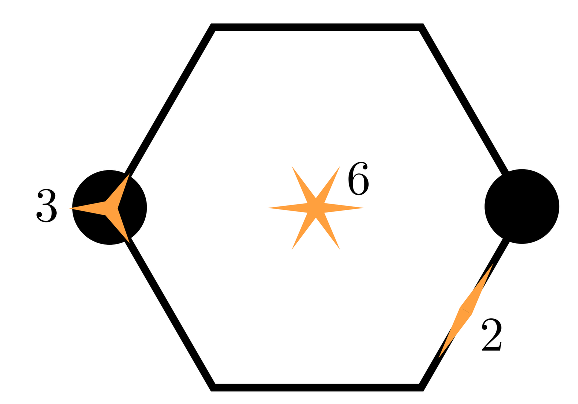
Implementation: SSMC

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

Methods for long-range interactions [6]

Approach: Reduce infinite system to finite system with replicas!

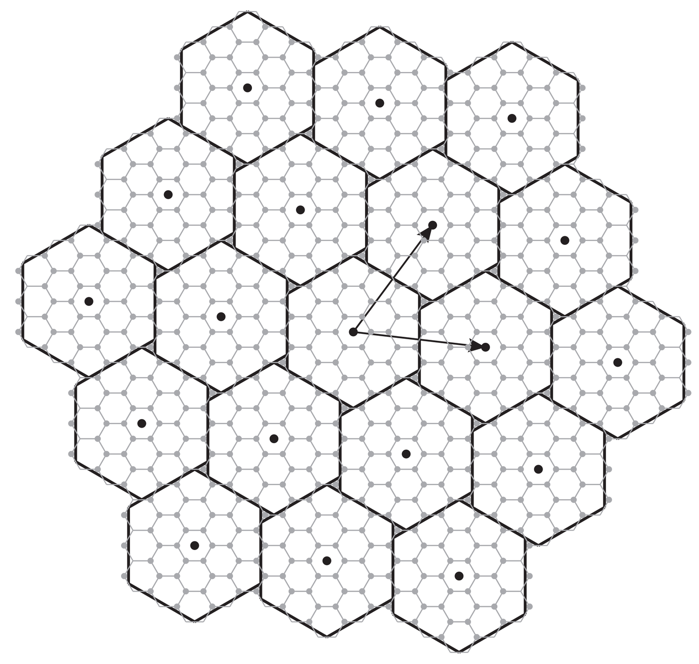
1. the system's shape must allow for tiling without gaps
2. the system's shape should reflect the symmetries of the underlying lattice



- 3-fold rotational symmetry around one of the basis atoms
- 6-fold rotational symmetry around the center of the unit cell
- 2-fold rotational symmetry around the center of nearest-neighbor connections

Extremely symmetric finite system with periodic boundary conditions:

- hexagonal arrangement of unit cells
- tiling of the replicas in analogy to tiling of the unit cells within the system



Maximum symmetry to prevent geometric frustration!

$\Rightarrow$ Use periodicity $S_i^z \equiv S^z(\vec{r}_i) = S^z(\vec{R}+\vec{r}_i)$ to rewrite the Hamiltonian:

$$H = -\sum_{i,j}\sum_{\vec{R}}\left[\Lambda(\vec{r}_i,\vec{R}+\vec{r}_j) + \Gamma(\vec{r}_i,\vec{R}+\vec{r}_j)\right] S_i^z S_j^z = -\sum_{i,j} J_{ij}^{\mathrm{eff}} S_i^z S_j^z$$

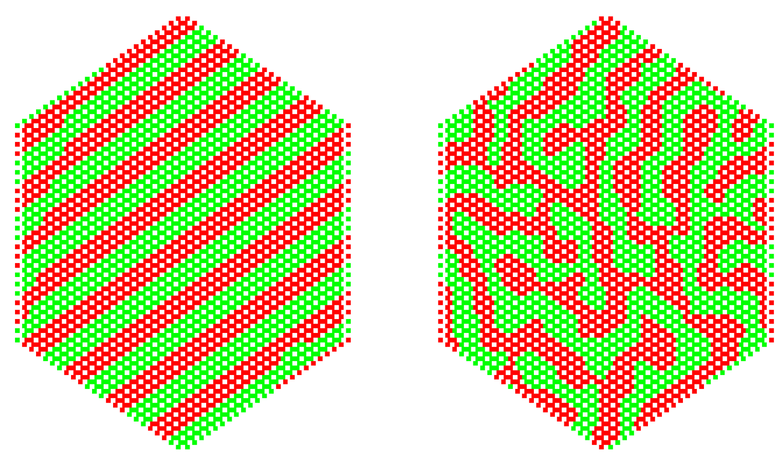
$$\text{with}\quad \Lambda(\vec{r}_i,\vec{R}+\vec{r}_j) = \begin{cases} J & \text{if } \vec{r}_i \text{ and } \vec{R}+\vec{r}_j \text{ are n.n.}\\ 0 & \text{otherwise}\end{cases}$$

$$\Gamma(\vec{r}_i,\vec{R}+\vec{r}_j) = \begin{cases} 0 & \text{if } \vec{r}_i = \vec{R}+\vec{r}_j\\ \frac{g}{|\vec{r}_i-\vec{R}-\vec{r}_j|^3} & \text{otherwise}\end{cases}$$

Honeycomb lattice results [6]

Procedure:

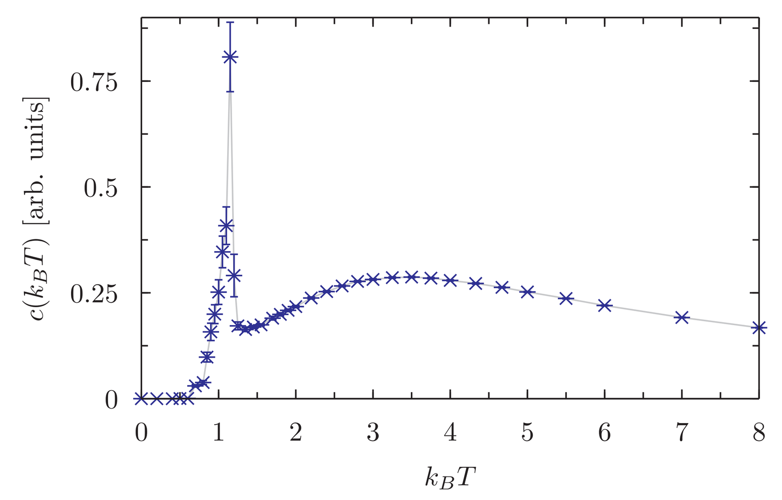
- perform simulated annealing to determine the ground state
- use obtained ground state to initialize equilibration period for simulations at constant temperature

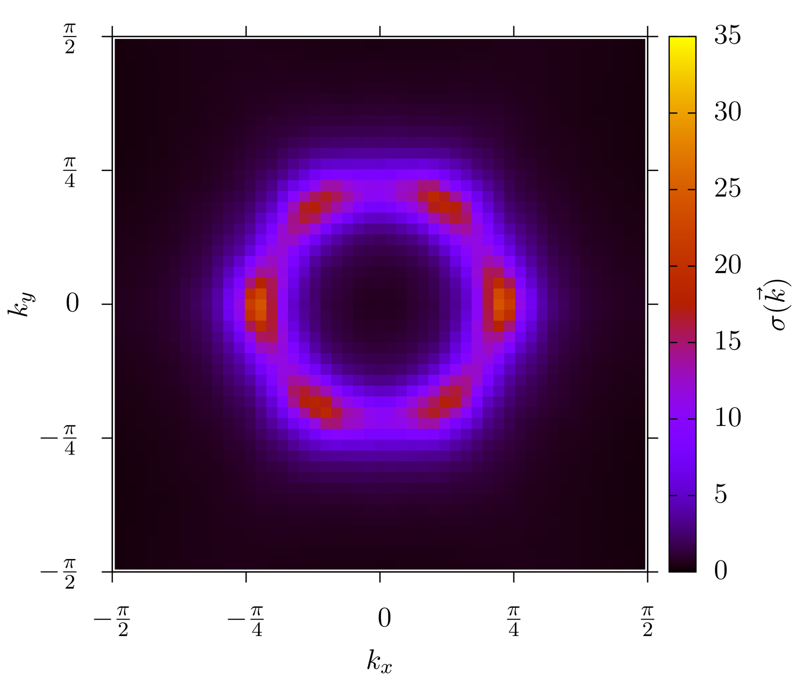


striped phase at $T=0.4$ — hexatic phase at $T=1.25$

Results:

- 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

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