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

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Motivation

... domain formation in two-dimensional magnets

Simple model for magnetic domain formation

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

- ferromagnetic exchange interaction ($J > 0$)
- dipolar interaction (antiferromagnetic $g < 0$, weak $|g| < J$)

Physical systems

- ultrathin metal films on metal substrates
- spin-$\frac{1}{2}$ and strong magnetocrystalline anisotropy
- ferromagnetic exchange interaction

Technical applications

- electronics
- data storage
- catalysis

Motivation

... known results for the square lattice

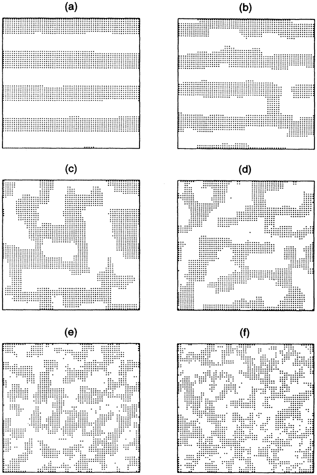


FIG. 1. Typical Monte Carlo magnetic moment configurations at various temperatures in a 64 × 64 system with $J/g = 8.9$. $kT/g = 3.0$ (a), 4.8 (b), 5.2 (c), 6.4 (d), 10.0 (e), and 13.0 (f).

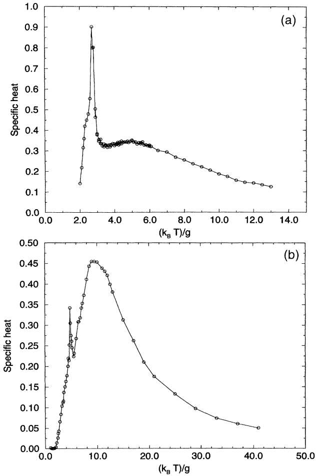


FIG. 2. Variation of the specific heat with temperature for a 64 × 64 system with $J/g = 6.0$ (a) and $J/g = 8.9$ (b).

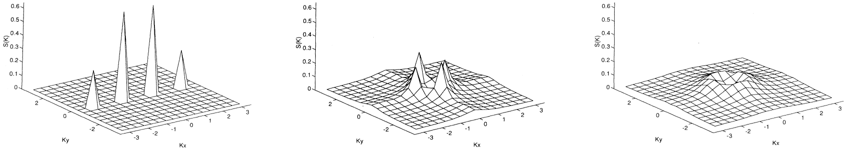
Phys. Rev. Lett. **75**, 950 (1995)

Motivation

... known results for the square lattice

The structure factor $S(\vec{k})$ as a quantitative measurement of rotational symmetry:

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



Phys. Rev. B **51**, 16033 (1995)

Motivation

... a remaining question

What effect does the underlying lattice
have on the emerging structures?

Methods

... how to deal with finite size effects?

Neighbor interactions

- Open boundary conditions are only slightly wrong.
  (only the edge spins are influenced directly)
- Implementation of periodic boundary conditions is usually trivial.

Long-range interactions

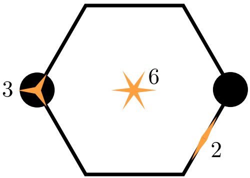
- Open boundary conditions completely wrong!
  (all spins are influenced directly)
- Implementation of periodic boundary conditions?

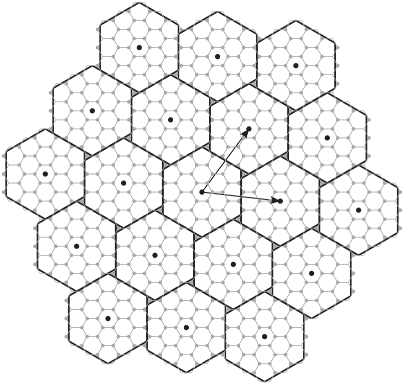
Common method: Tiling with replicas of the finite system!

Requirements for the system's shape:

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

Symmetries of the honeycomb lattice:





Methods

... using the periodicity

One can now use $S_i^z \equiv S^z(\vec{r}_i) = S^z(\vec{R} + \vec{r}_i)$ to rewrite the Hamiltonian:

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

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

$$\Rightarrow \quad H = -\sum_{i,j} J_{ij}^{\text{eff}} S_i^z S_j^z$$

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

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

Methods

... how to calculate effective interaction coefficients?

Usually: Ewald summation techniques ...

But: 2d system with r^{-3} potential $\Rightarrow$ series nicely convergent!

Straightforward evaluation of J_{ij}^{eff}

1. real space sum with cutoff (will underestimate dipolar part)
2. calculation of a single $J_{ii}^{\text{eff}\,\prime}$ using a much larger cutoff
3. add $J_{ii}^{\text{eff}\,\prime} - J_{ii}^{\text{eff}}$ to all effective interaction coefficients

Results

... the ground state

The low-temperature problem:

Low-temperature simulation initialized with an arbitrary state?
⇒ almost steepest descend in the energy landscape
⇒ **very** likely to be trapped in some **local** minimum
⇒ simulation results completely wrong!

Solution: use the ground state to initialize the simulation!

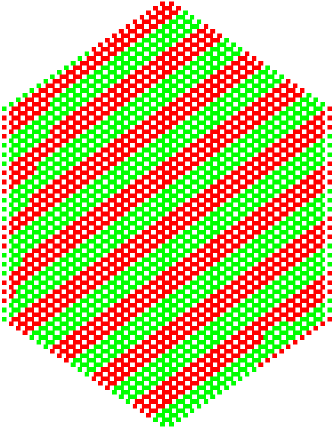
Practical realization?

perform a simulated annealing to get close to the ground state

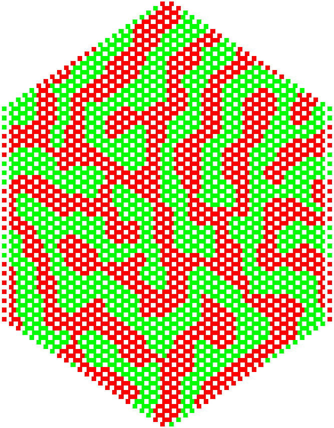
- good enough as the initial state
- information about the ground state can be extrapolated

Results

... the three phases



striped phase at $T = 0.4$

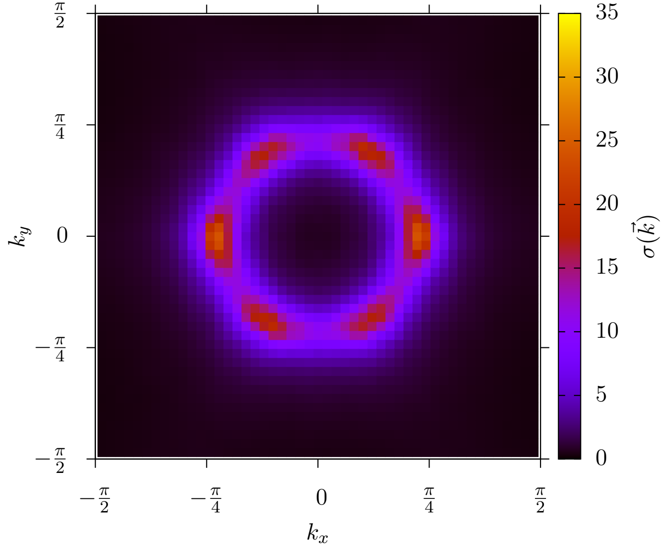


hexagonal phase at $T = 1.25$

+ disordered (paramagnetic) phase at $T \to \infty$

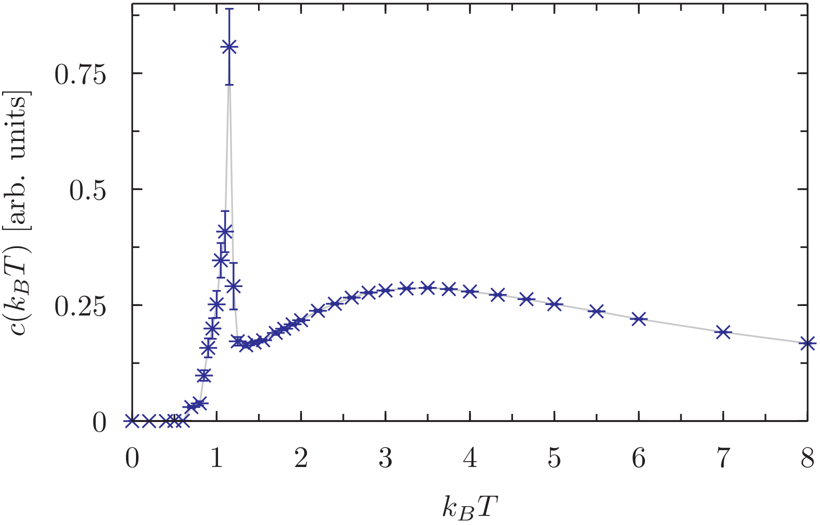
Results

... the hexagonal phase's structure factor



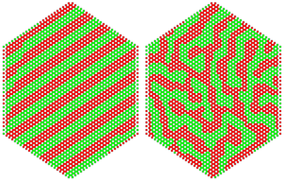
Results

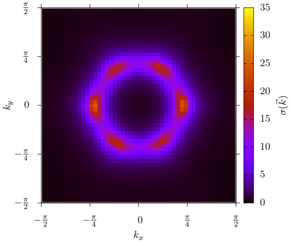
... the specific heat

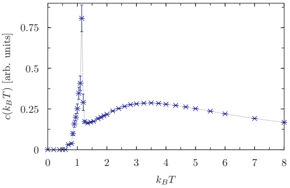


Summary of the results:

- three distinct phases: striped, hexagonal, paramagnetic
- hexagonal phase reflects the symmetries of the underlying triangular bravais lattice
- striped-hexagonal transition: sharp peak in the specific heat
- hexagonal-paramagnetic transition: broad shoulder in the specific heat







More information:

- Article published as Phys. Rev. B **86**, 024431 (2012)
- Source code available at `github.com/robertrueger/SSMC`
- Feel free to ask questions!