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

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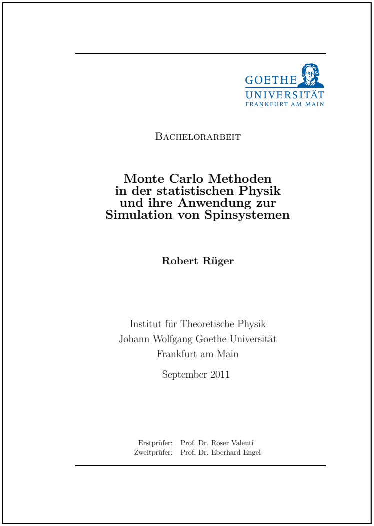
Motivation

… my personal view



GOETHE UNIVERSITÄT FRANKFURT AM MAIN

BACHELORARBEIT

Monte Carlo Methoden in der statistischen Physik und ihre Anwendung zur Simulation von Spinsystemen

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Zweitprüfer: Prof. Dr. Eberhard Engel

Bachelor thesis about Monte Carlo methods in statistical physics and their application to spin systems

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experimental lecture mentions the dipole-dipole interaction as the origin of magnetic domains

=

Monte Carlo simulation of magnetic domain formation?

Interesting!

Motivation

... my personal view

7 Ausblick: Ising-Modell mit Dipol-Dipol-Wechselwirkung

Dieses letzte Kapitel soll einen kleinen Ausblick auf die Untersuchung eines komplizierteren Ising-Modells mit mehreren Wechselwirkungen geben.

Das untersuchte System und dessen Grundzustand

Wir wollen ein zweidimensionales Ising-Modell betrachten, bei dem neben der Nächsten-Nachbarn-Wechselwirkung eine langreichweitige Dipol-Dipol-Wechselwirkung existiert. Zur Hamiltonfunktion aus Kapitel 6 müssen wir also noch den Term der Dipol-Dipol-Wechselwirkung addieren.

$$H = -J \sum_{\langle ij \rangle} S_i S_j - g \sum_{i \neq j} \frac{S_i S_j}{r_{ij}^3} - B \sum_i S_i \qquad (7.1)$$

Der Abstand r wird in Einheiten der Gitterkonstanten gemessen und die $i \neq j$ Summe soll über alle Spinpaare laufen, also jede Bindung nur einfach zählen. Es sei die Nächste-Nachbar-Wechselwirkung ferromagnetisch ($J > 0$) und die Dipol-Dipol-Wechselwirkung antiferromagnetisch ($g < 0$). Das Verhalten in einem externen Feld wäre zwar auch sehr interessant, wir beschränken uns aber zunächst auf den feldfreien Spezialfall ($B = 0$).

Welches System wird durch diese Hamiltonfunktion beschrieben? Das durch Gleichung 7.1 beschriebene System ist ein Modell für einen dünnen ferromagnetischen Film, bei dem die Ausrichtung der magnetischen Momente senkrecht zur Filmebene stattfindet. Neben der aus dem quantenmechanischen Austausch resultierenden Nächsten-Nachbar-Wechselwirkung berücksichtigt man aber noch die magnetische Dipol-Dipol-Wechselwirkung, die für zwei magnetische Momente $\vec{\mu}_1$ und $\vec{\mu}_2$ durch die folgende Gleichung für die potentielle Energie beschrieben wird.

$$V = \frac{\mu_0}{4\pi} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - \frac{3(\vec{\mu}_1 \cdot \vec{r}_{12})(\vec{\mu}_2 \cdot \vec{r}_{12})}{r_{12}^2}}{r_{12}^3} \qquad (7.2)$$

Durch das zweidimensionale Gitter und die dazu senkrechte Ausrichtung der magnetischen Momente stehen diese senkrecht auf ihrer Verbindung, sodass der Bruch im Zähler wegfällt und man direkt der Term aus Gleichung 7.1 erhält.

Das interessanteste an diesem System ist allerdings, dass es durch die beiden konkurrierenden Wechselwirkungen zur Bildung von magnetischen Domänen kommt. Als Domäne bezeichnet man einen Bereich, in dem alle Spins die gleiche Ausrichtung haben. Der Grund für die Ausbildung von Domänen ist, dass es wegen der ferromagnetischen Nächsten-Nachbarn-Wechselwirkung zwar energetisch günstig ist, wenn direkte Nachbarn die gleiche Orientierung haben, es aber aufgrund der langreichweitigen antiferromagnetischen Dipol-Dipol-Wechselwirkung extrem ungünstig wäre, wenn sich diese Ordnung über das

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Realizations:

- long-range interaction is hard to implement efficiently
- my primitive implementation is orders of magnitude too slow to be useful
- too ambitious for the thesis, revisit later ... ?

Hamiltonian

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

Interesting case:

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

$\Rightarrow$ simple model for magnetic domain formation

Physical systems?

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

Motivation
... results obtained by others

- multitude[1] of results are available for the square lattice
- rigorous proof[2], that the ground state is striped for all values of J
- three phases[3]: striped, tetragonal, paramagnetic
  phase transitions correspond to maxima in the specific heat
- tetragonal phase shows 4-fold rotational symmetry[2]
- nematic phase[4] [5] between striped and tetragonal phase for specific values of $J/|g|$

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[1] Rev. Mod. Phys. **72**, 225 (2000)
[2] Phys. Rev. B **51**, 16033 (1995)
[3] Phys. Rev. Lett. **75**, 950 (1995)
[4] Phys. Rev. B **73**, 184425 (2007)
[5] Phys. Rev. B **76**, 054438 (2007)

Motivation

... results obtained by others

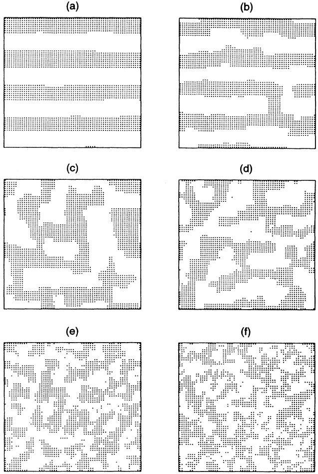


FIG. 1. Typical Monte Carlo magnetic moment configurations at various temperatures in a 64 × 64 system with $J/g = 8.9$. $kT/g = 3.0$ (a), 4.8 (b), 5.2 (c), 6.4 (d), 10.0 (e), and 13.0 (f).

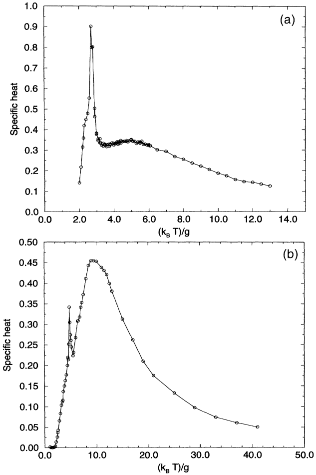


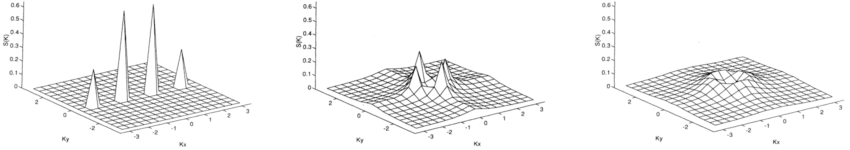
FIG. 2. Variation of the specific heat with temperature for a 64 × 64 system with $J/g = 6.0$ (a) and $J/g = 8.9$ (b).

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

Motivation
... results obtained by others

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?

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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?

Idea: Tiling with replicas of the finite system!

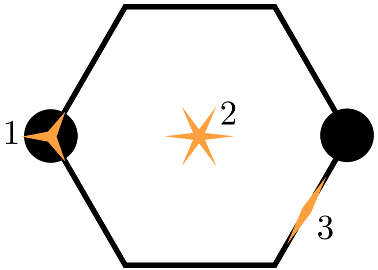
Issues:

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

   (we expect those symmetries to have an effect on the domain structure and don't want to introduce an artificial frustration)

Methods

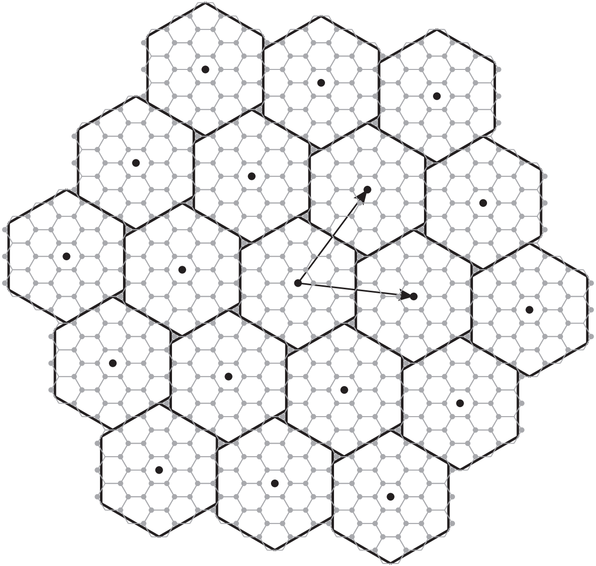
... rotational symmetries of the honeycomb unit cell



1. 3-fold rot. sym. around one of the basis atoms
2. 6-fold rot. sym. around the center of the unit cell
3. 2-fold rot. sym. around the center of nearest-neighbor connections

Methods

... introducing the "aggregation"



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:

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

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

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

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

Methods

... introducing effective interaction coefficients

The $\vec{R}$ summation is independent of the orientation of S_i^z and S_j^z, so it only has to be done once for every pair of spins!

General Ising model Hamiltonian

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

$$J_{ij}^{\text{eff}} = \sum_{\vec{R}} \left[\mathit{\Lambda}(\vec{r}_i, \vec{R} + \vec{r}_j) + \mathit{\Gamma}(\vec{r}_i, \vec{R} + \vec{r}_j) \right]$$

Effective interaction coefficient J_{ij}^{eff} includes:

- exchange interaction, if S_i^z and S_j^z (or any of its copies) are nearest neighbors
- dipole-dipole interaction of S_i^z with S_j^z and all copies of S_j^z

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. direct summation using a (n, m) aggregation for all J_{ij}^{eff}
   (will underestimate all coefficients)
2. calculation of a single $J_{ii}^{\text{eff}\,\prime}$ using a much larger (n, m') aggregation with $m' \gg m$
3. add $J_{ii}^{\text{eff}\,\prime} - J_{ii}^{\text{eff}}$ to all effective interaction coefficients

Simple!

Methods

Summary

- highly symmetric (n, m) aggregation
  - n controls size of the system and time required per MCS
  - m controls accuracy of the effective interaction coefficients
- general Ising model Hamiltonian with effective interaction coefficients
  - coefficients are calculated by direct summation
  - underestimation is approximately compensated in an additional step

Simulation code to be released as free software soon ...

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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!

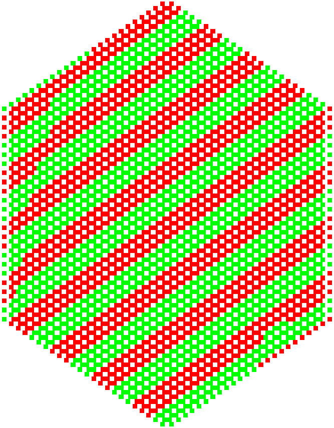
Practical realization?

perform a simulated annealing to get close to the ground state

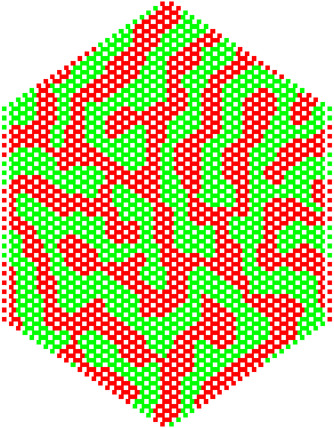
- good enough as the initial state
- information about the ground state can be extrapolated

Results

... the three phases



striped phase at $T = 0.4$

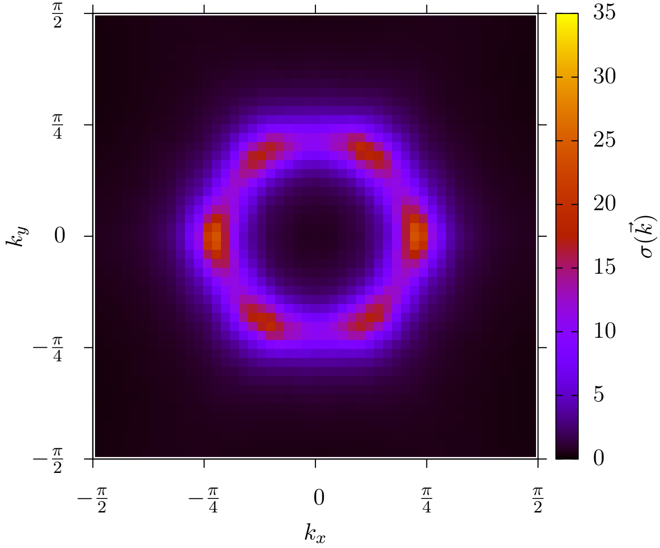


hexatic phase at $T = 1.25$

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

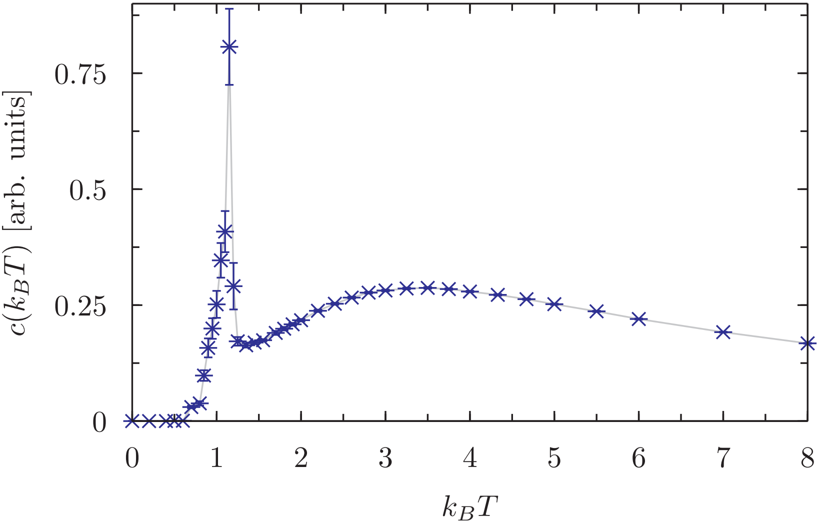
Results

... the hexatic phase's structure factor



Results

... the specific heat



Results
... a summary

- three distinct phases: striped, hexatic, paramagnetic
- hexatic phase reflects the symmetries of the underlying triangular bravais lattice
- striped-hexatic transition: sharp peak in the specific heat
- hexatic-paramagnetic transition: broad shoulder in the specific heat
- honeycomb lattice analogon to the square lattice's nematic phase?