Exercise class 2

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Solution exercise sheet 1

Exercise 1. Ising model

Goal: We start by simulating the 3D Ising model using the Metropolis-based single-spin flip Monte Carlo method. For those who attended last semester's lecture it is (to some degree) a revision.

Write a program for a Monte Carlo simulation to solve the three-dimensional Ising model with periodic boundary conditions. Implement the *single-spin flip* Metropolis algorithm for sampling. As you will have to reuse this code for upcoming exercise sheets, it might be worth to make sure that it is well-structured!

Task 1: Measure and plot the *energy* E, the *magnetization* M, the *magnetic susceptibility* χ and the *heat capacity* C_V at different temperatures T.

Task 2: Determine the critical temperature T_c.

Hint: You should obtain $T_c \simeq 4.51$.

Task 3: Study how your results depend on the system size.

Hint: Start with small systems to reduce the computation time.

Task 4 (OPTIONAL): Save computation time by avoiding unnecessary reevaluations of the exponential function. To achieve this, use an array to store the possible spin-flip acceptance probabilities.

Task 5 (OPTIONAL): Plot the time dependence of M for a temperature $T < T_c$.

Hint: For small systems you should be able to observe sign-flips in M.

Implementation

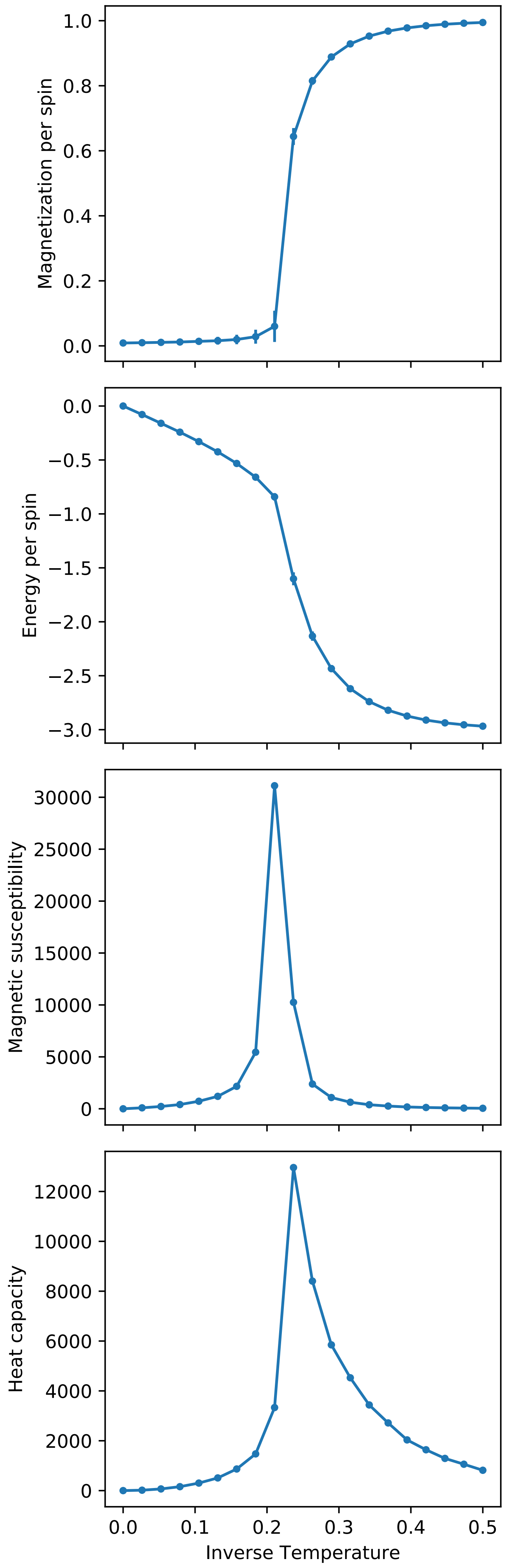
Show code

Compare with python

Results

Parameters:
L=20
$N_{thermalization}$=100L^3
N_{sample} = 3000
$N_{subsweep}$=3L^3

- $0.2 < 1/T_c = \beta_c < 0.25$
- Larger error at T_c
  → critical slowing down
- Larger system size: more abrupt phase transition
  → increased peaks of χ and C_V



Exercise sheet 2

Critical exponents

Behavior near T_c

- $M(T) \propto (T_c - T)^{\beta}, \, T < T_c$
- $M(T = T_c, H) \propto H^{1/\delta}$
- $\chi(T) \propto |T_c - T|^{-\gamma}$
- $C_V(T) \propto |T_c - T|^{-\alpha}$
- $\xi(T) \propto |T_c - T|^{-\nu}$

Exponent	$d = 2$	$d = 3$
α	0	0.110(1)
β	1/8	0.3265(3)
γ	7/4	1.2372(5)
δ	15	4.789(2)
η	1/4	0.0364(5)
ν	1	0.6301(4)

Describe behavior near phase transition

Scaling laws

The 6 critical exponents are connected:

$$\alpha + 2\beta + \gamma = 2 \quad \text{(Rushbrooke)},$$

$$\gamma = \beta(\delta - 1) \quad \text{(Widom)},$$

$$\gamma = (2 - \eta)\nu \quad \text{(Fisher)},$$

$$2 - \alpha = d\nu \quad \text{(Josephson)},$$

Number of independent critical exponents: 2

Universality

Critical exponents **only depend on fundamental system** properties such as dimension or symmetries.

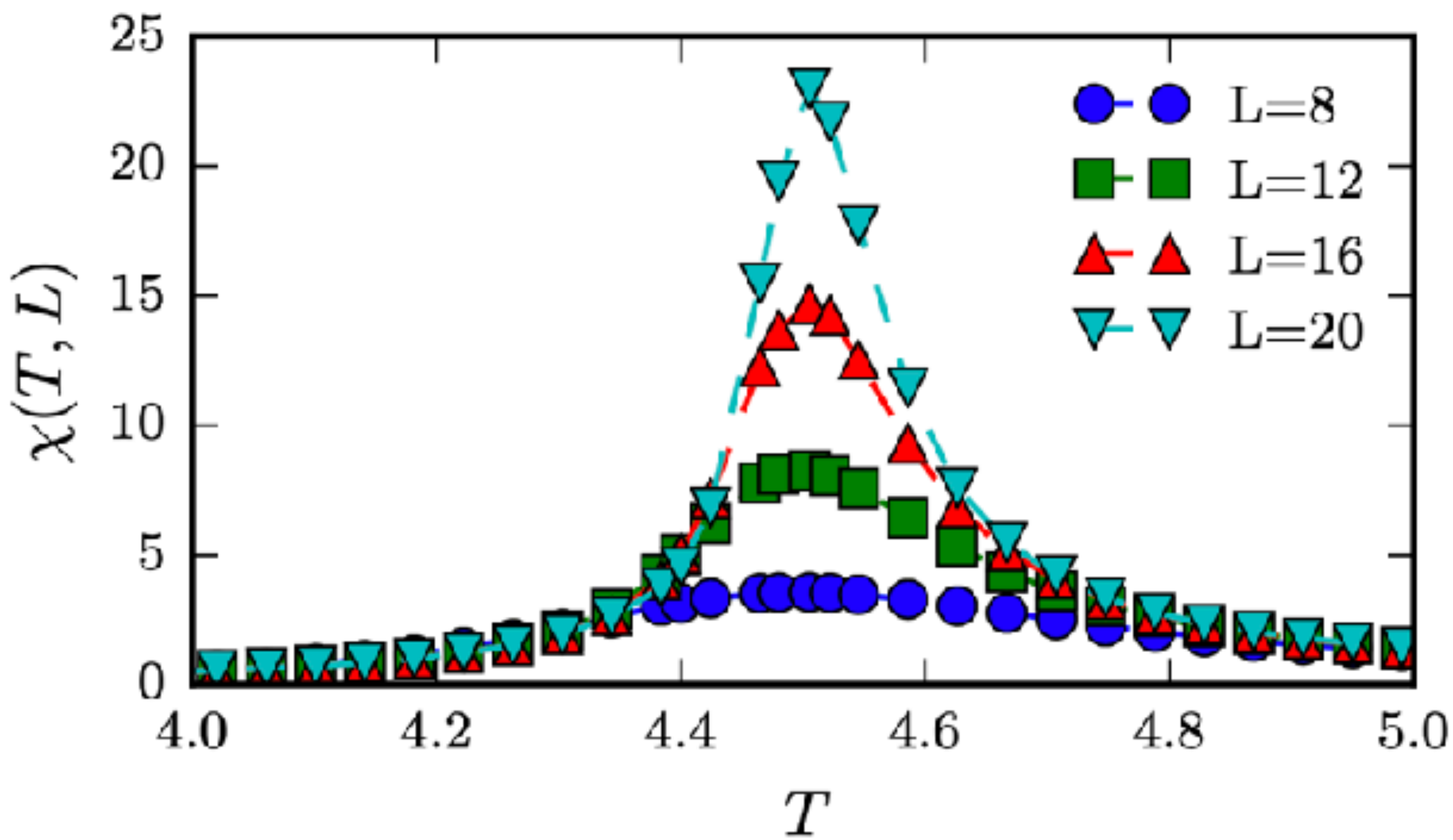
→ universal

All systems belonging to a certain universality class share the same **critical exponents**

Finite size scaling analysis

- χ, C_V and ξ diverge at T_c for $L \to \infty$
- Finite size:

$\propto L^{\gamma/\nu}$



Finite size scaling analysis

Problem:

- We have:

MC program for small Ising systems

- We want:

Behavior of large systems (thermodynamical limit)

Approach:

- Simulate small systems of different size
- Find critical exponents

→ Critical exponents allow predictions for large systems

Exercise sheet 2

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Exercise sheet 02

FS 2020
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Exercise 1. Ising model: Finite size scaling analysis

> *Goal: In numerical simulations we are only able to tackle relatively small system sizes whereas real physical systems are usually much larger.* Finite size scaling analysis *is a technique which allows us to get good approximations for the thermodynamic limit.*

Task 1: Use your program of the first exercise sheet to perform simulations of the 3D Ising system for different system sizes to determine the critical exponents γ and ν .

Hint: Use the finite size scaling relation of the magnetic susceptibility and the fact that the critical temperature is given by $T_c \approx 4.51$.

You might find the following points useful:

- You can get a first estimate for the ratio γ/ν by plotting $\chi_{\max}$ as a function of the system size.
- Vary γ/ν and $1/\nu$ until you get the best possible data collapse. Judge the quality of the data collapse "by eye".

Task 2 (OPTIONAL): Repeat the same process for the specific heat.

Instructions

- Simulate small 3D Ising systems of different size
- Use the scaling relation

$$\chi(T,L) = L^{\gamma/\nu} F_\chi\left((T-T_c)L^{1/\nu}\right)$$

to determine γ and ν

- $\max_T \chi(T,L) = \chi(T=T_c,L) \propto L^{\gamma/\nu}$

  → plot maxχ as a function of L (logarithmic) to obtain γ/ν
- plot $\chi(T,L)L^{-\gamma/\nu}$ as a function of $(T-T_c)L^{1/\nu}$

  → vary γ and ν to obtain the best data collapse