

# Exercise class 3

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# Solution exercise sheet 2

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Computational Statistical Physics

Exercise sheet 02

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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  $\gamma$  and  $\nu$ .

*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  $\gamma/\nu$  by plotting  $\chi_{\max}$  as a function of the system size.
- Vary  $\gamma/\nu$  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.

# Solution exercise sheet 2

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Goal: critical exponents  $\gamma$ ,  $\nu$  from finite size scaling

Approach

1. At  $T_c$ :  $\max_T \chi(T, L) = \chi(T = T_c, L) \propto L^{\gamma/\nu}$   
→ plot  $\max \chi$  as a function of  $L$  (logarithmic) to obtain  $\gamma/\nu$
2.  $\chi(T, L)L^{-\gamma/\nu}$  vs.  $(T - T_c)L^{1/\nu}$  is independent of  $L$   
→ vary  $\gamma$  and  $\nu$  to obtain the best data collapse

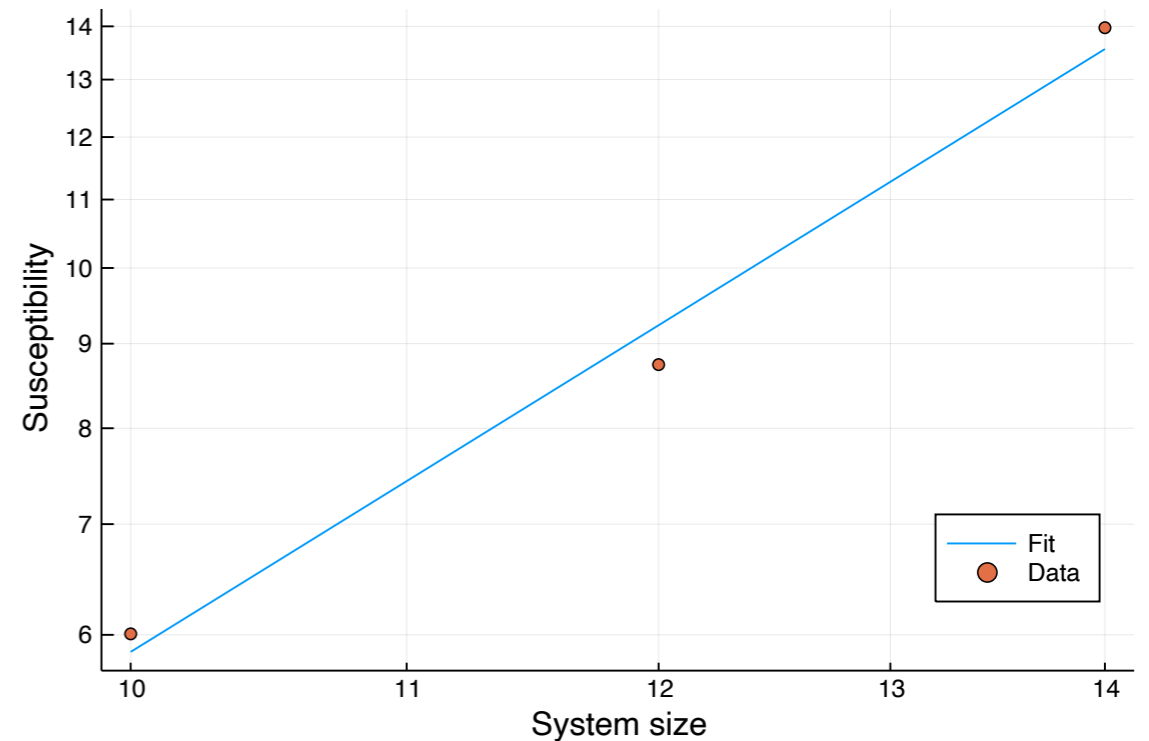
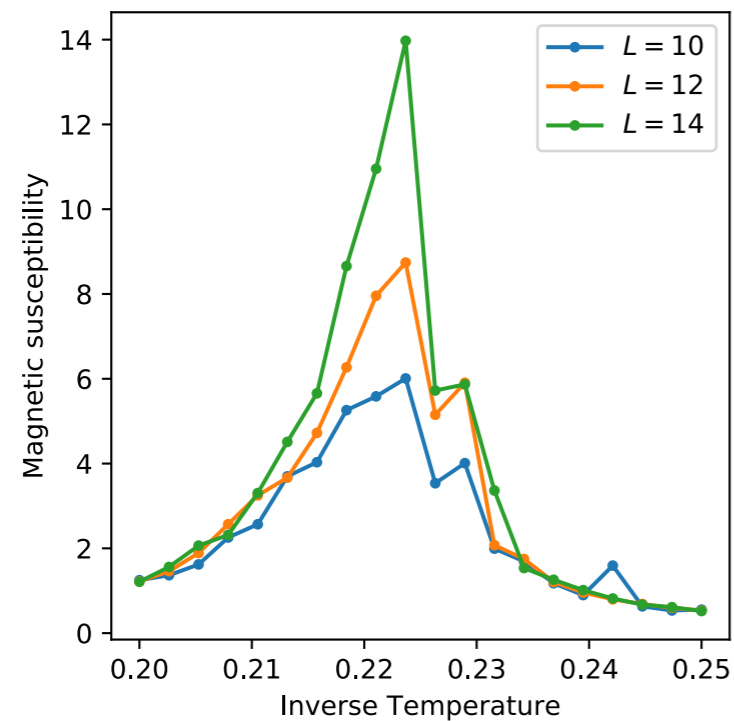
# 1. approach

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Solution:

Simulate system for  
 $L=10$ ,  $L=12$ ,  $L=14$

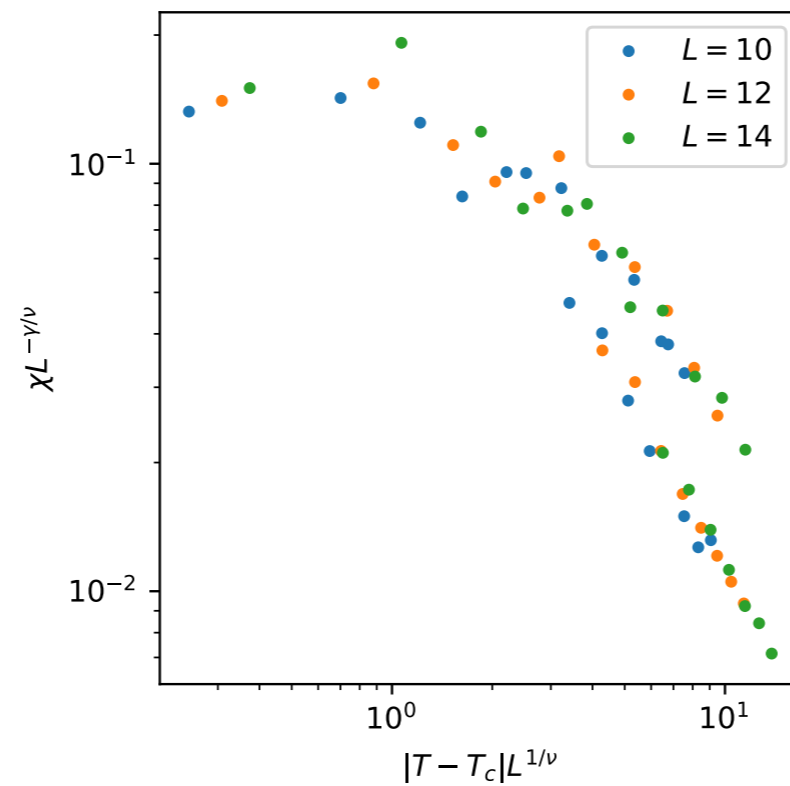
Loglog-plot of  $\chi_{max}$  vs  $L$   
slope:  $\gamma/\nu$



## 2. approach

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- Plot  $\chi(T, L)L^{-\gamma/\nu}$  vs.  $(T - T_c)L^{1/\nu}$
- Vary  $\gamma$  and  $\nu$  to obtain the best data collapse



# Exercise sheet 3

# Cluster algorithms

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- Larger system size  $\rightarrow$  longer simulation time
- Critical slowing down
- Wait long for statistically independent samples

Aim:

Reduce computation time by flipping multiple spins

Potts model: 
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j} - H \sum_i \sigma_i \quad \sigma_i \in \{1, \dots, q\}$$

For  $q=2$ : equivalent to Ising

# Swendsen-Wang algorithm

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## Swendsen-Wang algorithm

- Occupy the bonds with probability  $p = 1 - e^{-\beta J}$  if sites are in the same state.
- Identify the clusters with the Hoshen-Kopelman algorithm.
- Flip the clusters with probability  $1/2$  for Ising or always choose a new state for  $q > 2$ .
- Repeat the procedure.



# Wolff algorithm

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## Wolff algorithm

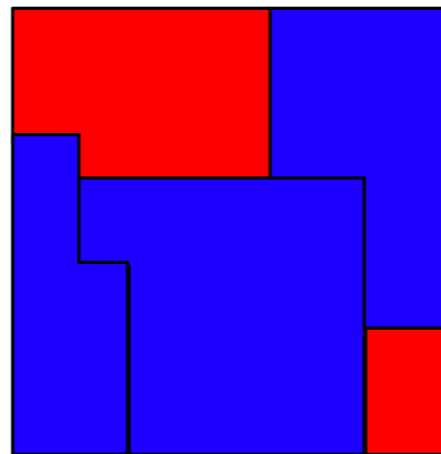
- Choose a site randomly.
- If the neighboring sites are in the same state, add them to the cluster with probability  $p = 1 - e^{-\beta J}$ .
- Repeat this for any site on the boundaries of the cluster, until all the bonds of the cluster have been checked exactly once.
- Choose a new state for the cluster. Flip cluster with  $p=1$
- Repeat the procedure.

# Comparison

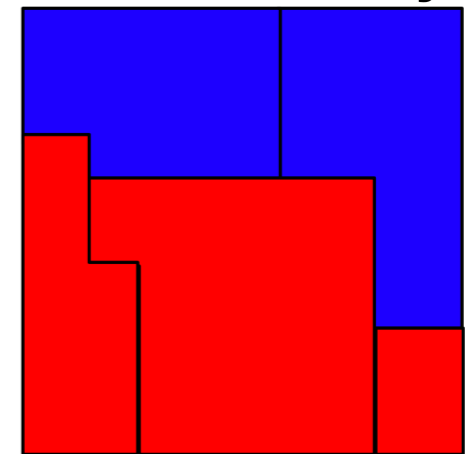
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Swendsen-Wang

Identify all clusters

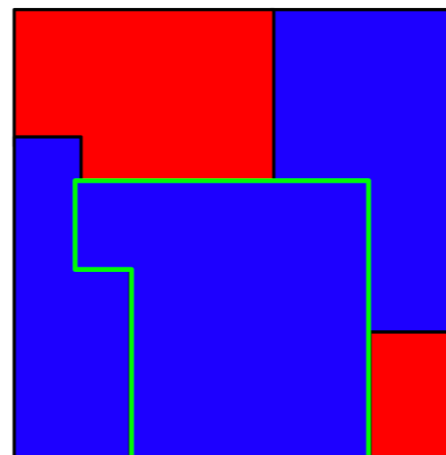


Flip each cluster randomly

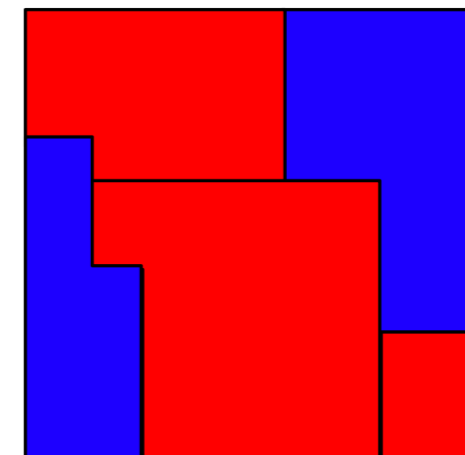


Wolff

Select a single cluster



Flip it



slightly better autocorrelation time by focusing on larger cluster and always accepting a flip

# Autocorrelation time

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MC measurements are correlated:

- Distribution correct
- Error scales as  $1/\sqrt{\text{independent}}$

Autocorrelation function:

$$\rho_{XX}(\Delta t) = \frac{\langle (X_t - \bar{X})(X_{t+\Delta t} - \bar{X}) \rangle_t}{\sigma^2}$$

Discrete time:

$$\hat{\rho}(k) = \frac{\sum_{s=1}^{n-k} (x_{s+k} - \bar{x})(x_s - \bar{x})}{\sum_{t=1}^n (x_t - \bar{x})^2}, \text{ for } k = 1, \dots, n-1$$

Julia: using StatsBase: autocor

# Autocorrelation time

- The autocorrelation time can be obtained from the exponential ansatz:  $\rho = e^{-t/\tau}$
- Alternative: integrated autocorrelation time

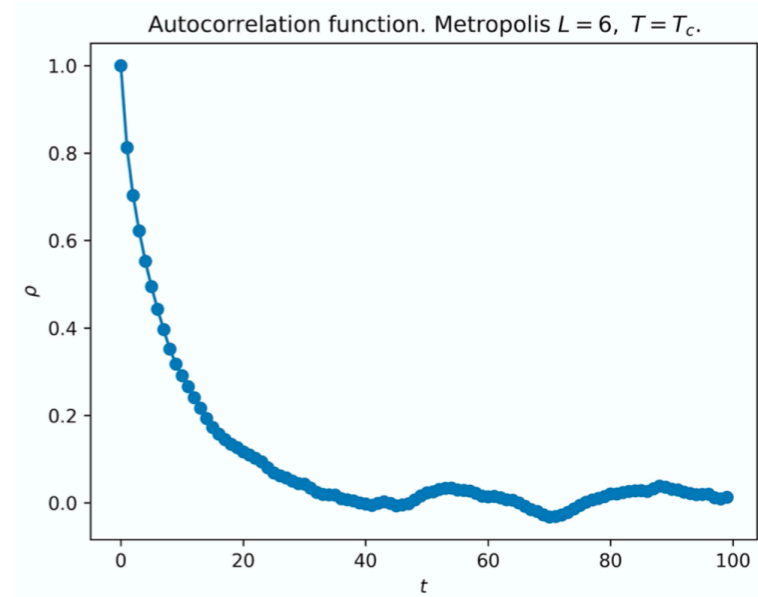
$$\tau_{\text{int}} = 1 + 2 \sum_{t=1}^{N_{\text{cut}}} \left(1 - \frac{t}{N}\right) \rho(t)$$

$$\text{For } \tau_{\text{int}} \gg 1 \\ \tau_{\text{int}} \approx 2 \tau_c$$

For both methods a cutoff is needed:

- Noisy at large time gaps
- Compensation issue

$$\sum_{k=1}^{n-1} \hat{\rho}(k) = -\frac{1}{2}$$



# Exercise 3

## Cluster algorithms

Cluster algorithms can be used to reduce the critical slowing down substantially. In this task you have to simulate either the 3D Ising model or the Potts model with  $q = 2$ . Choose either the Swendsen-Wang or the Wolff algorithm and compare with the Metropolis algorithm from exercise sheet 1. Optionally implement all three.

The difference between the two cluster algorithms is that in Swendsen-Wang all clusters will be determined and flipped with a probability  $1/2$  (Ising model), or randomly get a new value (Ising or Potts model). In the Wolff algorithm only one cluster is chosen by randomly choosing a spin on the lattice. In this case the cluster will be flipped (Ising model) or gets a new state (different from the old one) (Ising or Potts model).

- (a) Remember from the lecture that in the Potts model the probability for connecting sites in the same state is :

$$p = 1 - \exp(-\beta J) \quad (1)$$

What is the connection probability in the Ising model?

- (b) Implement Swendsen-Wang or Wolff (optionally both).  
(c) Check your code by plotting the binder cumulants or the magnetic susceptibility around  $T_c$ .  
(d) Compare the performance of the algorithm and show that in the cluster algorithms the critical slowing down is substantially reduced. Measure the runtime and compute the linear autocorrelation time  $\tau$ , relative to the observable E or M, of the cluster algorithm and compare with Metropolis.

Remember that you can extrapolate  $\tau$  from the autocorrelation series

$$\rho_{XX}(\Delta t) = \frac{\langle (X_t - \bar{X})(X_{t+\Delta t} - \bar{X}) \rangle_t}{\sigma^2} \quad (2)$$

Report a table with  $\tau$  and the Monte Carlo speed defined as

$$MC_{\text{speed}} = \frac{\text{sweeps}}{\text{time}} \frac{1}{\tau} \quad (3)$$

for at least three temperature values, say  $T_c$ ,  $T_c + 1$ ,  $T_c - 1$ , and fixed size. Make another table with temperature fixed at  $T_c$  and varying lattice size. Interpret the results.

- (e) Optional: include the timing of the official solution to exercise 01 in your table, so that you have a fixed reference point on your hardware. Mind that the code is very likely not optimal, and if yours outperforms it, you should submit it to the TAs.

# Instructions

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- Implement Swendsen-Wang or Wolff
- Check your code and compare  $\chi$
- Measure the runtime
- Calculate the autocorrelation series  $\rho$
- Calculate the autocorrelation time
- Calculate the  $MC_{speed}$
- Look at different temperatures around  $T_c$
- Look at different L