Free-energy barriers in spin glasses: mean-field vs short-range models

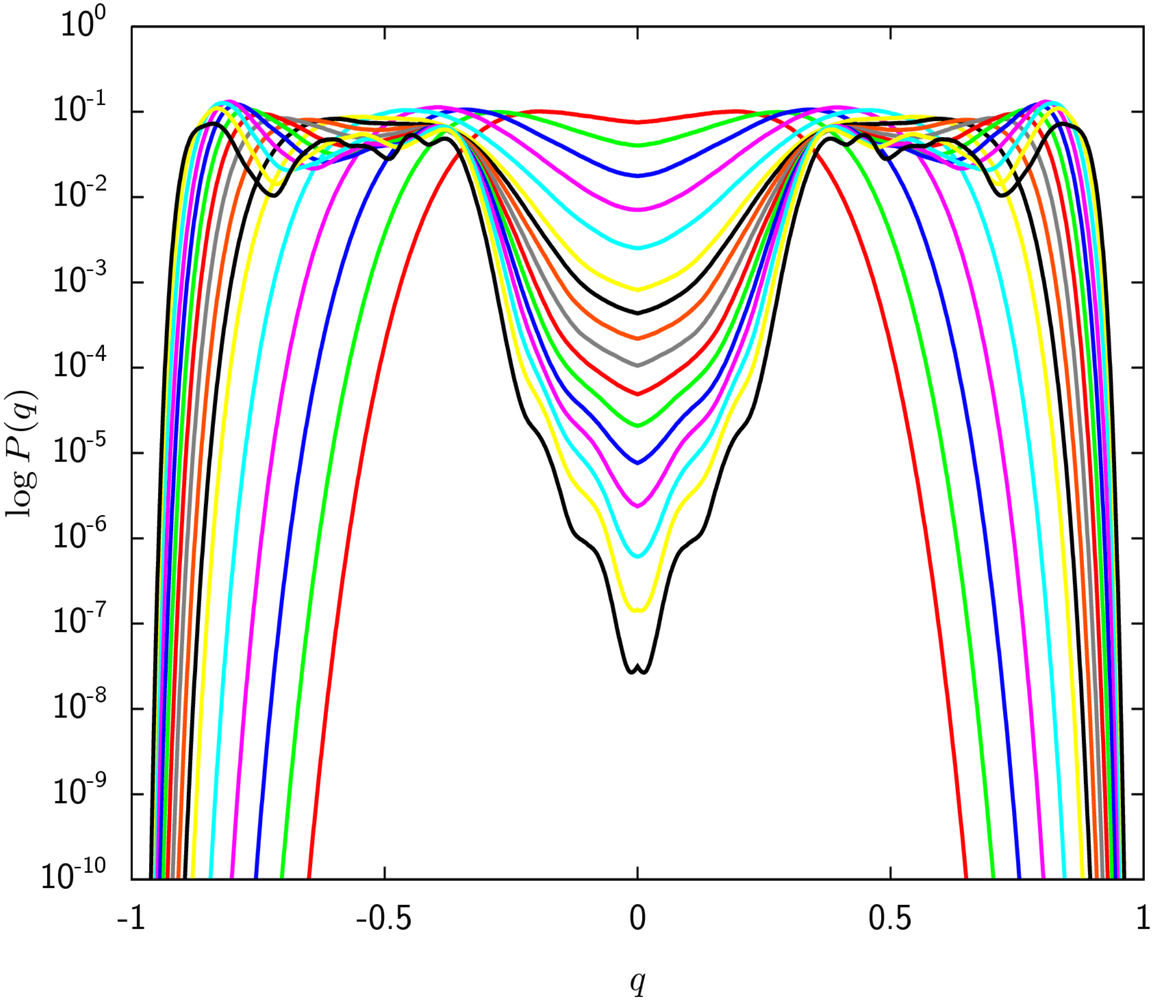
Elmar Bittner
Universität Leipzig

Collaborators: A. Nußbaumer and W. Janke

Spring School on Monte Carlo Simulations of Disordered Systems
Leipzig, April 4, 2008.

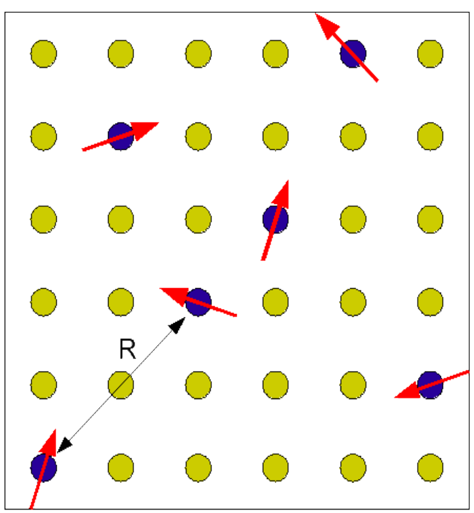
Outlook

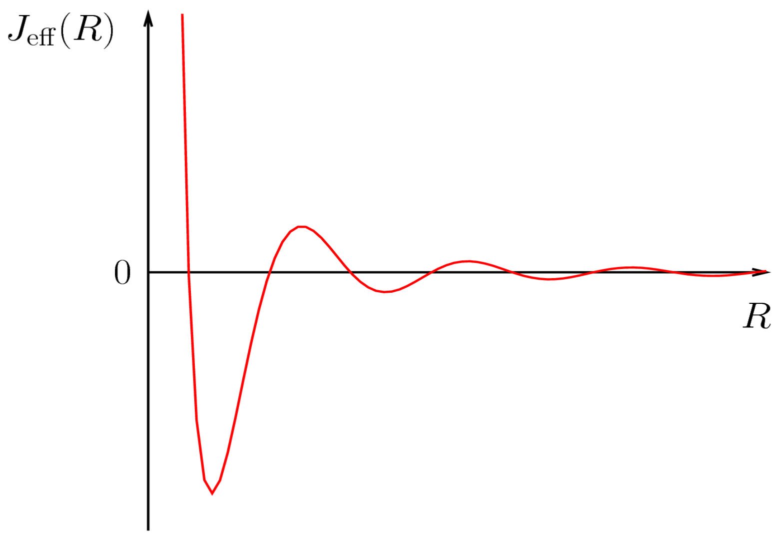
- Intro
- Models
- Problems
- Algorithms
- Motivation
- Results



Spin Glass Systems

- **There are real experimental spin glass systems.**
  (dilute solutions of magnetic transition metal impurities in noble metal hosts, for instance Au-2.98% Mn or Cu-0.9% Mn)

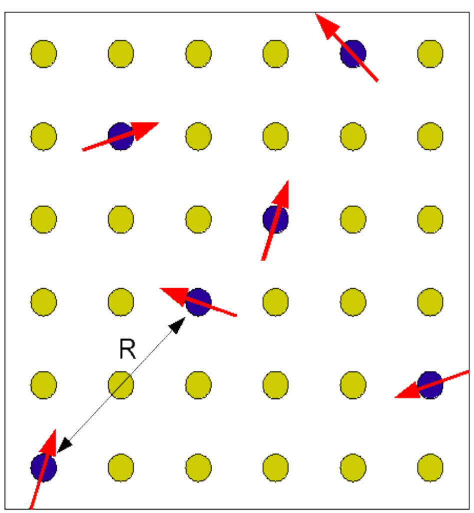


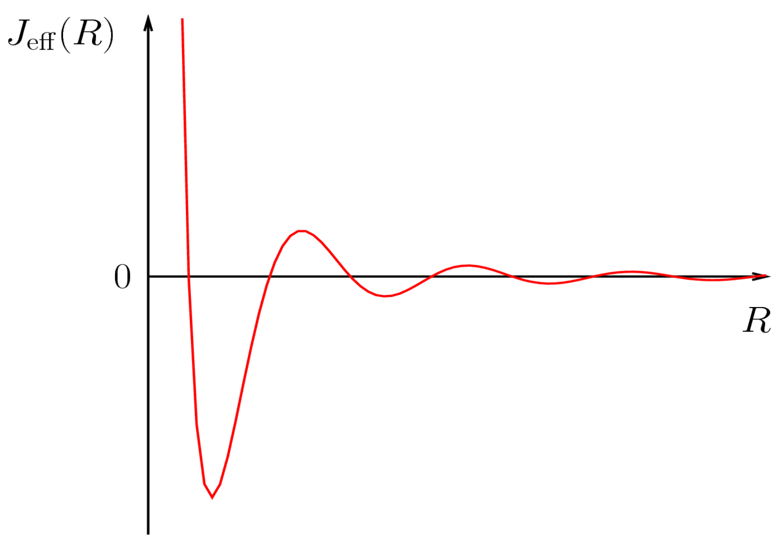


RKKY interaction: $J_{eff}(R) = J_0 \frac{\cos(2k_F R)}{R^3}, k_F R \gg 1, k_F$ **Fermi wave number**

Basic ingredients for spin-glass behaviour

- **randomness** in course of the dilution process the positions of the impurity moments are randomly distributed
- **competing interactions** due to the oscillations in the effective interaction as a function of the distance R





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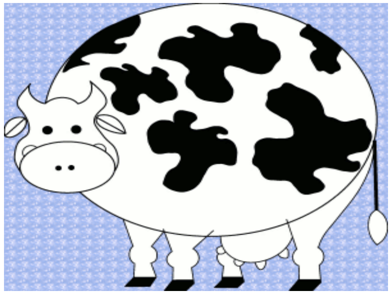


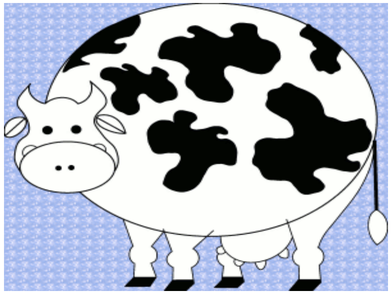
Spherical Cow

Most theory uses the simplest model with these ingredients:

the Edward-Anderson Model (EA)

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i h_i S_i$$

with $S_i = \pm 1$ lie on a regular lattice and the quenched coupling constants J_{ij}.



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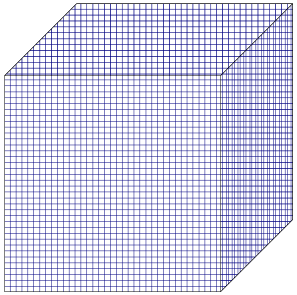
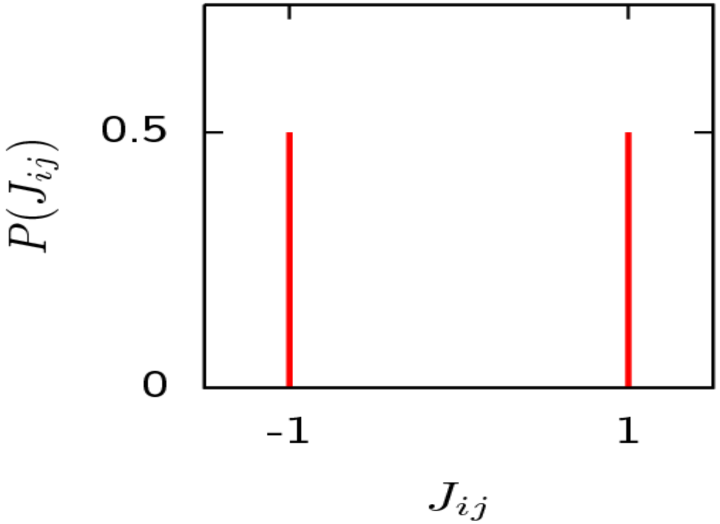


$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i h_i S_i$$

bimodal distribution $J_{ij} = \pm 1$



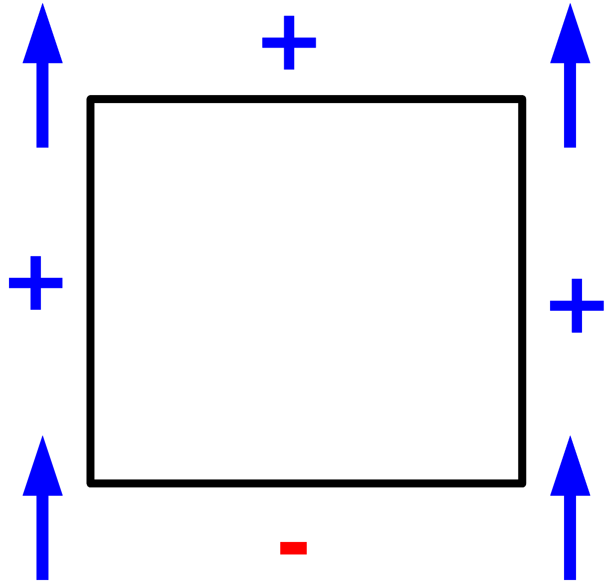
3D: $T_c \sim 1.16, h_i = 0$

[M. Palassini and S. Caracciolo, Phys. Rev. Lett. 82, 5128 (1999)]

no solution

What is a spin glass?

A system with disorder (randomness) and frustration.



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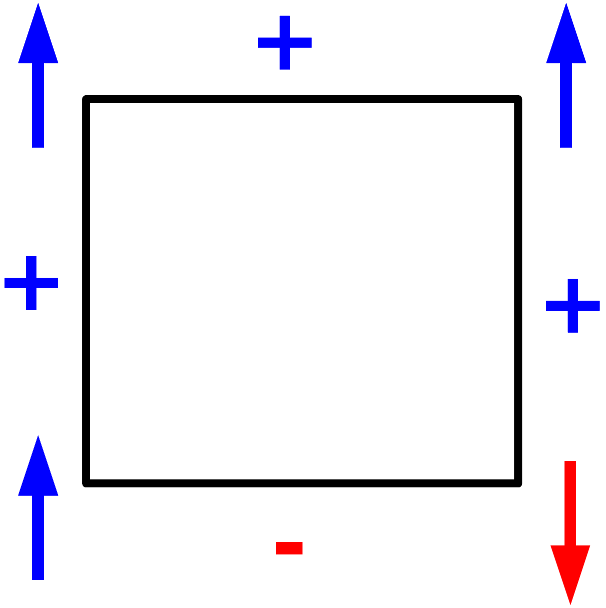
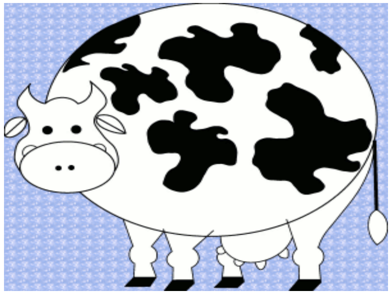
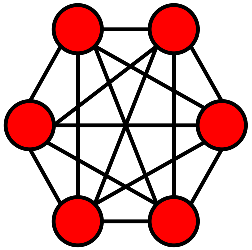




Another Cow

fully connected



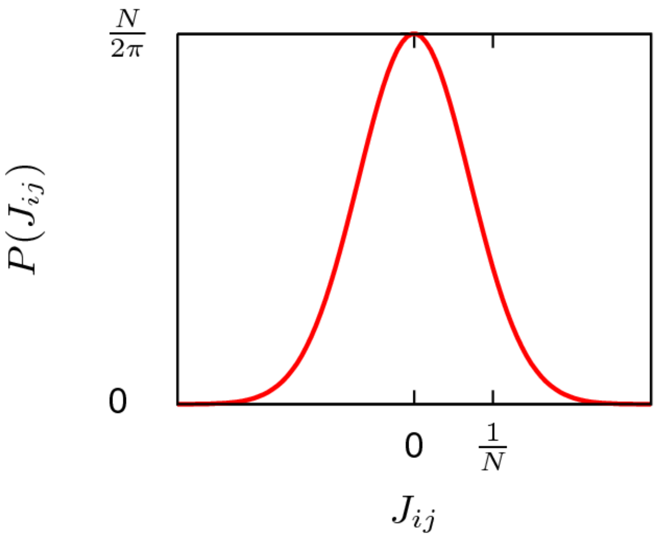
the Sherrington-Kirkpatrick Model (SK)

$$H = -\sum_{i<j} J_{ij} S_i S_j - \sum_i h_i S_i$$

Gaussian distribution with:

$$\langle J_{ij} \rangle = 0$$

$$\langle J_{ij}^2 \rangle - \langle J_{ij} \rangle^2 = \frac{J}{N}$$



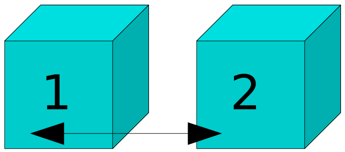
N is the number of spins.

$$T_c = 1, h_i = 0$$

mean field, Parisi's replica solution [PRL 43 (1979) 1754]

Overlap parameter

$$q = \frac{1}{N} \sum_{i=1}^{N} S_i^1 S_i^2$$



for to (real) replica S_i^1, S_i^2 **and given coupling constants** $J = \{J_{ij}\}$

$P_J(q)$ **probability density of** q

$x_J(q) = \int dq' P_J(q')$ **cumulative distribution of** $P_J(q)$

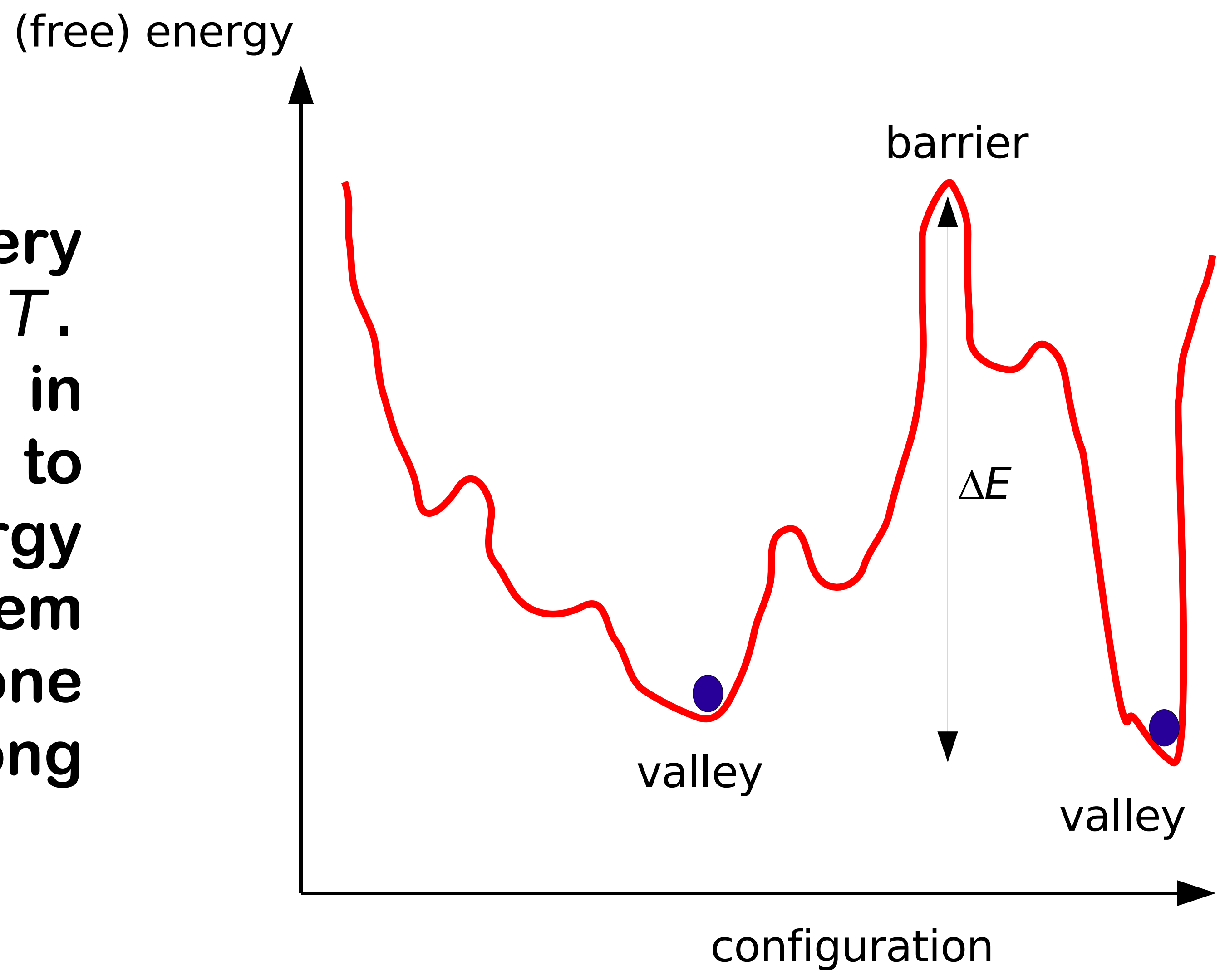
average over the disorder

$$P(q) = [P_J(q)]_{av} = \frac{1}{N_J} \sum_J P_J(q)$$

$$x_J(q) = [x_J(q)]_{av} = \frac{1}{N_J} \sum_J x_J(q)$$

Slow Dynamics

The dynamics is very slow at low *T*. System is not in equilibrium due to complicated energy landscape: system trapped in one "valley" for long times.



Algorithms

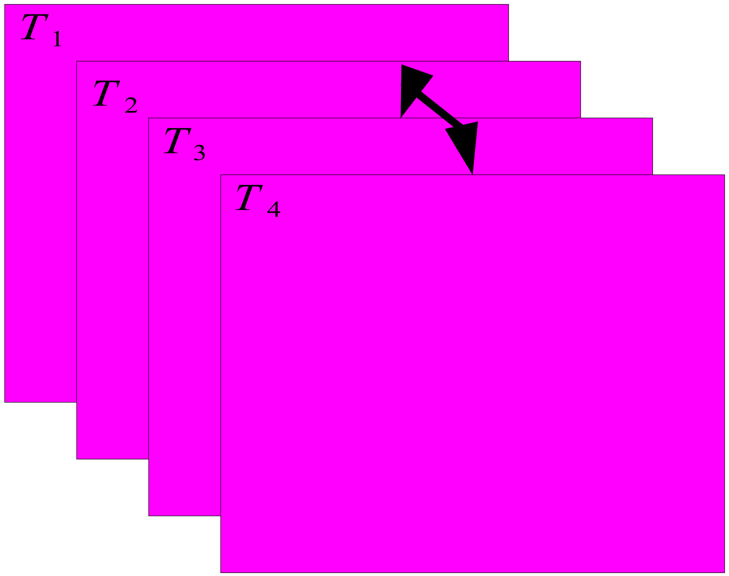
Parallel tempering (PT)

Exchange at regular intervals system i and $i+1$ with

$$P(i, i+1) = \min[1, \exp(\Delta\beta\Delta E)]$$

expectation values for single system:

$$\langle A \rangle_{T_i} = \langle A_i \rangle$$



System can decorrelate at high T

[K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. 65 (1996) 1604]

Talk of H. Katzgraber

Algorithms

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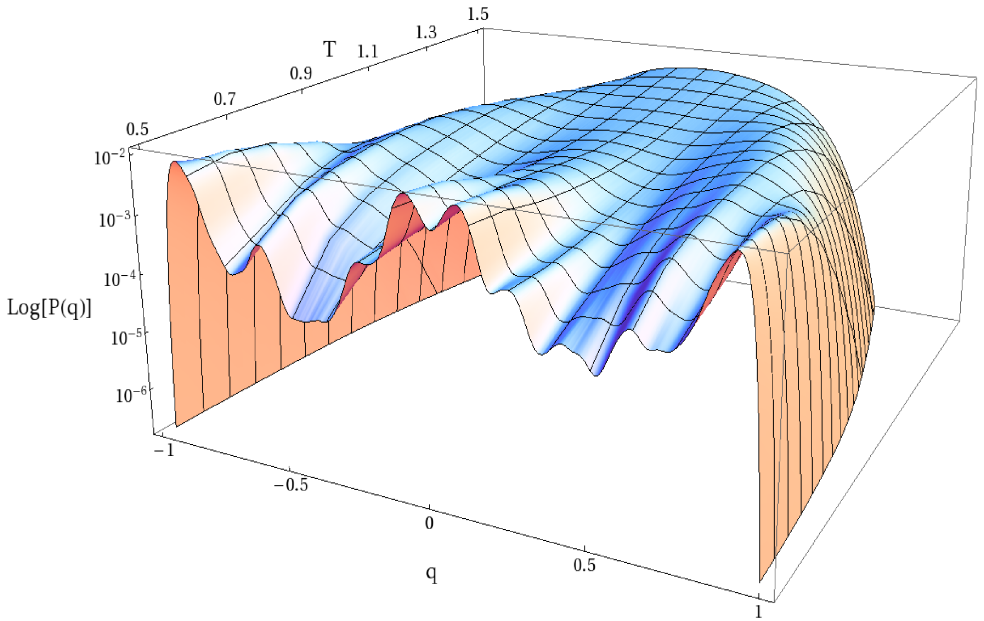

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Algorithms

Multioverlap Algorthim (MuQ)

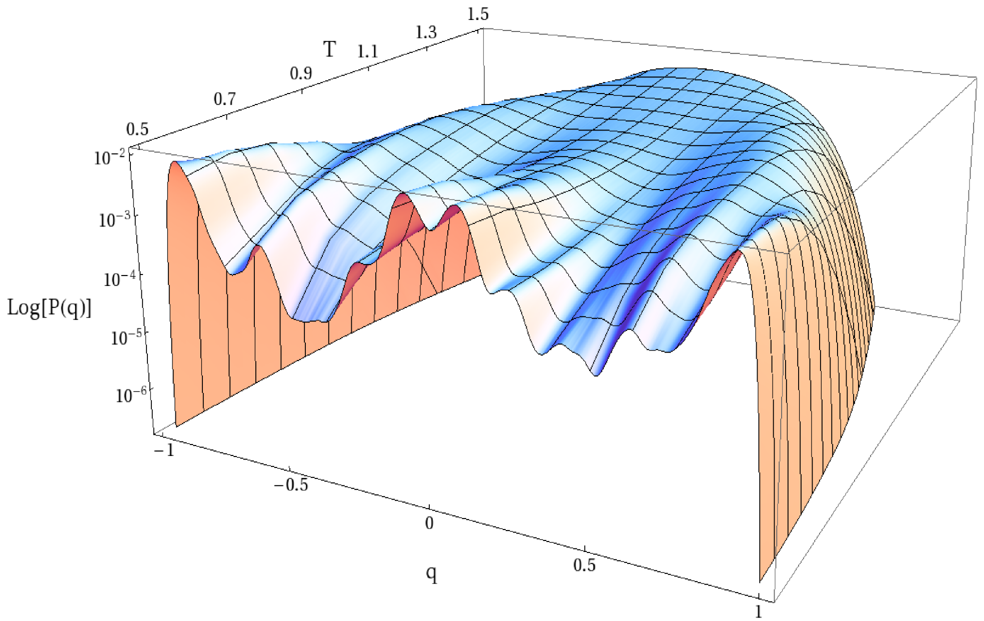
non-Boltzmann sampling with multioverlap weights $W(q)$**:**

$$\exp[-\beta H] W(q)$$

canonical expectation values:

$$\langle O \rangle^{\mathrm{can}} = \frac{\langle W O \rangle}{\langle W \rangle}$$

[B. Berg, W. Janke, PRL 80 (1998) 4771]



System can reach highly suppressed states

Algorithms

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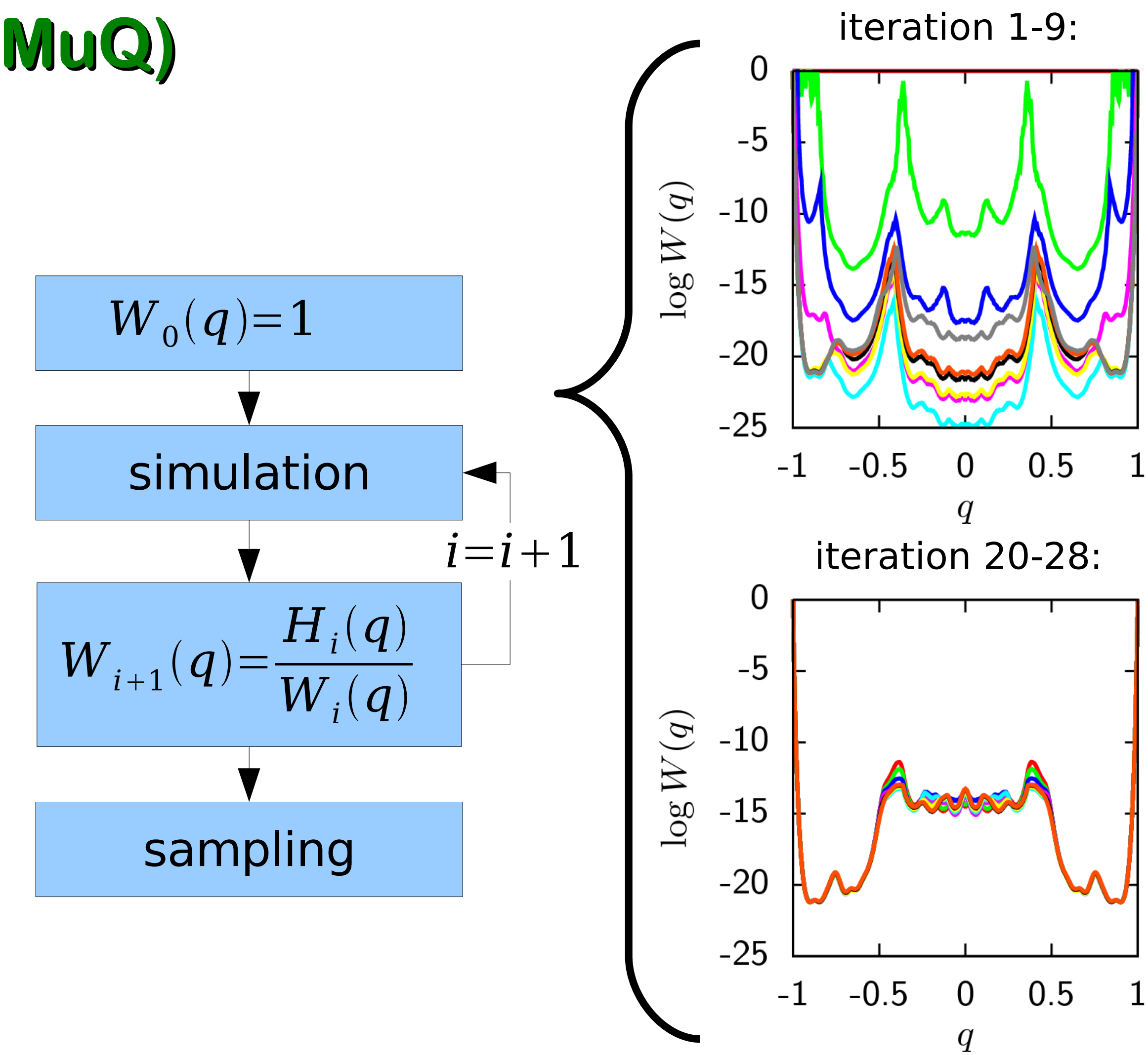

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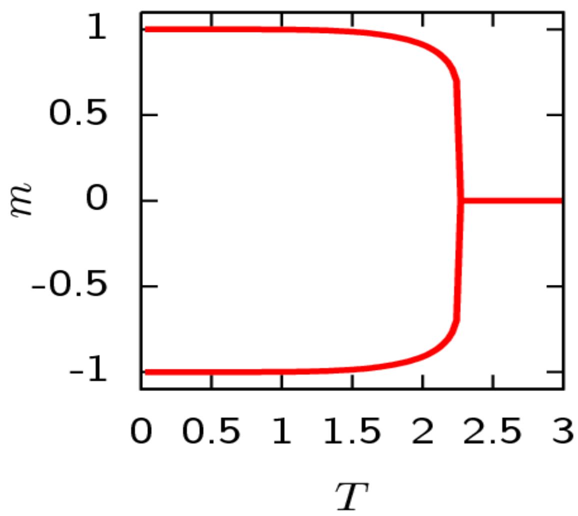
The 2D Ising Model

$$H = -\sum_{\langle i,j \rangle} J S_i S_j$$

$$S_i = \pm 1$$



$$T_c = \frac{2}{\log(\sqrt{2}+1)} = 2.269\ldots$$

$$m_0 = (1 - \sinh^{-4}(\frac{2}{T}))^{\frac{1}{8}}$$

Onsager solution, Onsager-Yang solution

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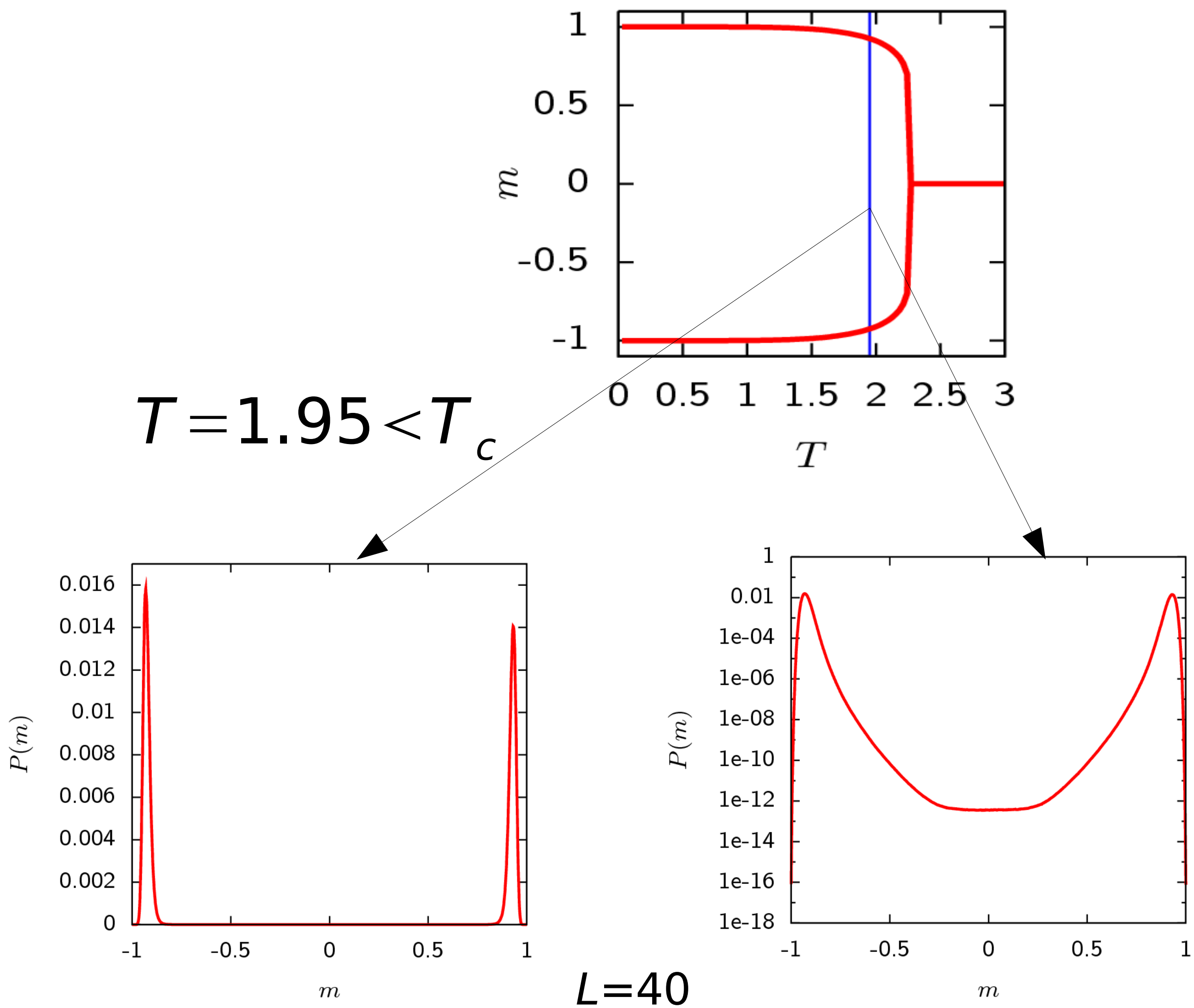

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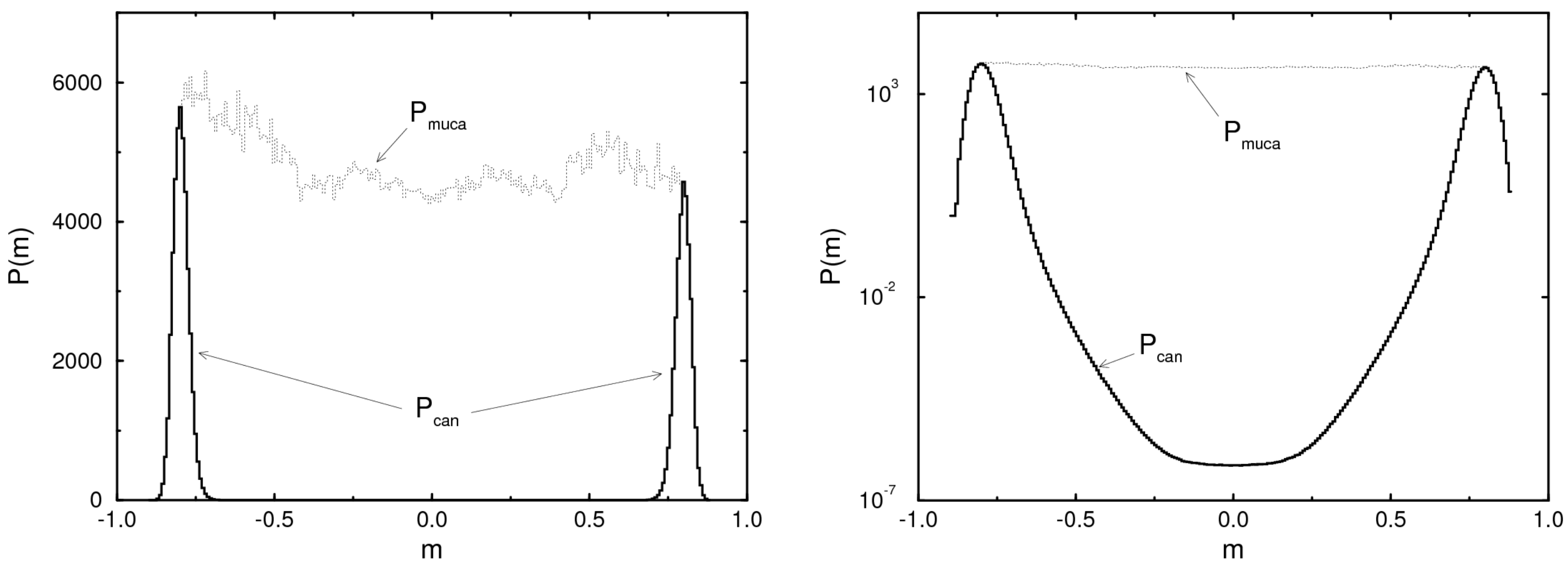
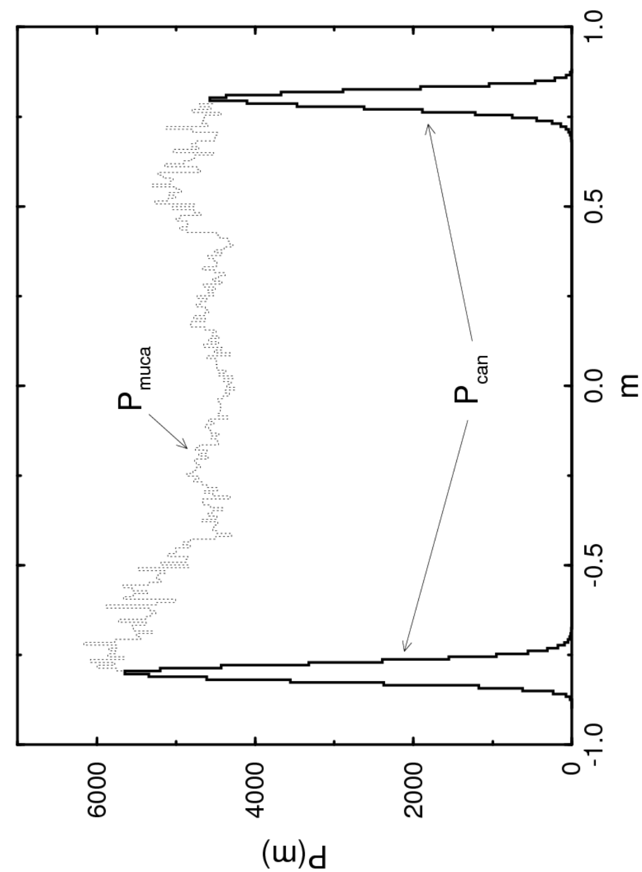
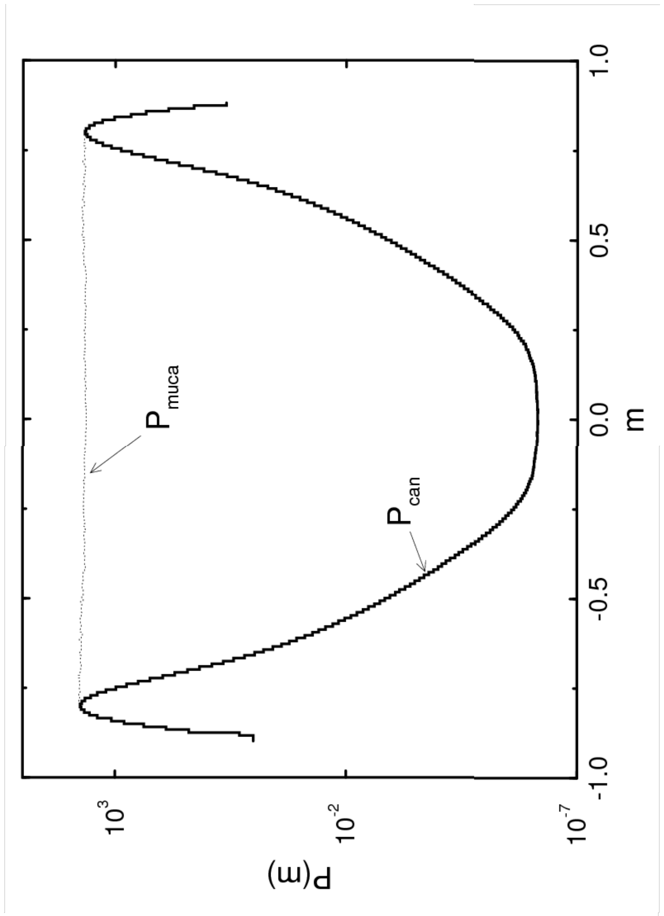


multimagnetical simulation

The 2D Ising Model





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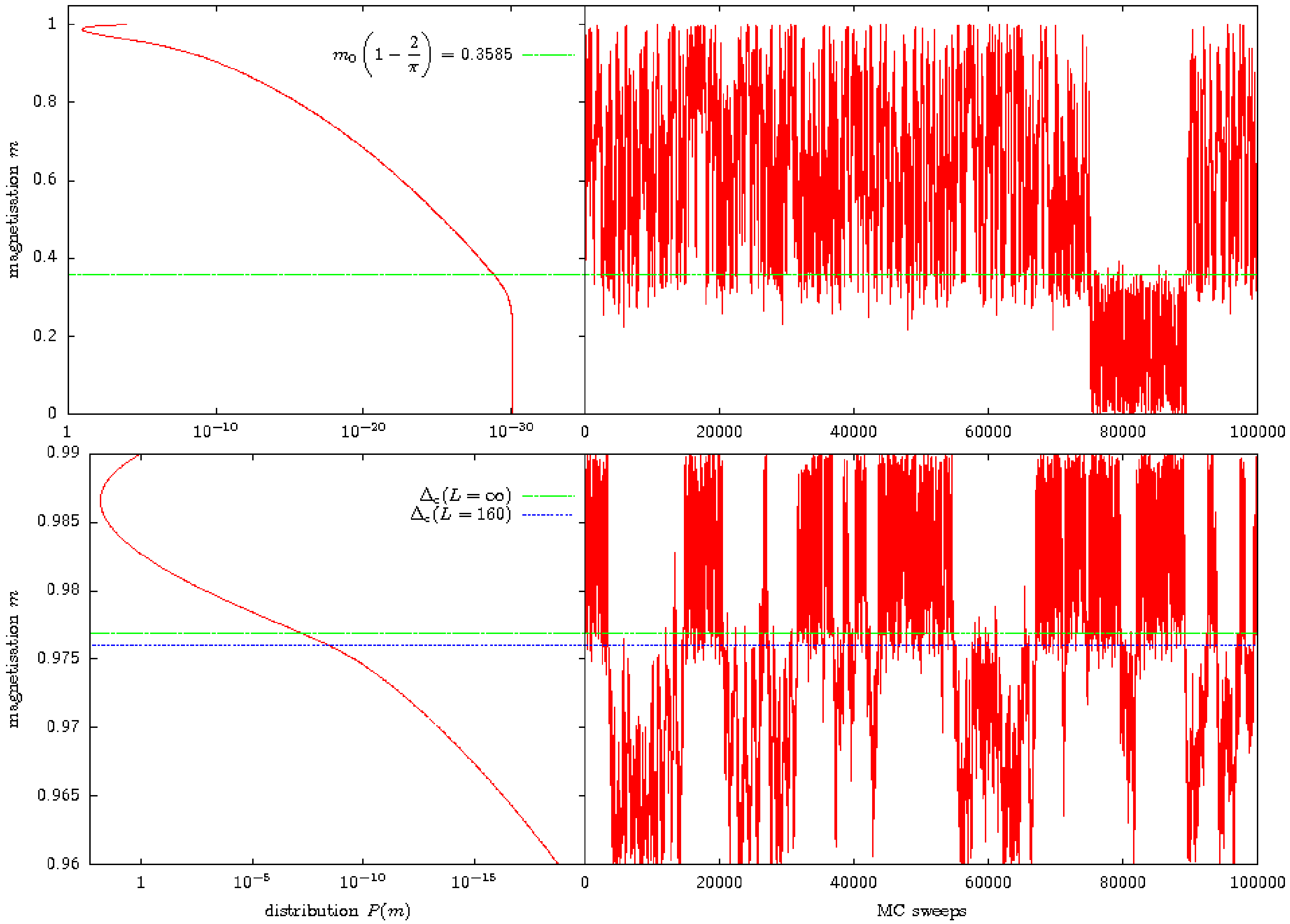
The 2D Ising Model

But there are still problems:



droplet/strip

evaporation/
condensation

The 2D Ising Model

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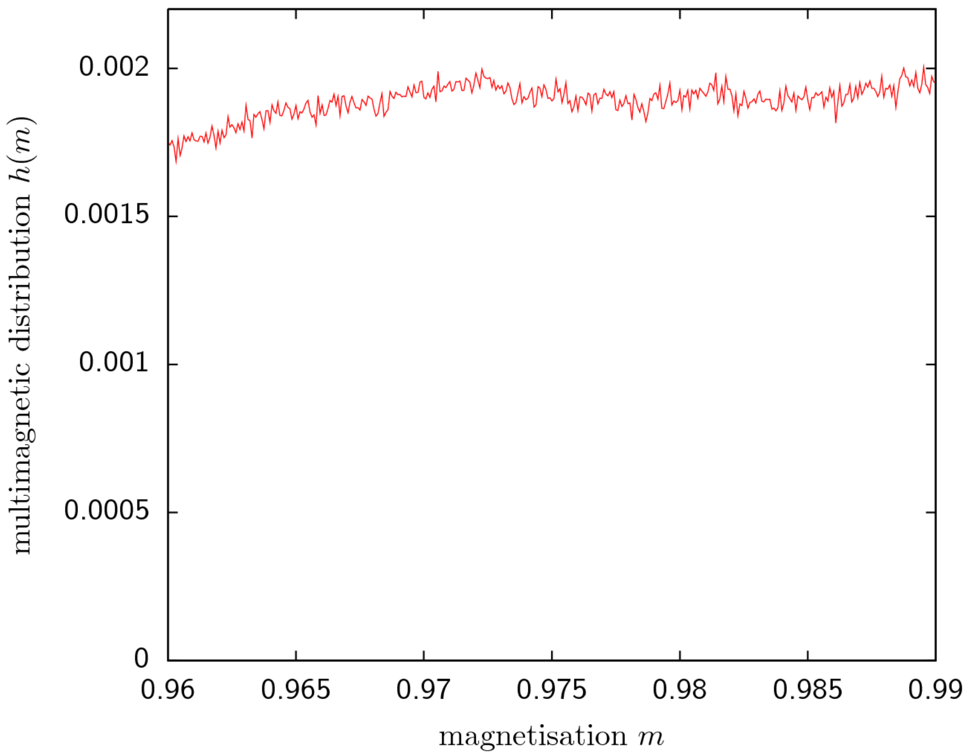

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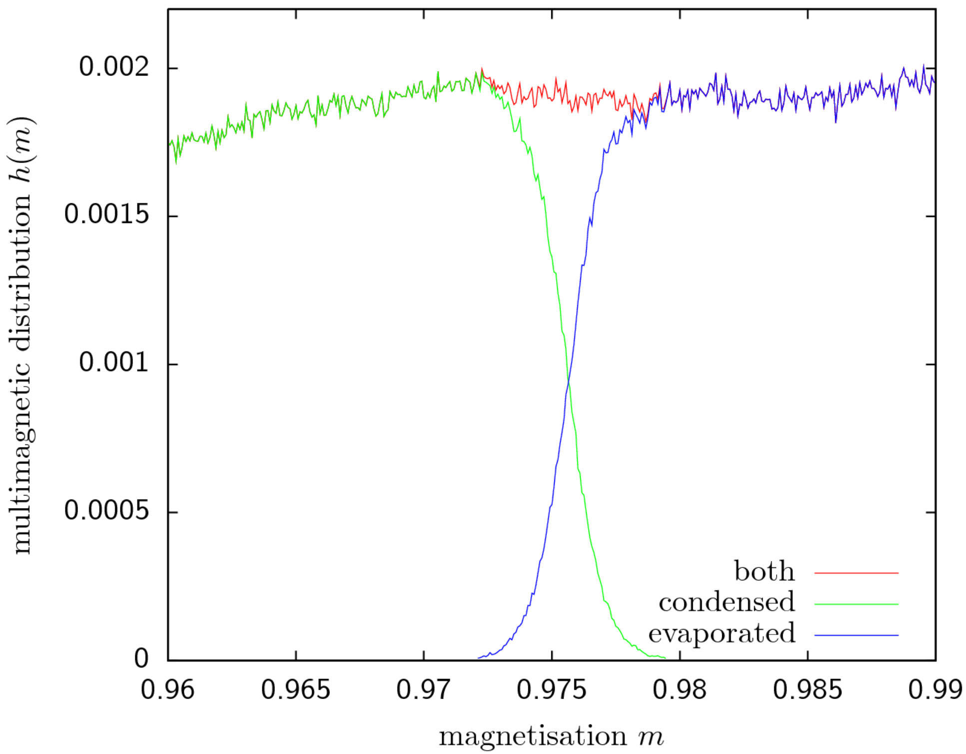
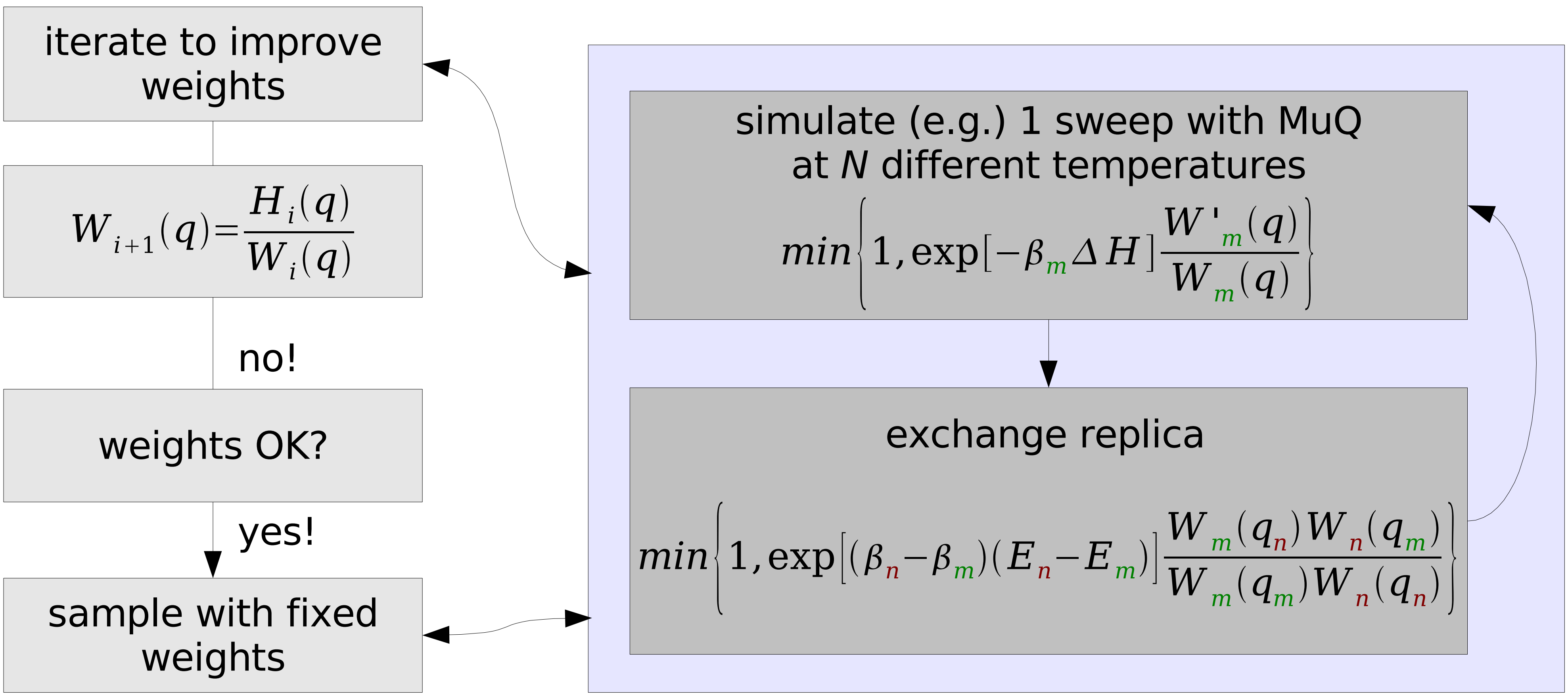


T. Neuhaus and J. S. Hager, J. Stat. Phys. 116 (2003) 47,
see also poster from A. Nußbaumer

Algorithms

combination of both methods: PT-MuQ



[E. Bittner, A. Nußbaumer, W. Janke, in preperation]

Algorithms

combination of both methods: PT-MuQ

iterate to improve weights

$$W_{i+1}(q) = \frac{H_i(q)}{W_i(q)}$$

no!

weights OK?

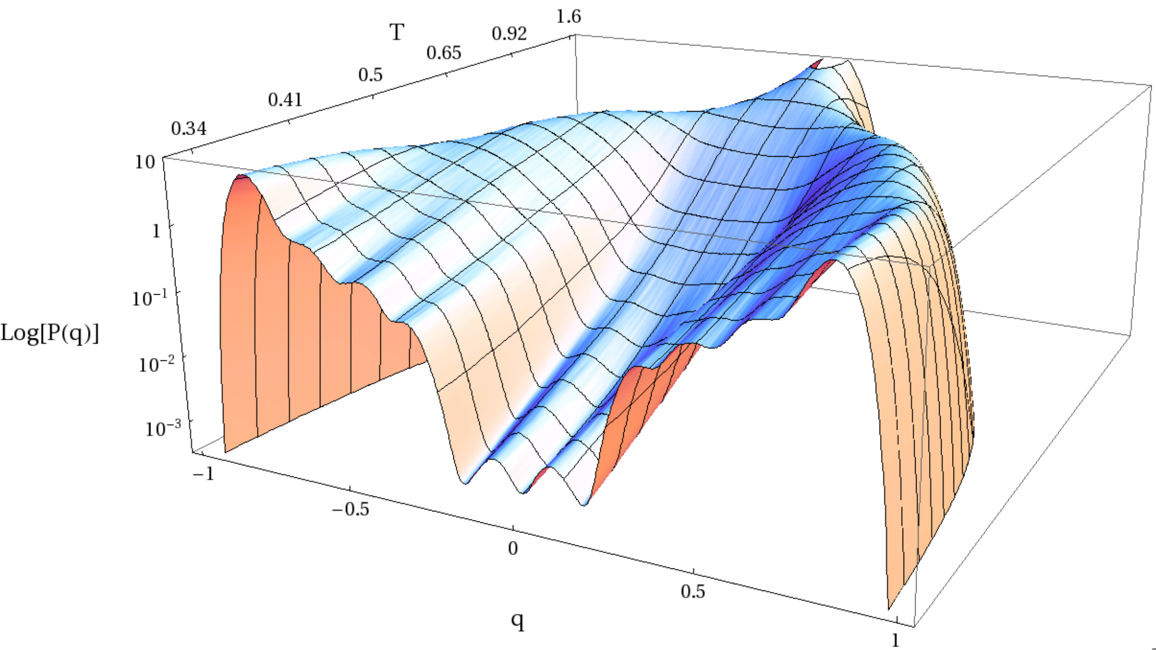
yes!

sample with fixed weights

- weights "belong" to a temperature β_m W_m
- if every replica is simulated on a different computer, all nodes have to have all weights
- in reality weights are computed with a more "sophisticated" approach

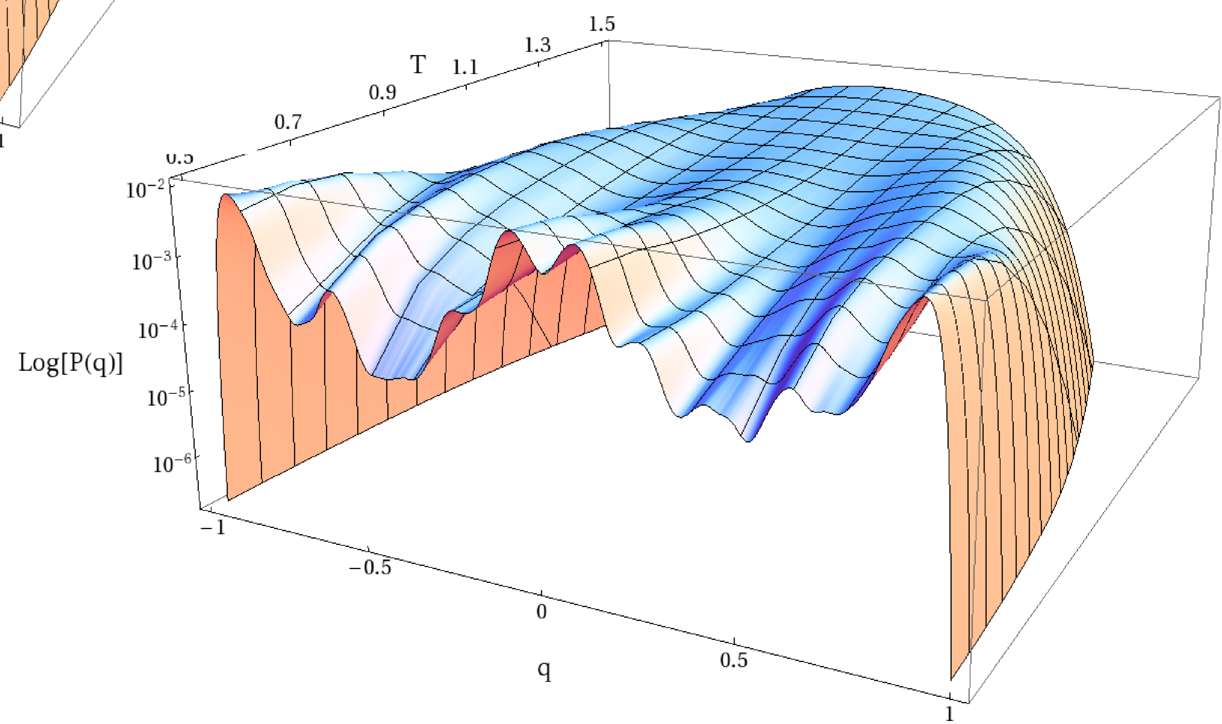
[E. Bittner, A. Nußbaumer, W. Janke, in preperation]

Algorithms



SK model, N=512

EA model, V=8x8x8



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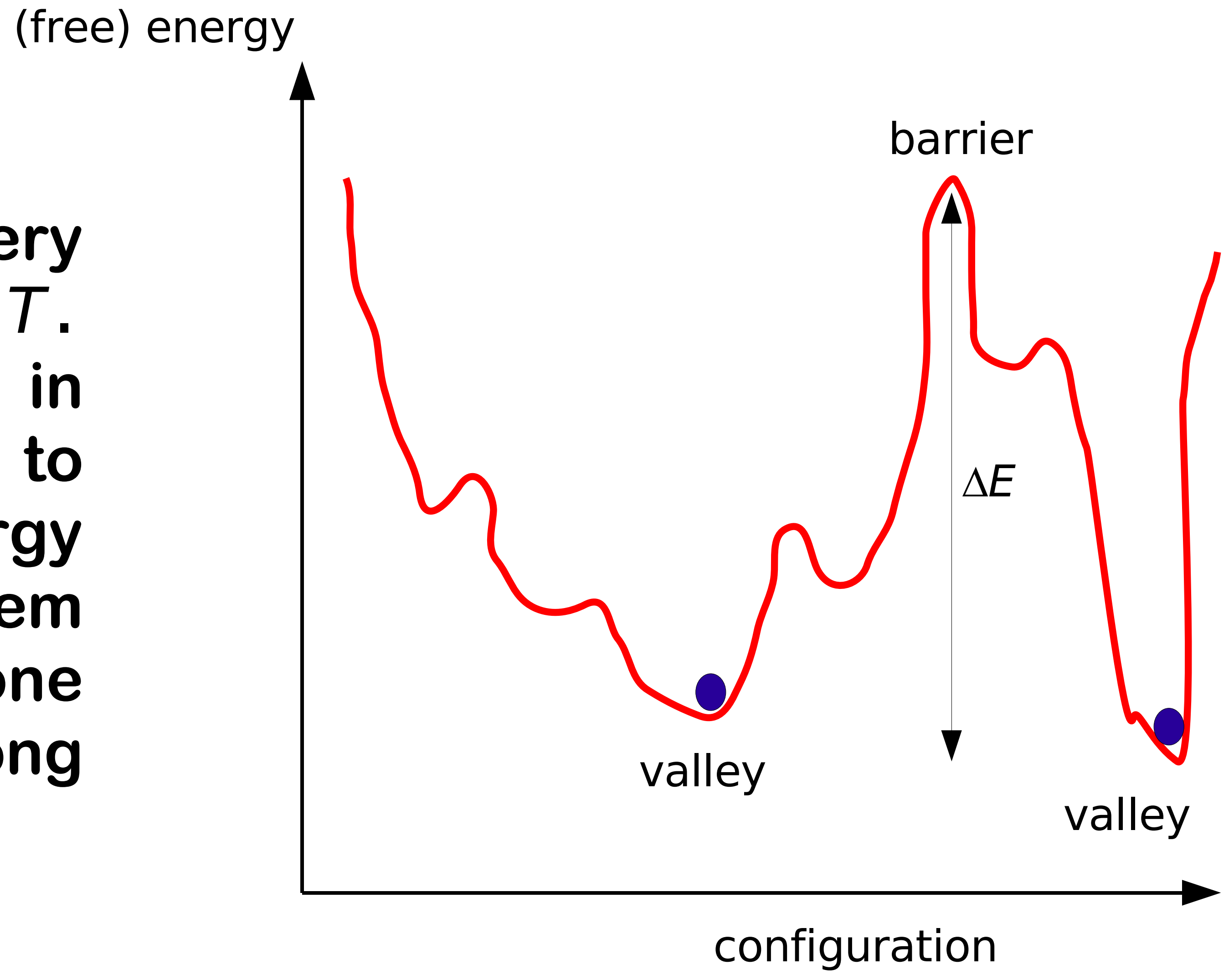


Main objective: barrier heights

2D Ising Model

$$H = -\sum_{\langle i,j \rangle} J S_i S_j$$

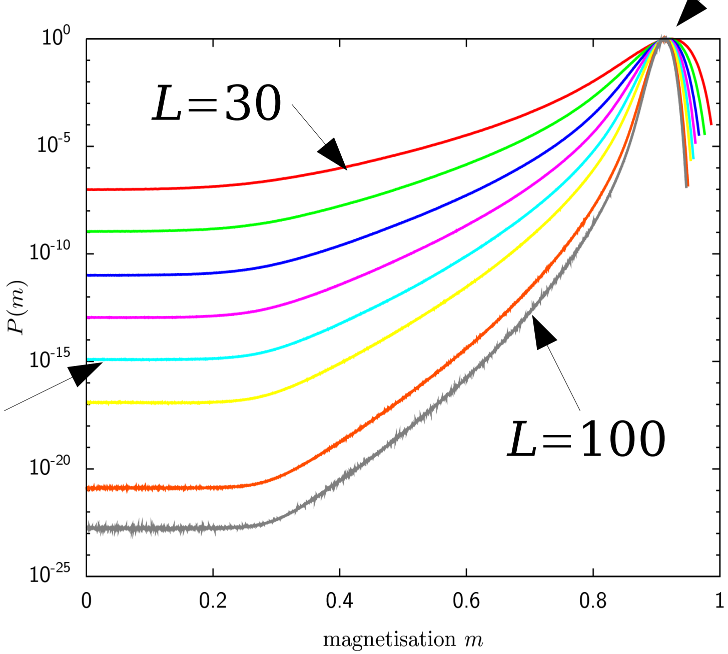
$$\frac{P_{\max}(L)}{P_{\min}(L)} \sim \exp\left[F_{\mathrm{B}}(L)\right] \equiv \tau(L)$$

$$S_i = \pm 1$$

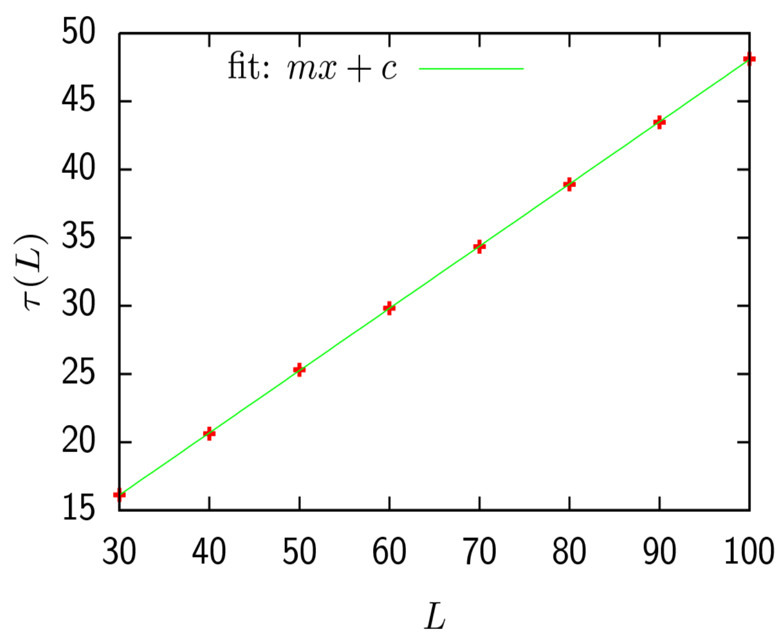
$P_{\max}(L)$

$$F_{\mathrm{B}} \sim \sigma(L) \sim 2L$$

$P_{\min}(L)$

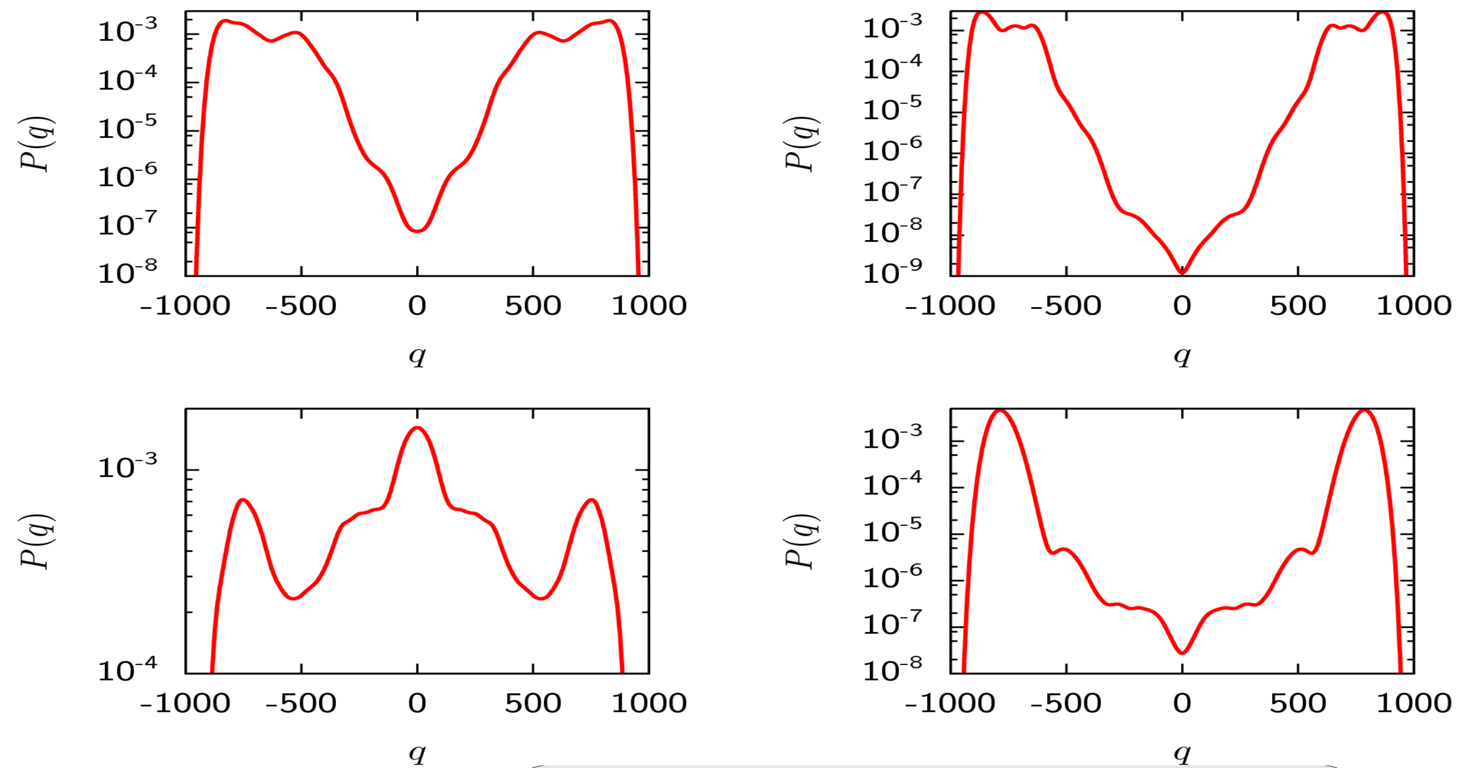


$$T < T_c$$



Main objective: barrier heights

Spin glasses:



$T < T_c$

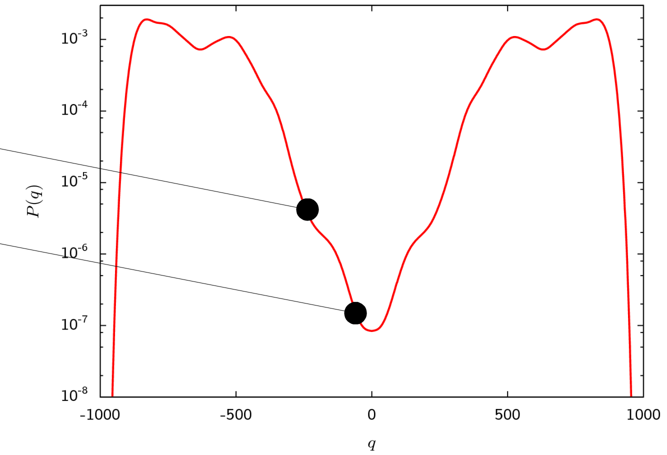
How do we measure the size of the largest barrier?

1d Markov chain/transition matrix

Definition:

$$T=\begin{pmatrix} 1-w_{1,2} & w_{1,2} & 0 & \cdots \\ w_{2,1} & 1-w_{2,1}-w_{2,3} & w_{2,3} & \cdots \\ 0 & w_{3,2} & 1-w_{3,2}-w_{3,4} & \cdots \\ 0 & 0 & w_{4,3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$w_{i,j}=\frac{1}{2}\min\left[1,\frac{P(q_j)}{P(q_i)}\right]$$



[B.A. Berg, A. Billoire and W. Janke, PRB 61 (2000), 12143]

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T **fulfills detailed balance → only real eigenvalues**

autocorrelation time for *q*: $\tau_B^q=\frac{1}{N\,log(\lambda_1)}$

λ_1 **second largest eigenvalue** $(\lambda_0=1)$

Motivation

theoretical predictions for mean-field model (SK): barrier between time-reversed states scales with system size as

$$N^{1/3}$$

(Rodgers and Moore, 1988)
(Kinzelbach and Horner, 1991)

results for short-ranged models (EA) are far away from the mean-field theory limit

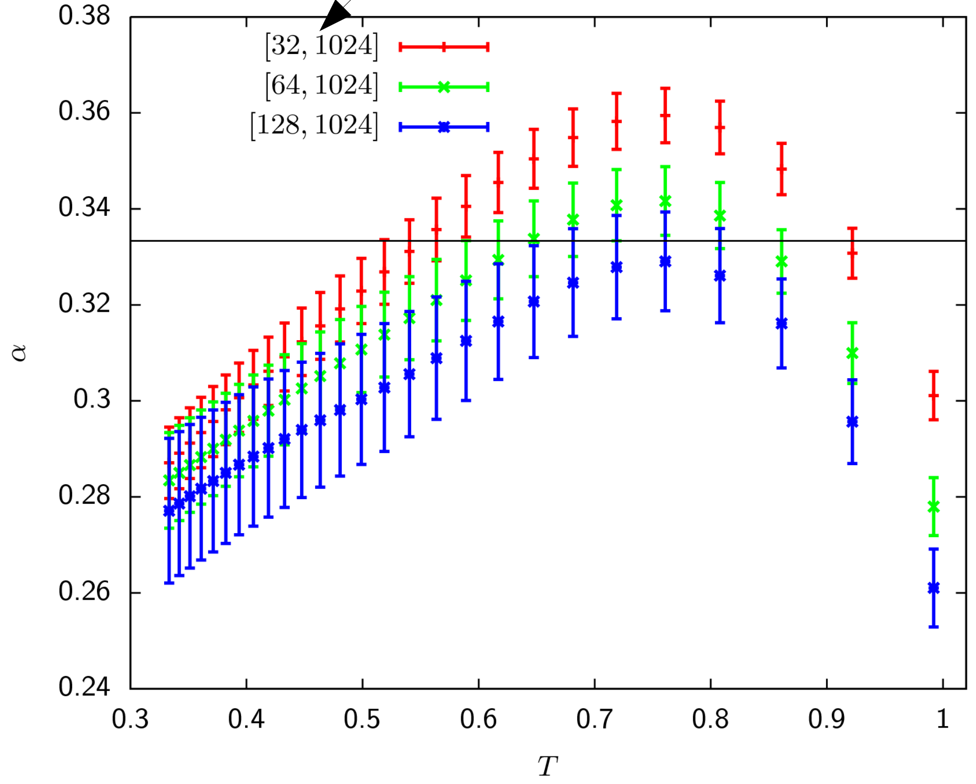
$$c_1 + c_2 \ln(N)$$

(Berg, Billoire, and Janke, 2000)

Results for the SK Model

$$\tau_B \propto \exp(cN^{\alpha})$$

fit rage



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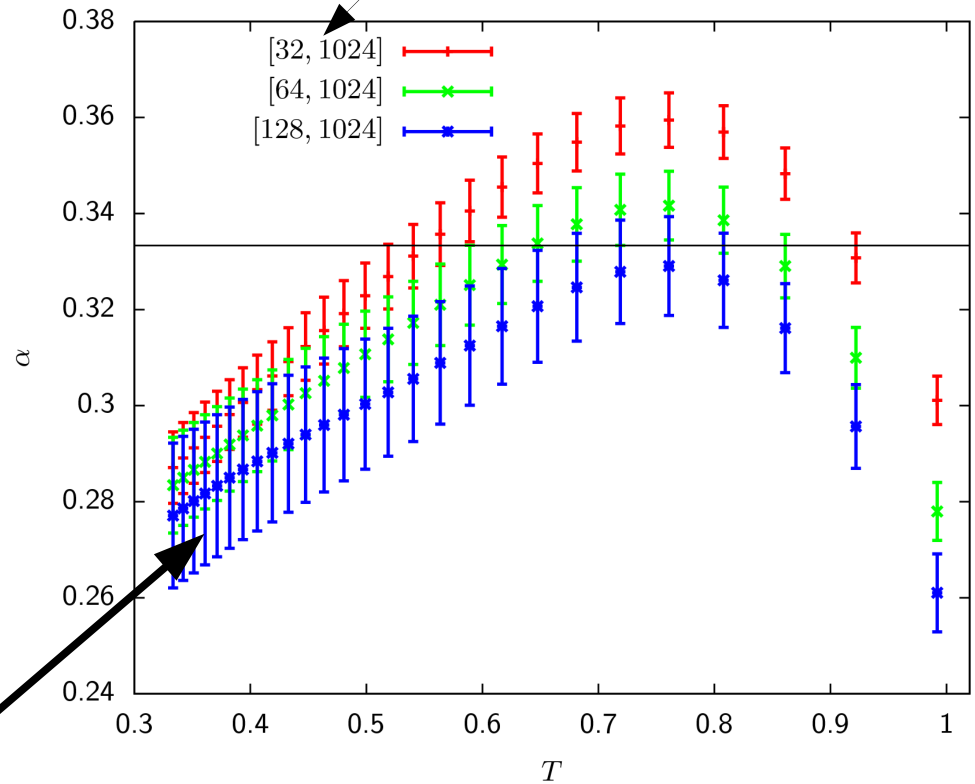
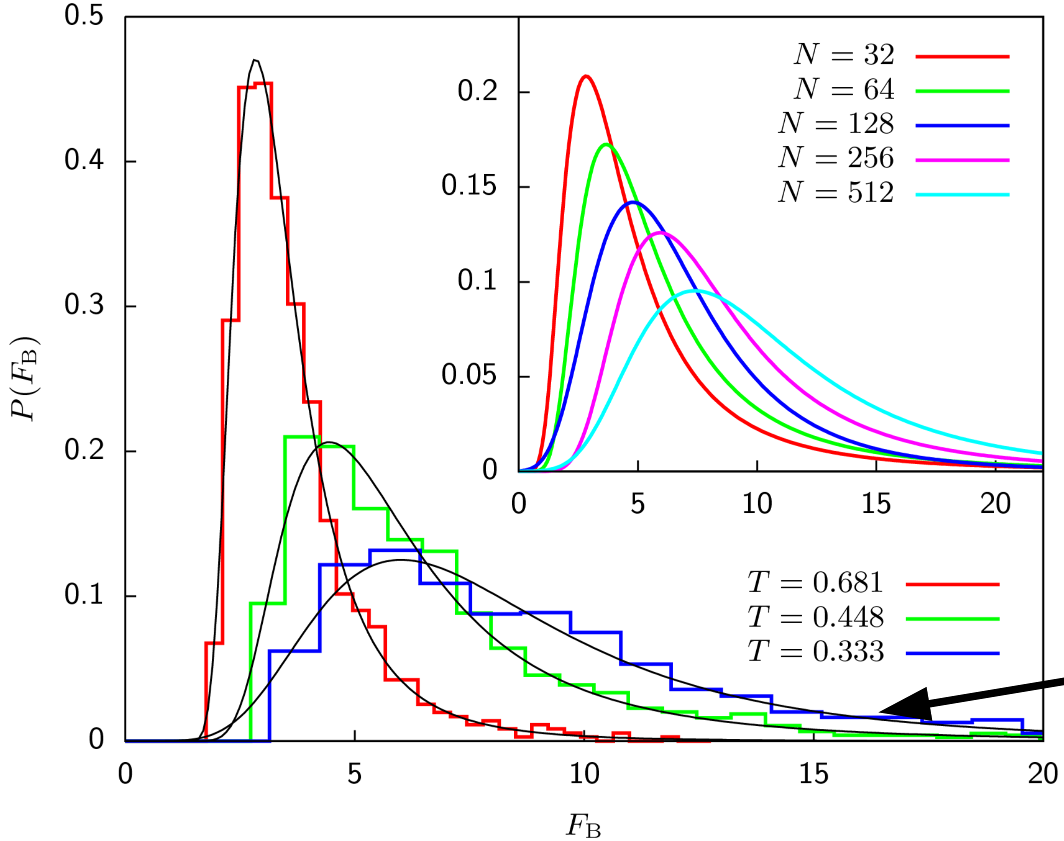


non-self-averaging (SK)

[L.A. Pastur and M.V. Shcherbina, J. Stat. Phys. 62 (1992) 1]

Results for the SK Model



extreme-value distribution

fat tails

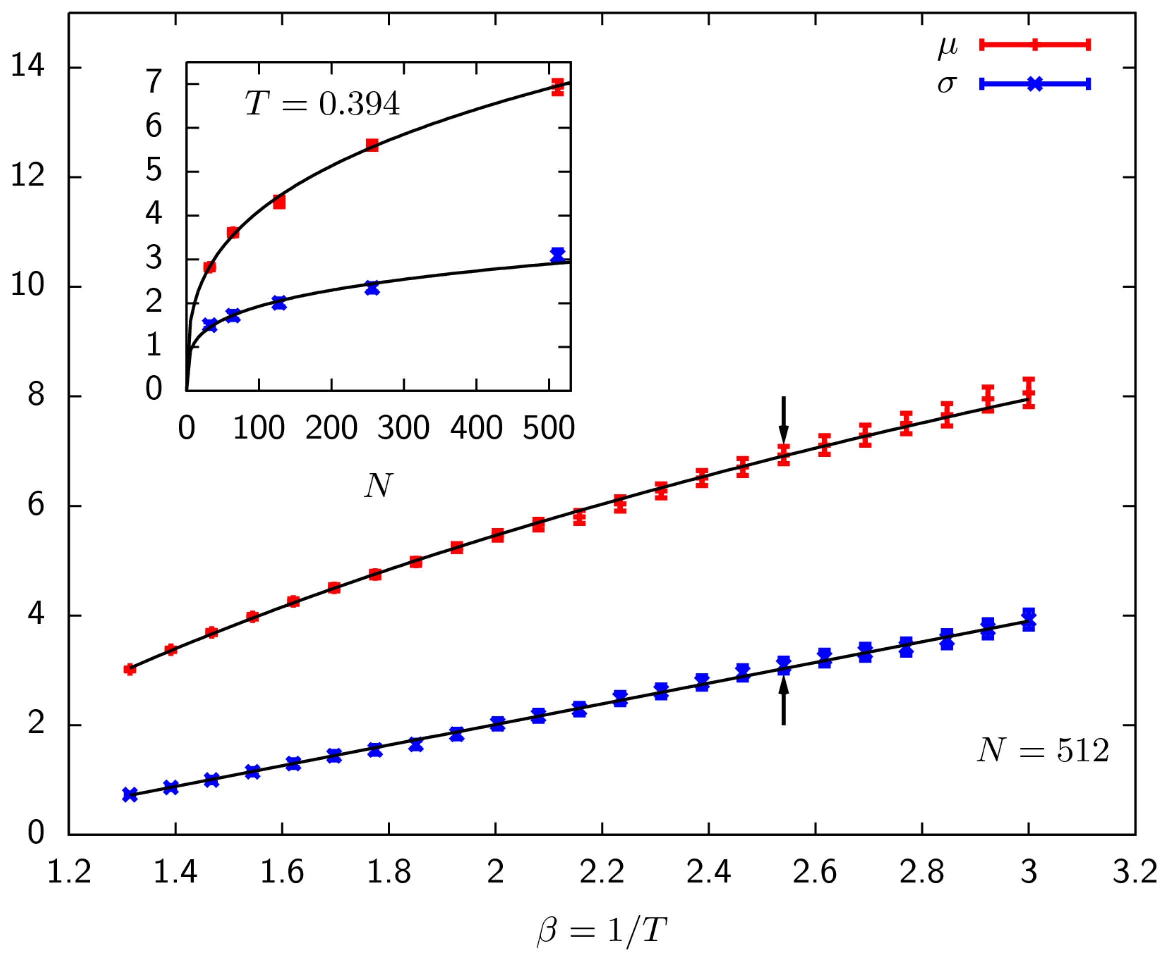
Fit integrated probability density:

$$F_{\xi;\mu;\sigma}(x) = \exp\left[-\left(1 + \xi \frac{x-\mu}{\sigma}\right)^{-1/\xi} \right]$$

$T < T_c$ → $\xi > 0$

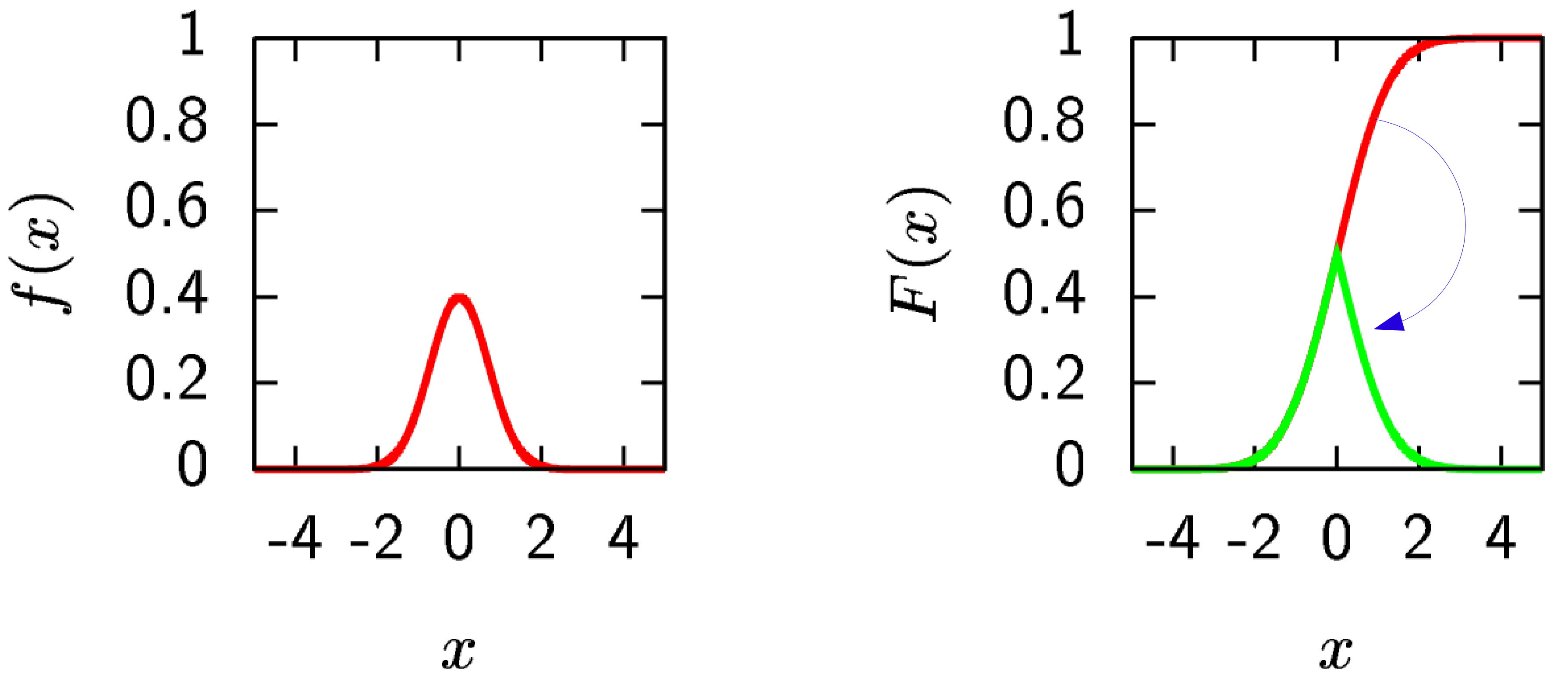
→ **fat tailed (algebraic)**
Fréchet distribution

Results for the SK Model



Results for the SK Model

Peaked probability distribution $D(F_B/F_{B_{\text{med}}})$



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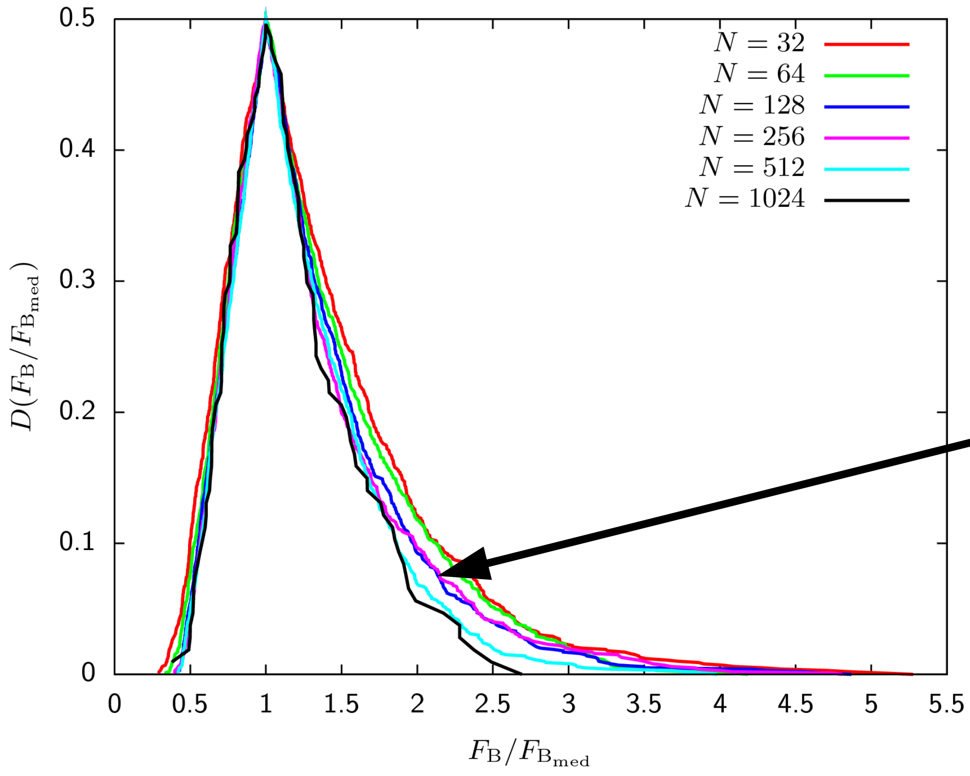

no scaling,
i.e. non-self-averaging

Results for the SK Model

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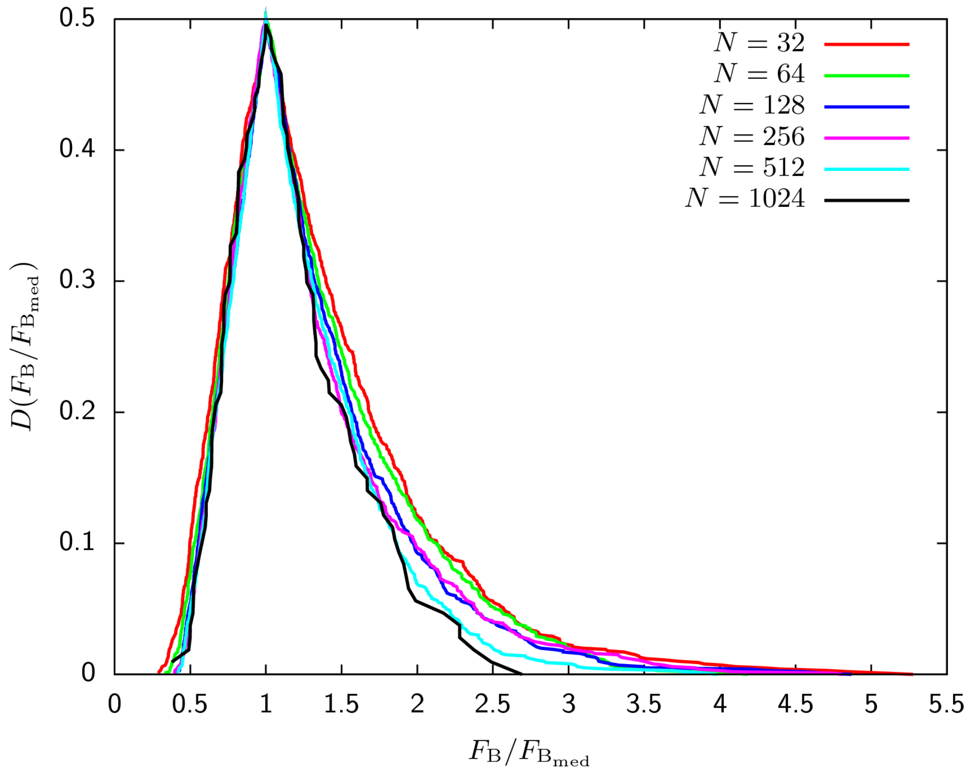
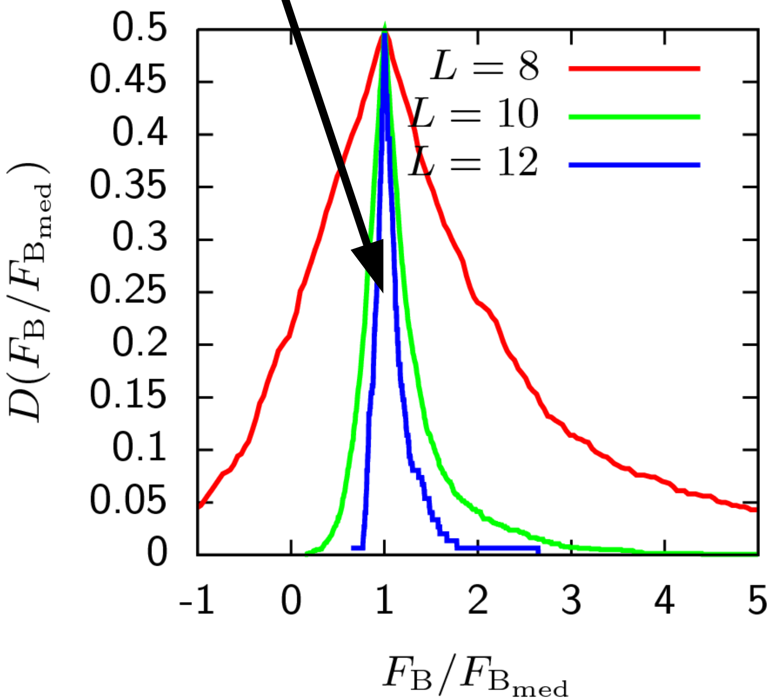


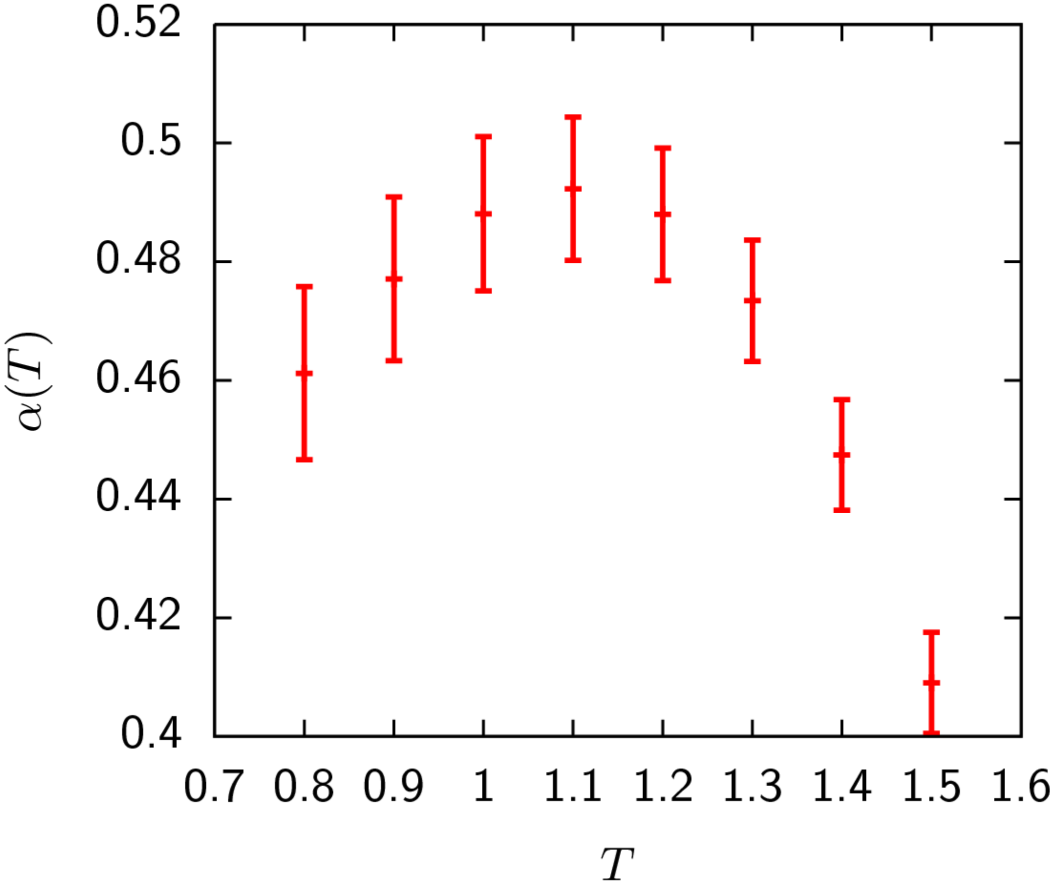
scaling,
i.e. self-averaging

(**EA Model**)



Results for the EA Model

$$\tau_B \propto \exp(cN^{\alpha})$$



but goodness of fit ...

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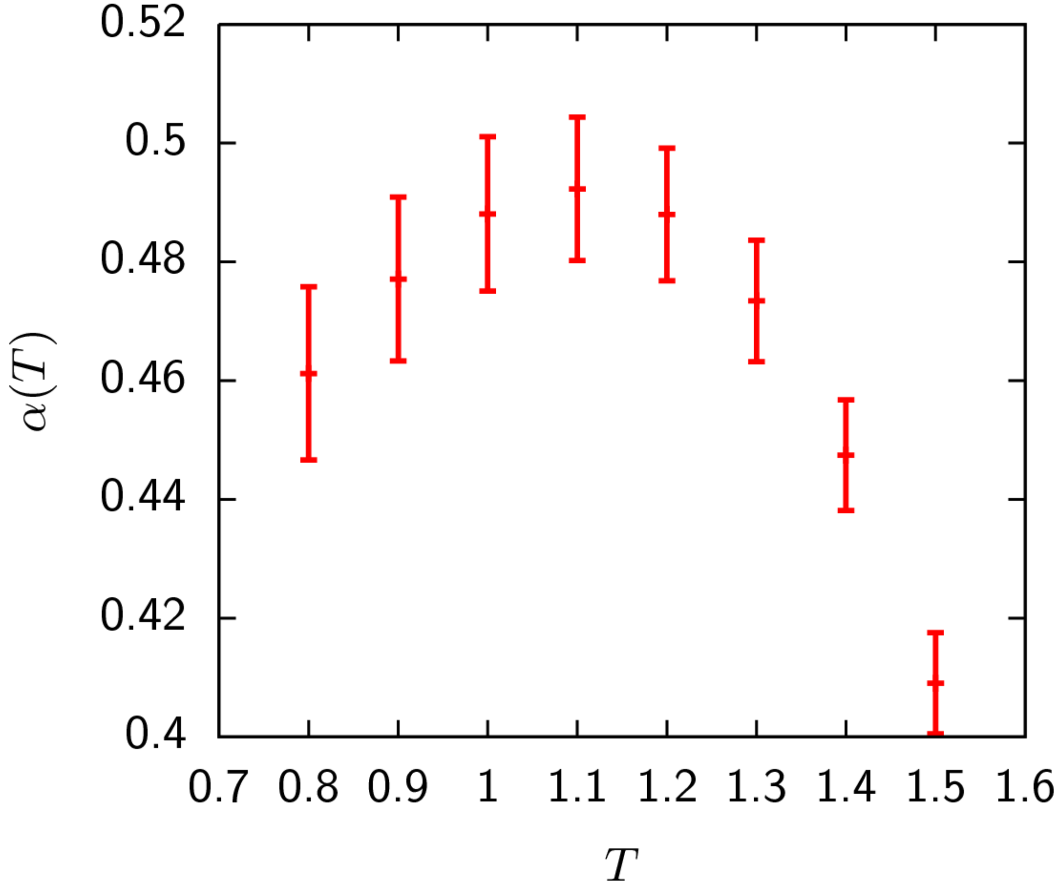

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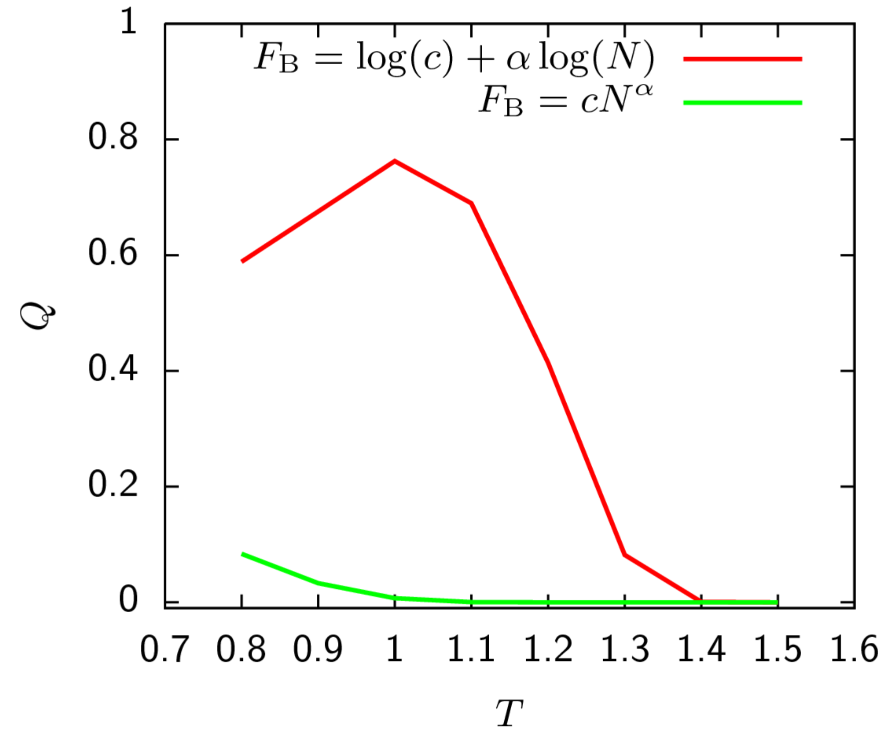

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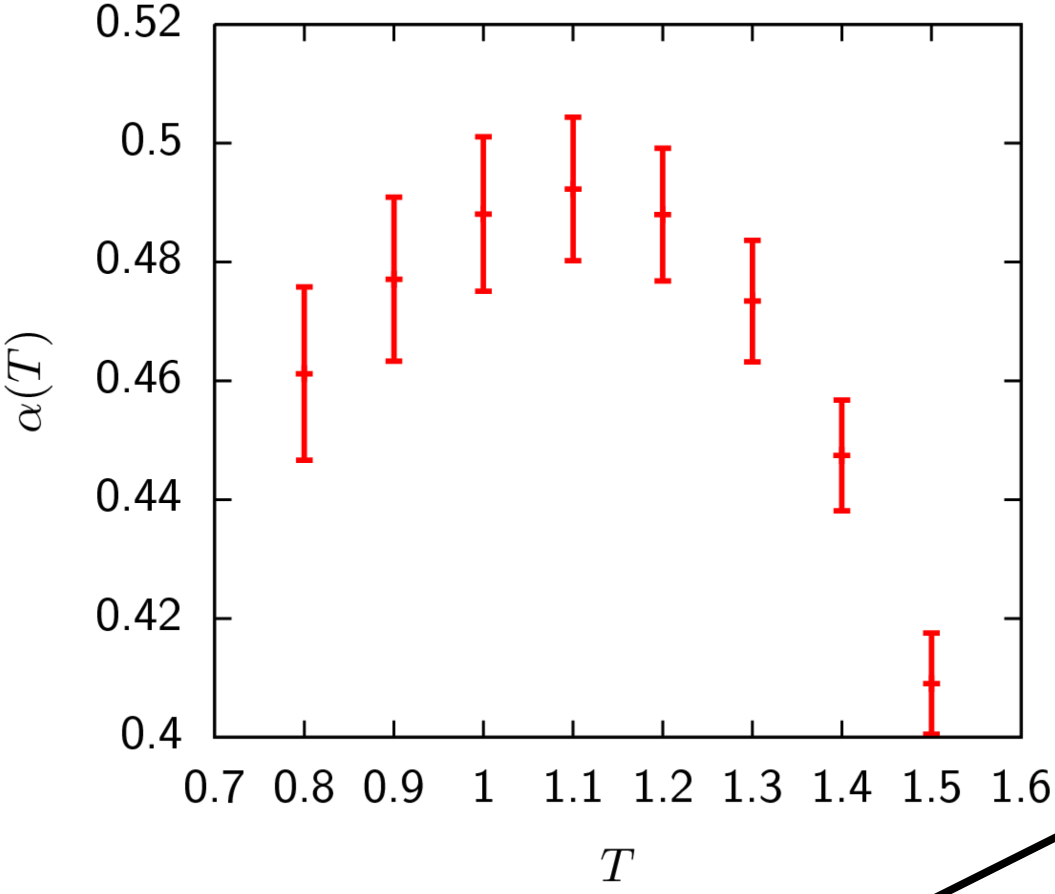
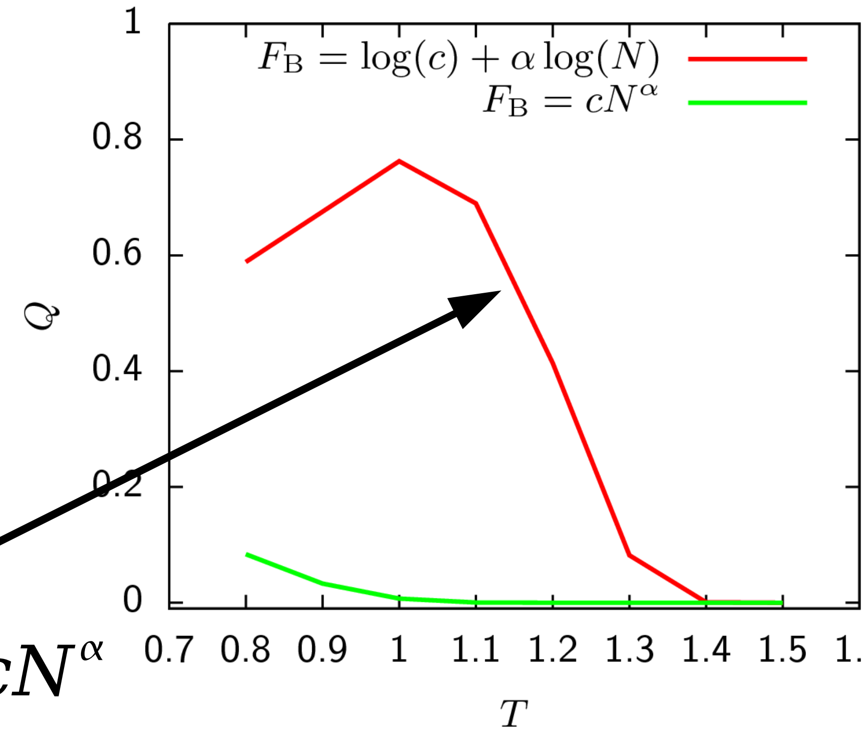


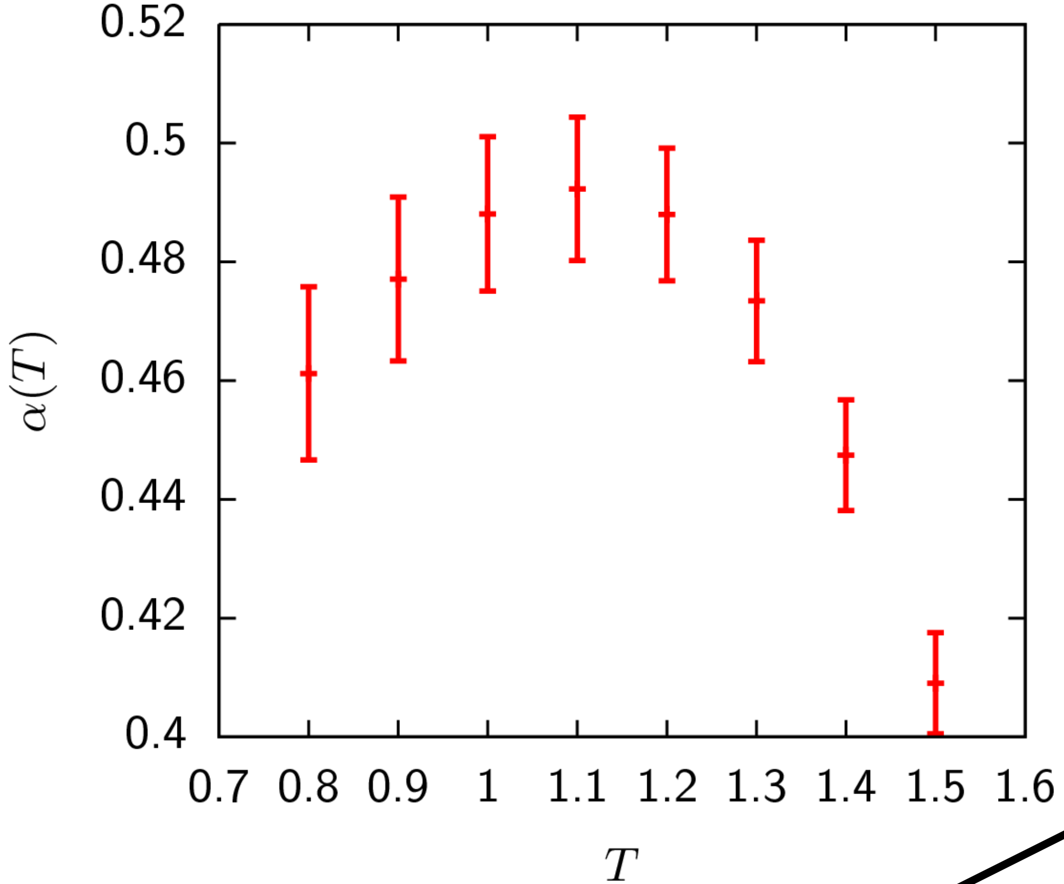
but goodness of fit ...



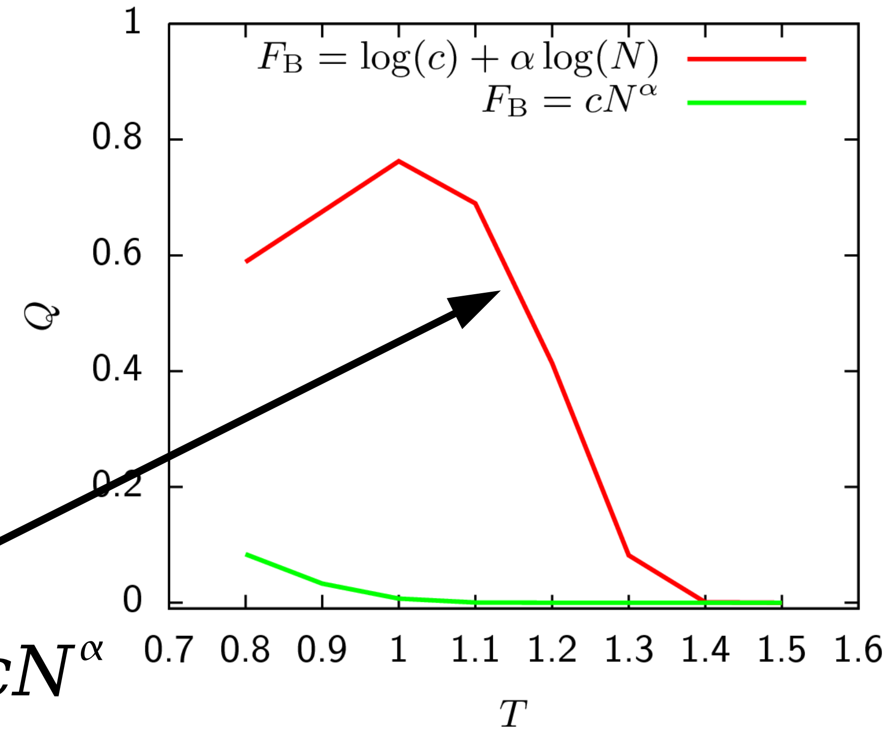
therefore, different fit: $\tau_B \propto cN^\alpha$

Results for the EA Model

$\tau_B \propto \exp(cN^{\alpha})$



but goodness of fit ...



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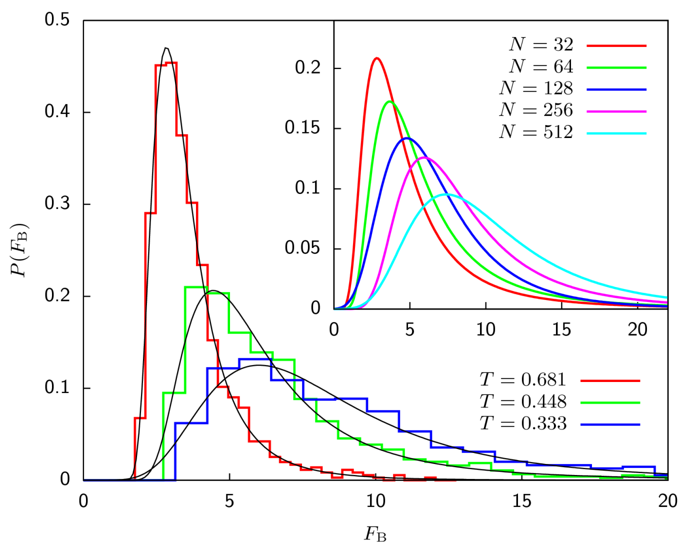
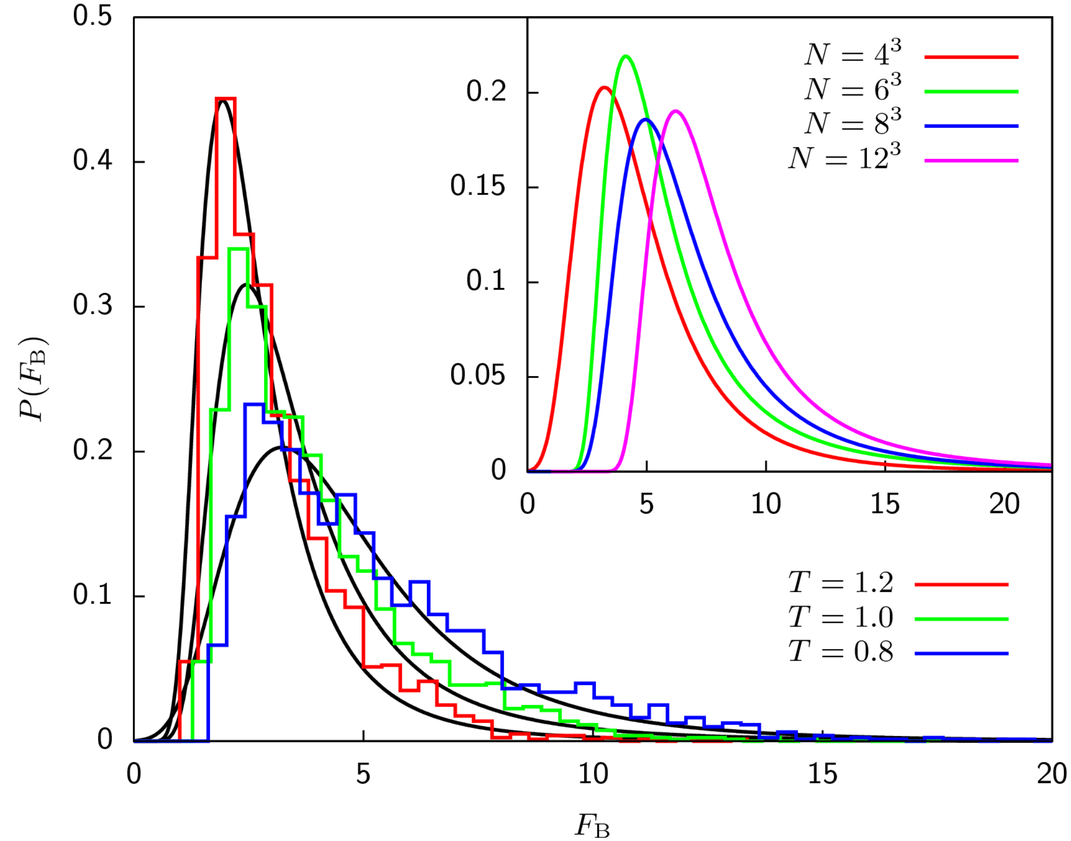
Results for the EA Model



SK Model



EA Model

Fit integrated probability density:

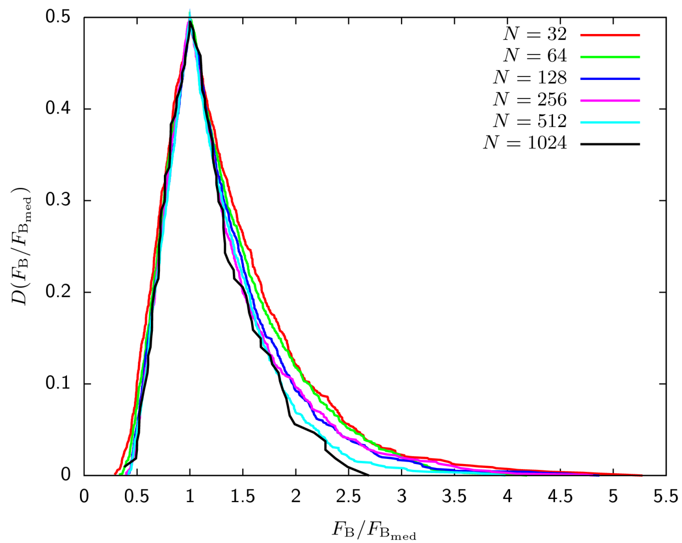
$$F_{\xi;\mu;\sigma}(x) = \exp\left[-\left(1+\xi\frac{x-\mu}{\sigma}\right)^{-1/\xi}\right]$$

$T < T_c$ → $\xi > 0$

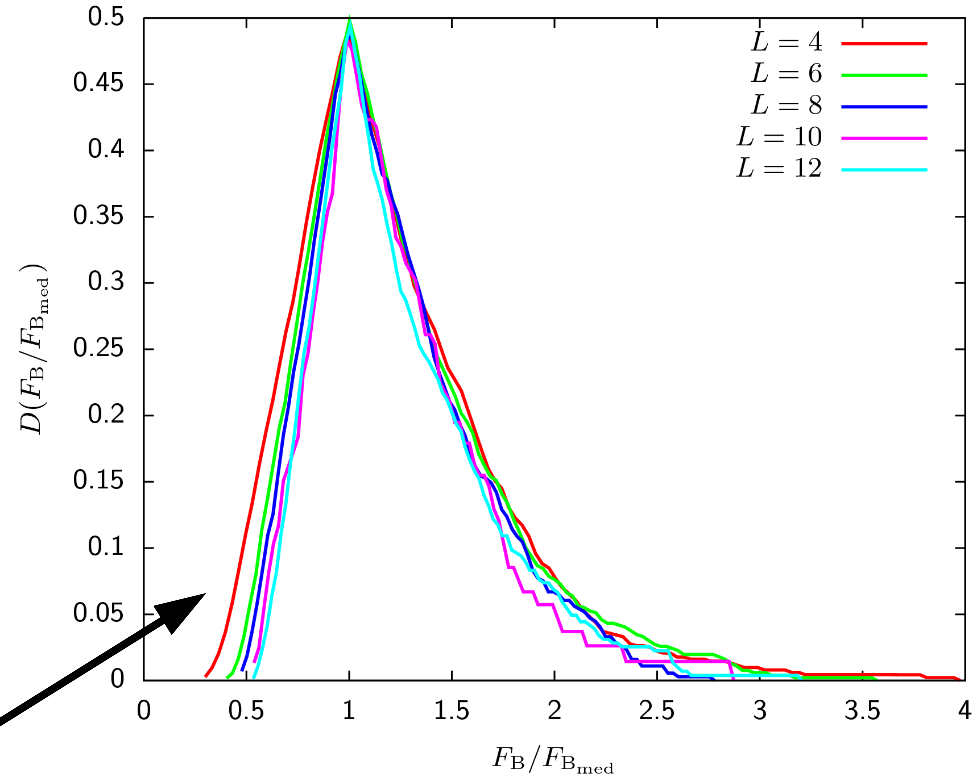
→ **fat tailed (algebraic) Fréchet distribution**

Results for the EA Model

Peaked probability distribution $D(F_B/F_{B_{\mathrm{med}}})$



SK Model



no scaling,
i.e. non-self-averaging

EA Model

Conclusion

- **Algorithmic**
  - PT is good to decrease the autocorrelation time
  - MuQ gives the full $P(q)$ information
  - the combination of PT+MuQ makes it possible to get $P(q)$ down to $T \approx 0.5\,T_{\mathrm{c}}$

- **Physical**
  - the free energy barriers of the SK and EA model are
    - a) non-self-averaging
    - b) follow the Fréchet extreme-value distribution
  - the free energy barriers of the SK model diverge with an exponent of $\alpha = 1/3$
  - the last is not true for the EA model

Thank you!