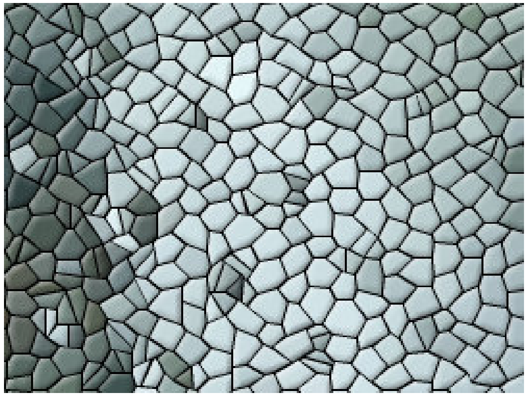
Free-energy barriers of spin glass (in 3D)

A. Nußbaumer, Elmar Bittner and Wolfhard Janke

CompPhys08, Leipzig 29th Nov. 2008

Experimental Part :-)

Question: What is a spin glass (for us)?

<u>Answer</u>:
collection of spins with a low-T state that is $\underbrace{\text{frozen disordered}}$

per site magnetisation: $m_i = \langle \sigma_i \rangle \neq 0$ (like ferrormagnet)

no net magnetsiation: $m = \frac{1}{N} \sum_i m_i = 0$ (unlike ferrormagnet)

exact: of order $\frac{1}{\sqrt{N}}$

(ferromagnet has completely ordered low-T state, i.e. a net magnetisation)

Q: Looking at a single spin, can I decide if he belongs to a spin glass?
A: NO!

What exactly do we want to calculate?

to quench=abschrecken
(im Sinne eines gekochten Eis)

From experiment:
impurities move slowly/not at all
spins change much faster

$\Big\}$ quenched couplings

① draw some J_{ij}
② keep them fixed
③ calculate some quantity, e.g

$$F = -T \log Z = -T \log \sum_{\{\sigma\}} e^{-\beta H(\sigma_1, \ldots, \sigma_N)}$$

④ do average over couplings = [...]

$$[F] = -T[\log Z] = -T\left[\log \sum_{\{\sigma\}} e^{-\beta H(\sigma_1, \ldots, \sigma_N)}\right]$$

Is this averaging allowed?
After all, there is only **one** set of couplings in a real SG:

free energy/degree of freedom:

$$\frac{F(\boldsymbol{J})}{N} = f(\boldsymbol{J})$$

at thermodynamic limit ($N \to \infty$):

$$f(\boldsymbol{J}) = [f]$$

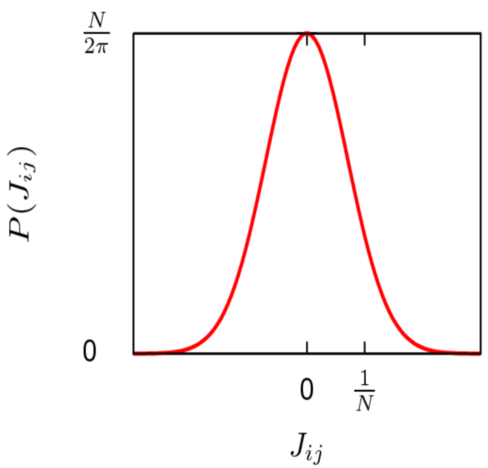
self-averaging of the free energy (density)

We are looking at two models:

a) Sherrington-Kirkpatrick (SK) model
[D. Sherrington and S. Kirkpartick, PRL 35 (1975) 1792]

$$H_{\mathrm{SK}} = -\sum_{i<j} J_{ij} s_i s_j$$

Gaussian distribution with:



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

$$\langle J_{ij} \rangle^2 - \langle J_{ij}^2 \rangle = \frac{1}{N}$$

Note:
both types of couplings are believed to show the same physics at finite temperatures!
this is just our choice

mean field

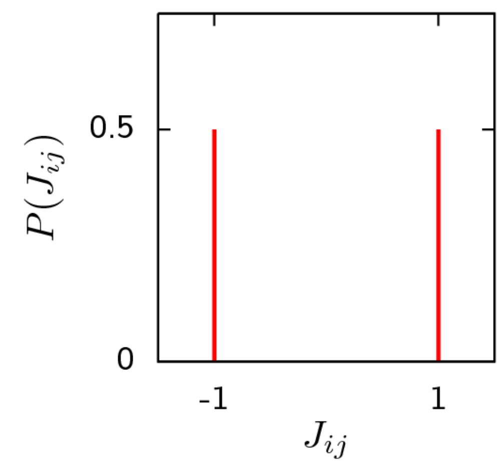
$T_c = 1$

Parisi's replica solution [PRL 43 (1979) 1754]
or mathematical: M. Talagrand, C. R. Acad. Sci. Paris, Ser. I 337 (2003) 111

b) Edwards-Anderson (EA) model
[S. F. Edwards and P. W. Anderson, J. Phys. F: Metal Phys. 5 (1975) 965]

$$H_{\mathrm{EA}} = -\sum_{\langle ij \rangle} J_{ij} s_i s_j$$

Bimodal distribution:



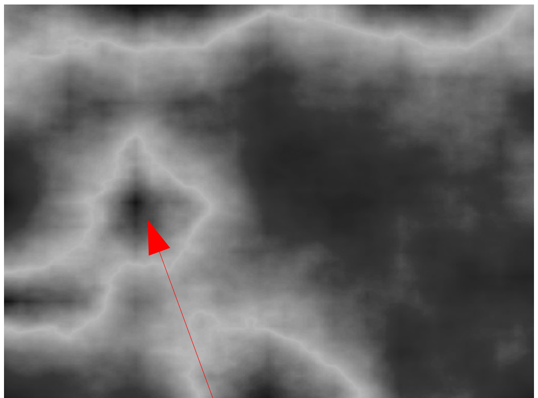
3 dimensions

$T_c \approx 1.10$ from MC [M. Hasenbusch, A. Pelissetto and E. Vicari, J. Stat. Mech. (2008) L02001]

no solution, problem is NP hard

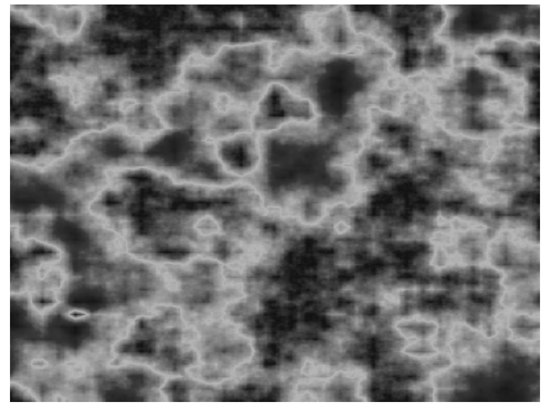
Multi-Valley picture

microscopically

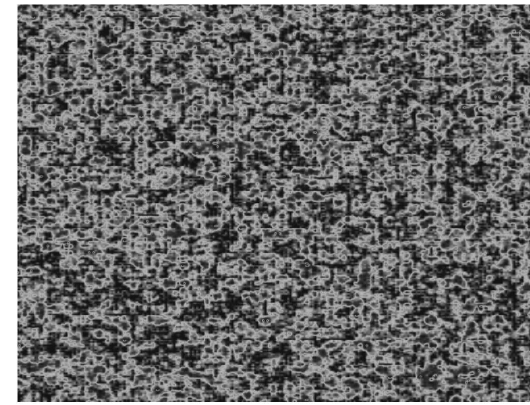


“valley”

intermediate



macroscopically



$P_a = e^{-\beta F_a}$ statistical weight of valley *a*

Now, quantities in terms of valleys:

e.g. site-magnetisation: $m_i^a = \langle \sigma_i \rangle_a$

average over all valleys

$$m_i = \sum_a P_a \cdot m_i^a$$

define OVERLAP of valley a and b: $q_{ab} = \frac{1}{N} \sum_i m_i^a m_i^b$

a and b are in the same valley: $a = b \rightarrow q_{aa} = q_{\mathrm{EA}}$

<u>completely</u> different valleys: $a \neq b \rightarrow q_{ab} = ?$

define OVERLAP distribution: $P_J(q)=\sum_{ab} P_a \cdot P_b \cdot \delta(q-q_{ab})$ and $P(q)=\left[P_J(q)\right]$

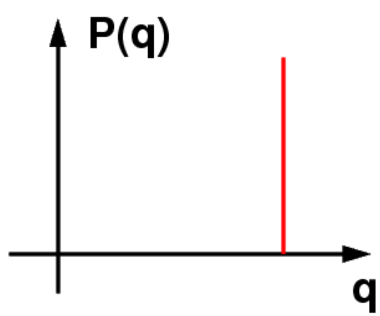
probability that valleys a and b (=pure states a and b) have mutual overlap q

the OVERLAP is the <u>physical</u> order parameter

So, and what happens in less than ∞ dimensions?

Bray/Moore & Fisher/Huse droplet picture/scaling theory		Parisi Replica Symmetry Breaking
$E\sim L^{\theta},\ \theta>0$ $\Rightarrow E\to\infty$	system-size excitations for $L\to\infty$	$E\sim L^{\theta},\ \theta=0$ $\Rightarrow E\to E_0$
fractal $d_s<d$	dimension of excitations	space filling $d_s=d$

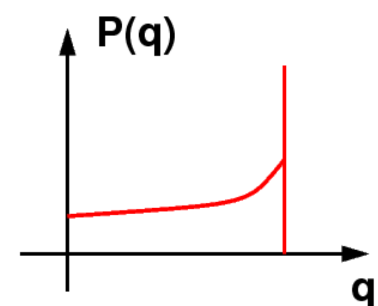
trivial



$P(0)\sim L^{-\theta}$

GS structure

non-trivial



$P(0)\sim L^{0}$

...

What can be done to verify 3D behavior:

<u>Measure with the computer ...</u>

stiffness exponents

e.g. apply two different boundary conditions

susceptibilities,

correlation functions: $[\langle s_i s_j \rangle^2] - [\langle s_i \rangle^2][\langle s_j \rangle^2] \sim T / Y R^{\theta}$ R :distance between i and j, average in a single pure state

distribution of overlap parameter $P(q)$

and check what happens at $q=0$

<u>Use "advanced" algorithms such as ...</u>

parallel tempering

multi-overlap

Wang-Landau in E and q

n-fold-way

waiting-time method

...

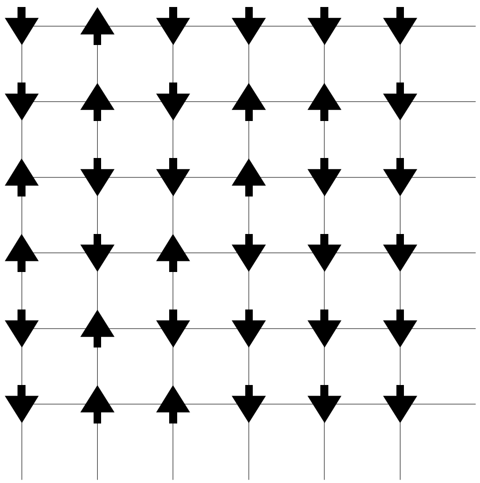
or combinations of the above as

n-fold-way+multi-overlap+parallel tempering

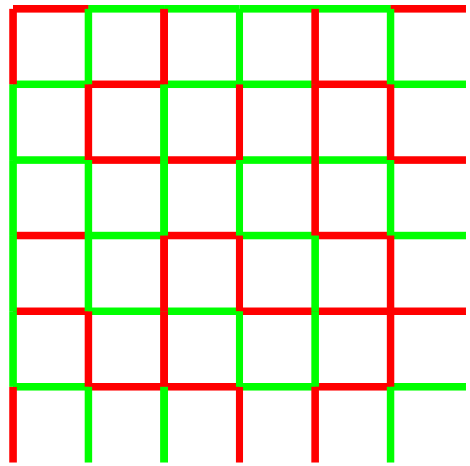
How to practically measure the overlap for the 3D EAI?

Recipe:

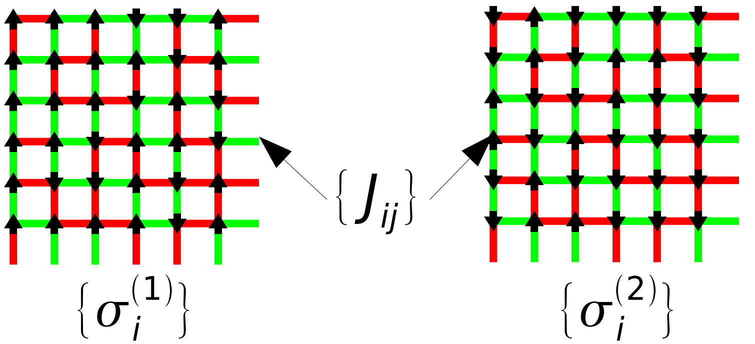
① take normal Ising model with spins $\{\sigma_i^{(1)}\}$



② draw random couplings $\{J_{ij}\}$ for every pair of spins



③ introduce second "independent" system $\{\sigma_i^{(2)}\}$ **with the same set of couplings** $\{J_{ij}\}$



④ choose "advanced" algorithm and do thermalisation

⑤ simulate one sweep of system 1

⑥ simulate one sweep of system 2

⑦ measure overlap

$$q = \frac{1}{N}\sum_i^N \sigma_i^{(1)}\sigma_i^{(2)}$$

repeat the measurement/simulation quite often!

Note,
we measure: $q = \frac{1}{N} \sum_{i}^{N} \sigma_i^{(1)} \sigma_i^{(2)}$

$$q(t) = \frac{1}{N} \sum_{i}^{N} \sigma_i^{(1)}(t) \sigma_i^{(2)}(t)$$

This is the overlap distribution from 4 pages ago!

$$P_J(q) = \frac{1}{T} \sum_{t=1}^{T} \delta[q - q(t)] = \sum_{ab} P_a \cdot P_b \cdot \delta(q - q_{ab})$$

[A. P. Young, PRL 51 (1983) 1206]

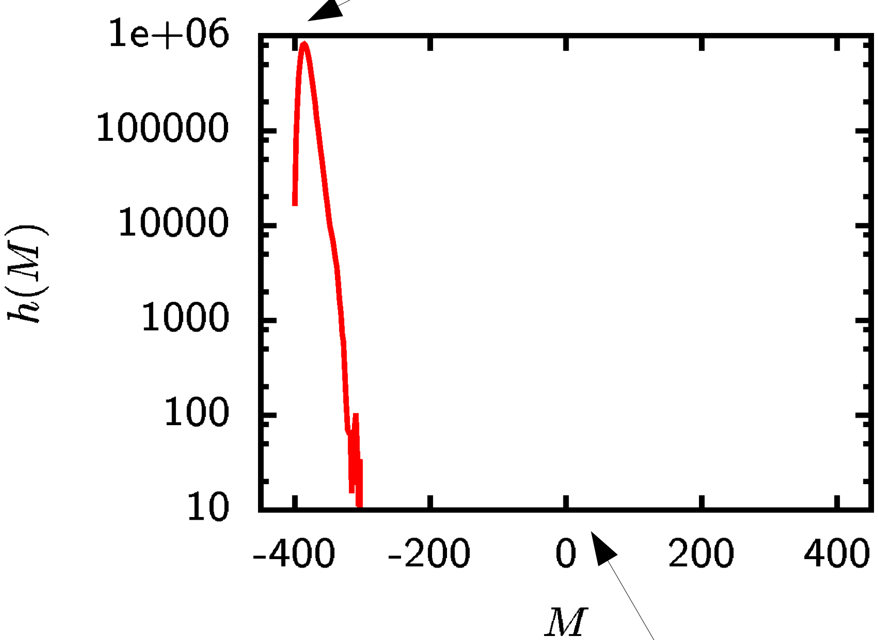
for N "very large"

Multimagnetic algorithm (MuM) 1:

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

A <u>canonical</u> simulation of the magnetisation

spontaneous magnetisation



no information here,
states are
<u>highly suppressed</u>

IDEA:
don't sample <u>Boltzmann</u> but <u>artifical</u> distribution

$$P(m)=\Omega(m)\exp[-\beta H] \Rightarrow \Omega(m)\exp[-\beta H]W(m)$$

<u>about $W(m)$:</u>

order parameter:

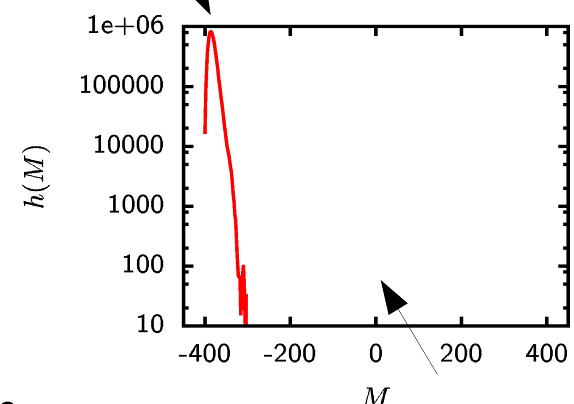
$$q=\sum_{i=1}^{V} s_i^{(1)} s_i^{(2)}$$

① is called “weights”
② can have <u>arbitrary</u> values
③ canonical expectation values can be recovered:

$$\langle A\rangle^{\mathrm{can}}=\frac{\langle W^{-1}A\rangle}{\langle W^{-1}\rangle}$$

use weights to make distribution
“simpler” to sample

sample “less” here



sample “more” here

Multimagnetic algorithm (MuM) 2:

use iterative approache

Which weights are good?

Def.: we want to sample a “flat” histogram

$$h(m) \approx \text{const.}$$

Optimal: inverse weights: $W(m) = 1/P(m)$

small problem: we don't know this function
(otherwise the problem already solved)

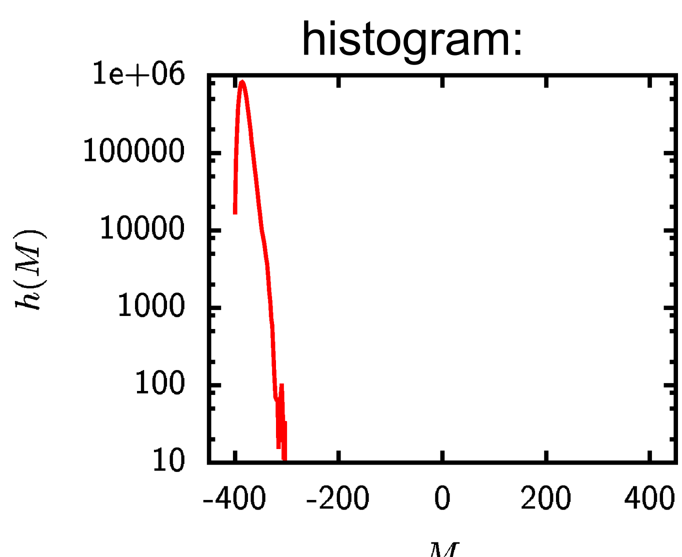
$$W_0(m) = 1$$

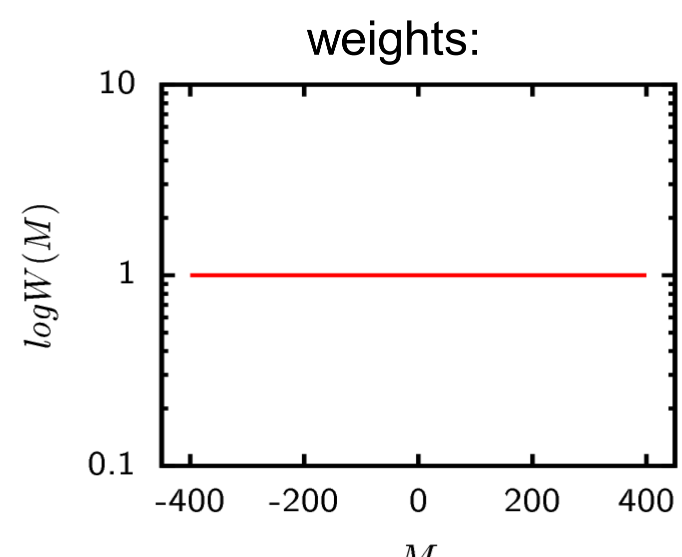
simulation

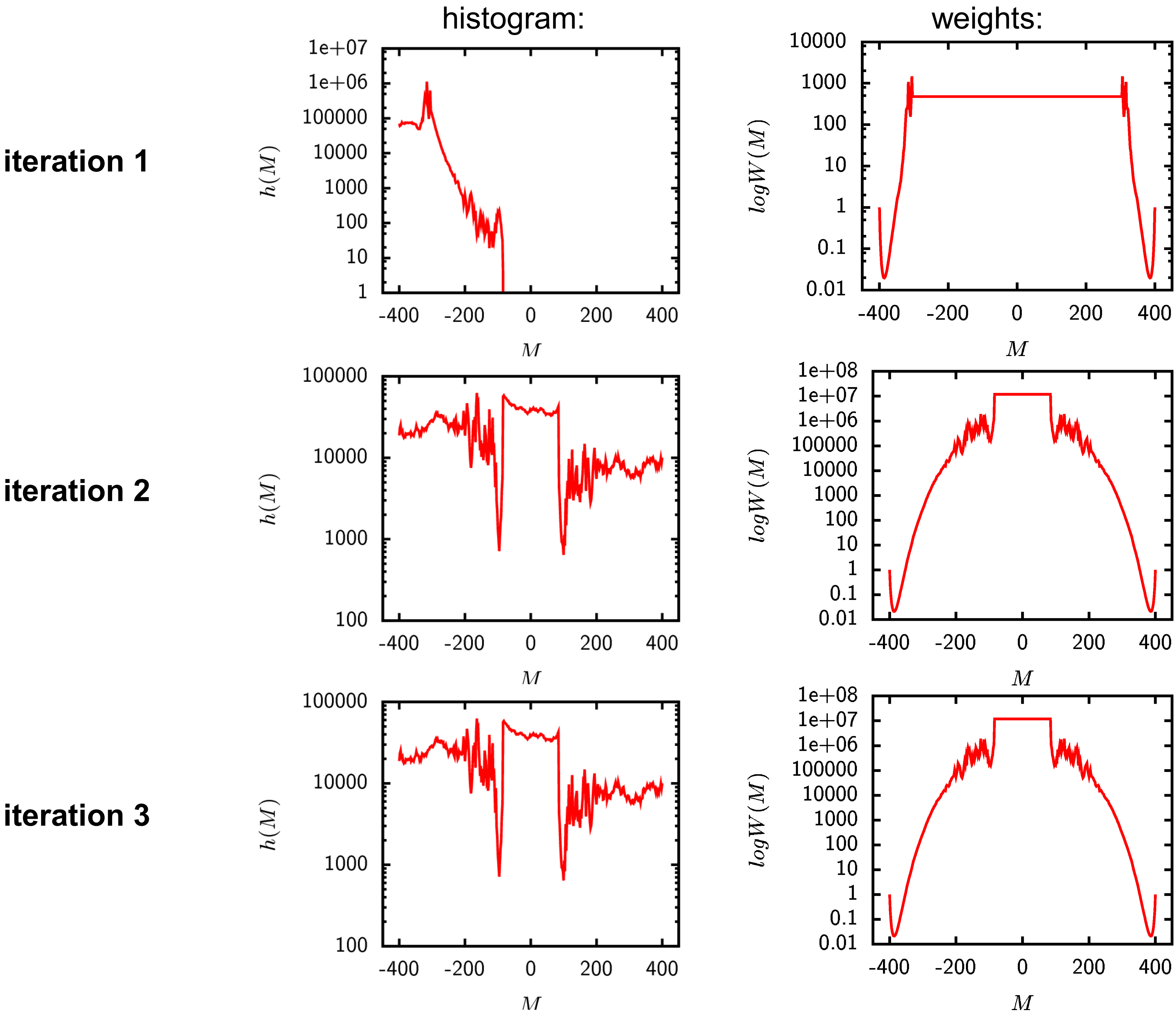
$$W_{i+1}(m) = \frac{H_i(m)}{W_i(m)}$$

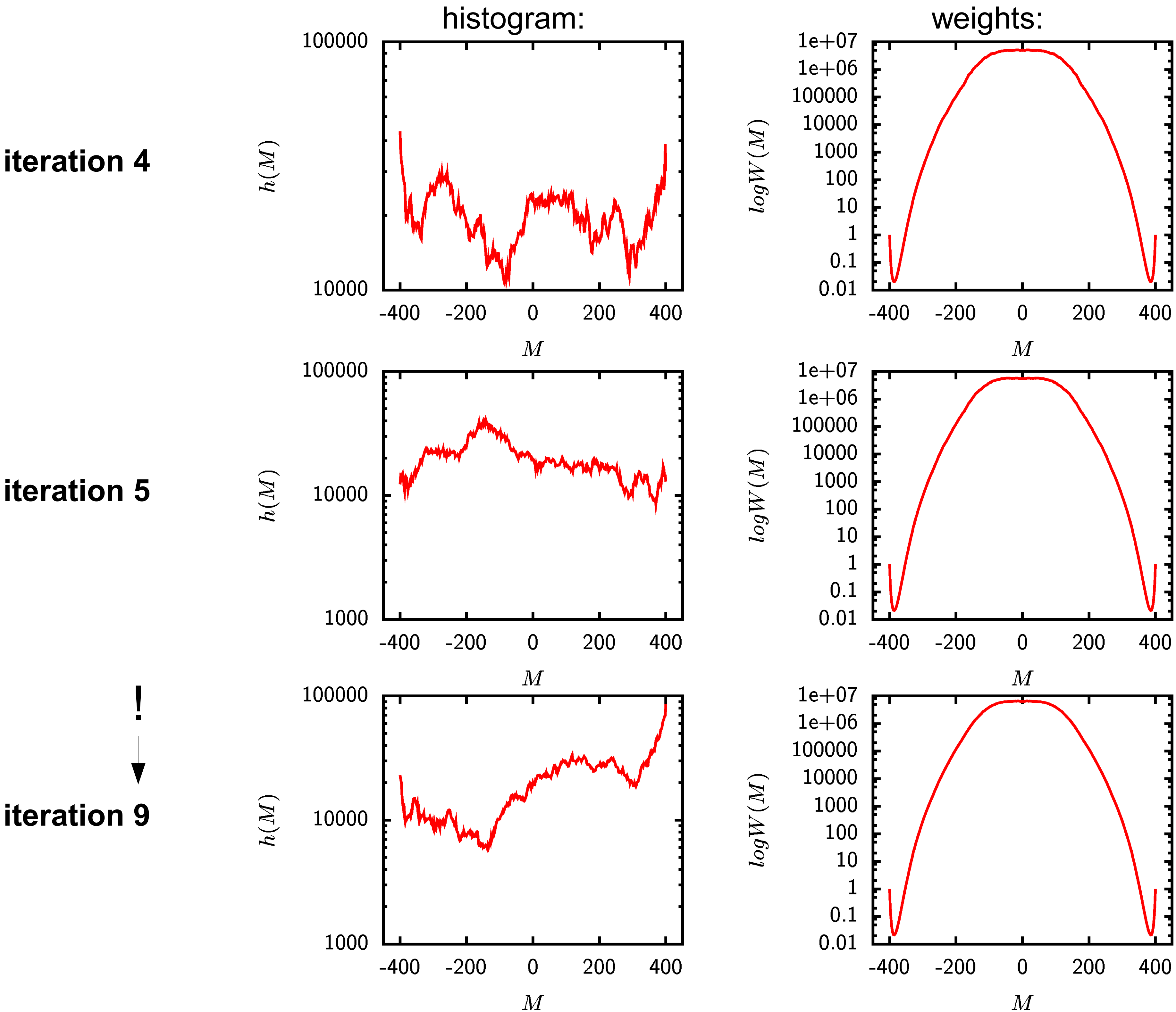
sampling

This seems to a bit strange, but it works:






histogram:
weights:
iteration 1
iteration 2
iteration 3
h(M)
logW(M)
M
1e+07
1e+06
100000
10000
1000
100
10
1
0.1
0.01
1e+08
-400
-200
0
200
400



histogram:
weights:
iteration 4
iteration 5
!
iteration 9
h(M)
logW(M)
M
100000
10000
1000
1e+07
1e+06
100000
10000
1000
100
10
1
0.1
0.01
-400
-200
0
200
400

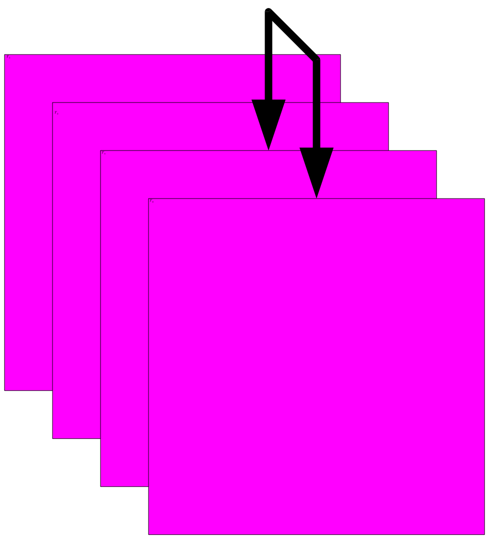
We use:
Parallel tempering (PT) + multioverlap (MuQ)

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

Idea:
Simulate larger system with
N “replica” at different *T*

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

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



note:

① replica can decorrelate at high temperatures

② expectation values for at a specific temperature

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

③ there is the freedom to adjust the number of temperatures (replicas) and the values

Now: combination of both (aka PT-MuQ)

iterate to improve weights

❷

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

no!

weights OK?

yes!

❸

sample with fixed weights

❶

❹

simulate (e.g.) 1 sweep with MuQ
at *N* different temperatures

$$min\left\{1, \exp[-\beta_m \Delta H] \frac{W'_m(q)}{W_m(q)}\right\}$$

exchange replica

$$min\left\{1, \exp\left[(\beta_n - \beta_m)(E_n - E_m)\right] \frac{W_m(q_n) W_n(q_m)}{W_m(q_m) W_n(q_n)}\right\}$$

<u>Note:</u>
weights “belong” to a temperature

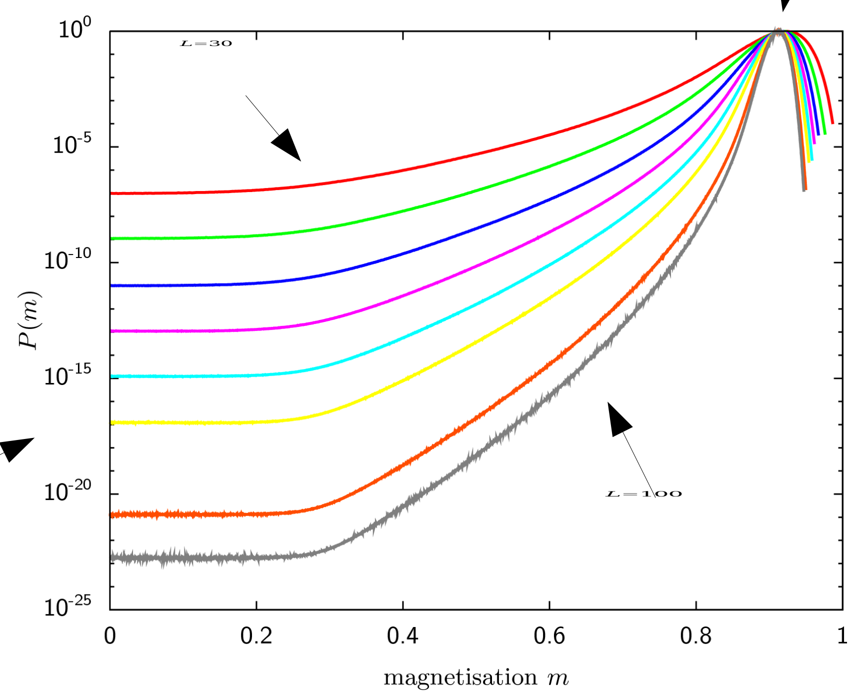
β_m W_m

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

Main objective: barrier heights

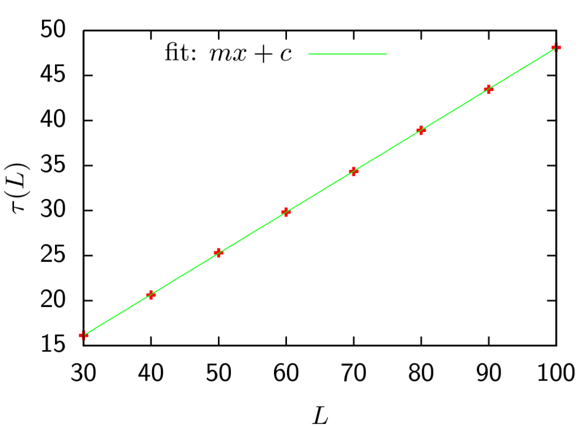
<u>Example: 2D Ising!</u>

$P_{\max}(L)$



$P_{\min}(L)$

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

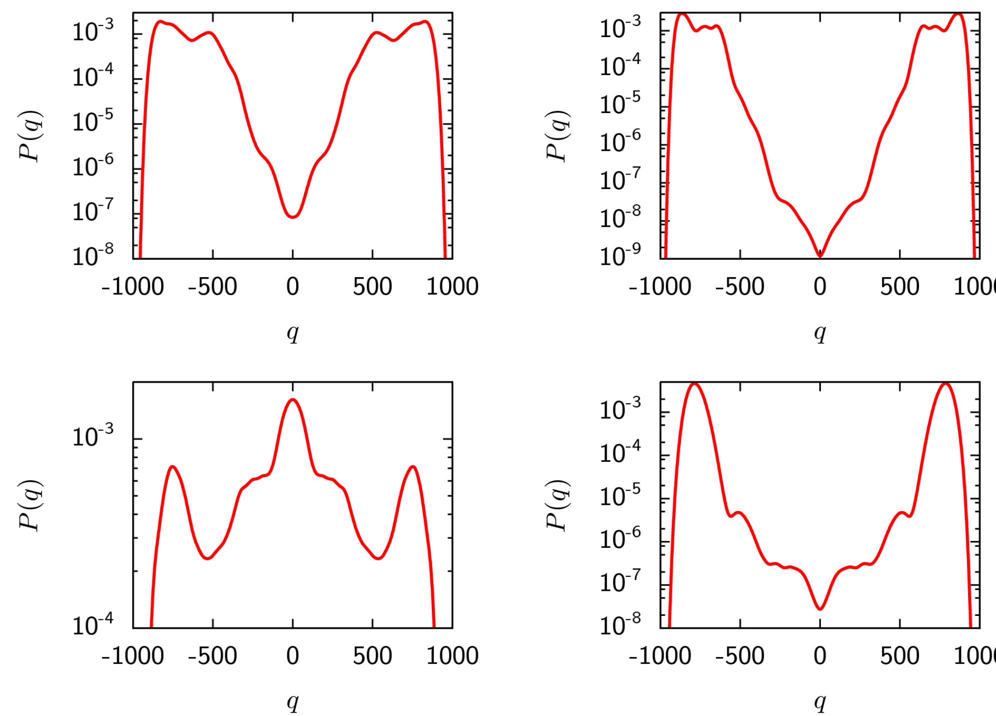


<u>fit:</u>
for 2D Ising the function is well known

$$F_B \sim \sigma(L) \sim 2L$$

<u>Spin glasses:</u>

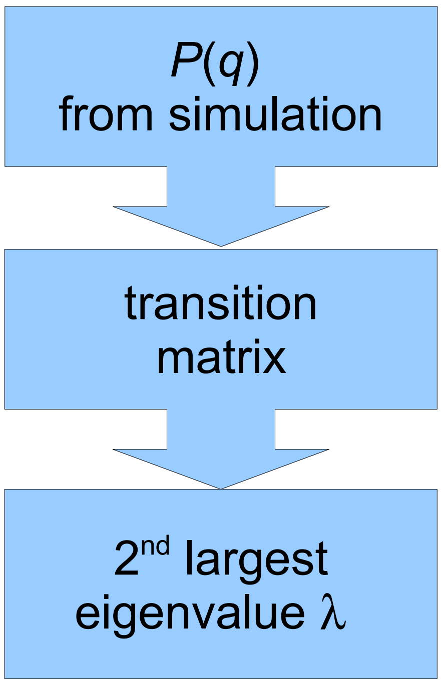
difficult structure, maxima/minima are scattered around



<u>Question</u>:
how do we measure the <u>size</u> of the <u>largest barrier</u>?

Idea: 1d Markov chain/transition matrix

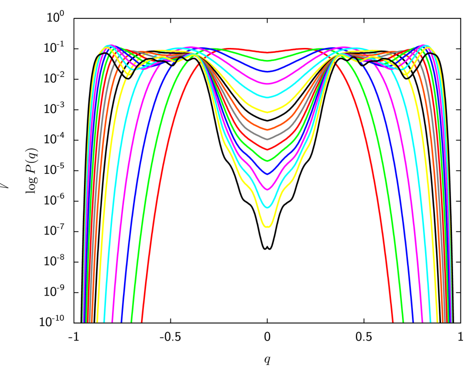
[B.A. Berg, A. Billoire and W. Janke, PRB 61 (2000), 12143]



Definition:

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

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



Simple example:
random walk

flat distribution

$$P(x_i)=\frac{1}{N}$$

$$w_{i,j}=\frac{1}{2}\min\left[1,\frac{1/N}{1/N}\right]=\frac{1}{2}$$

$$T=\begin{pmatrix} 1/2 & 1/2 & 0 & \cdots \\ 1/2 & 0 & 1/2 & \cdots \\ 0 & 1/2 & 0 & \cdots \\ 0 & 0 & 1/2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

with equilibrium distribution $A=\begin{pmatrix} 1/n \\ 1/n \\ \vdots \end{pmatrix}$ follows $TA=A$ ✓

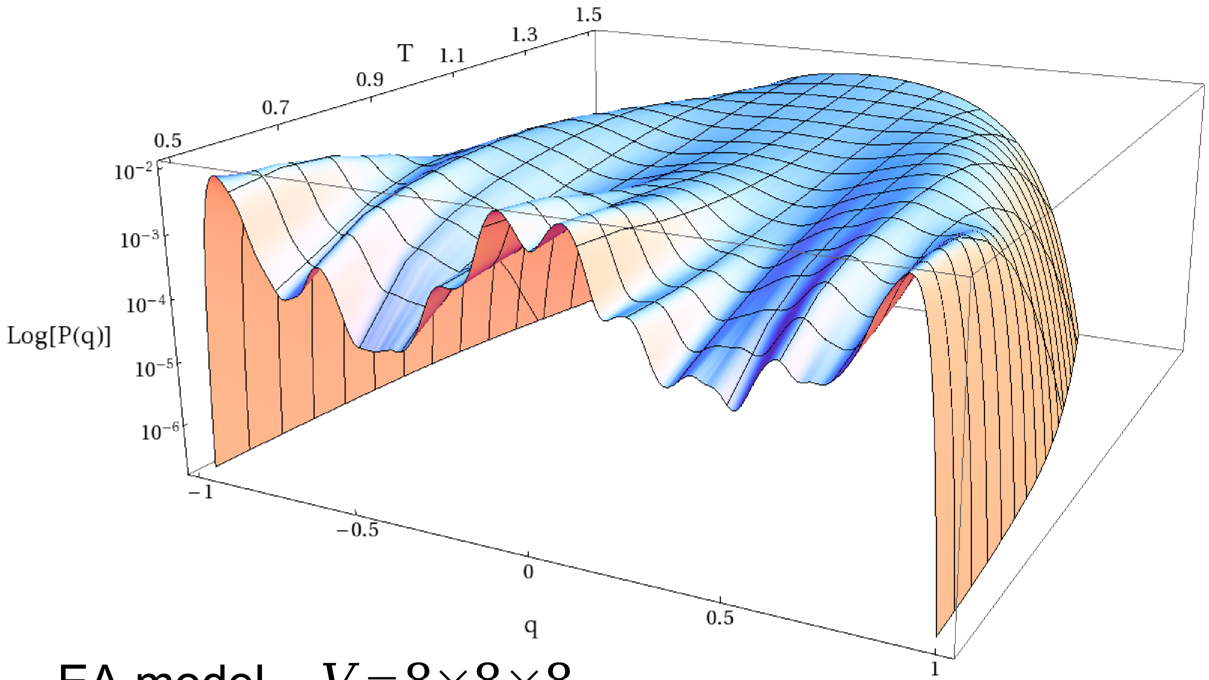
autocorrelation time for q:

$$\tau_B=\frac{1}{N\log\lambda}$$

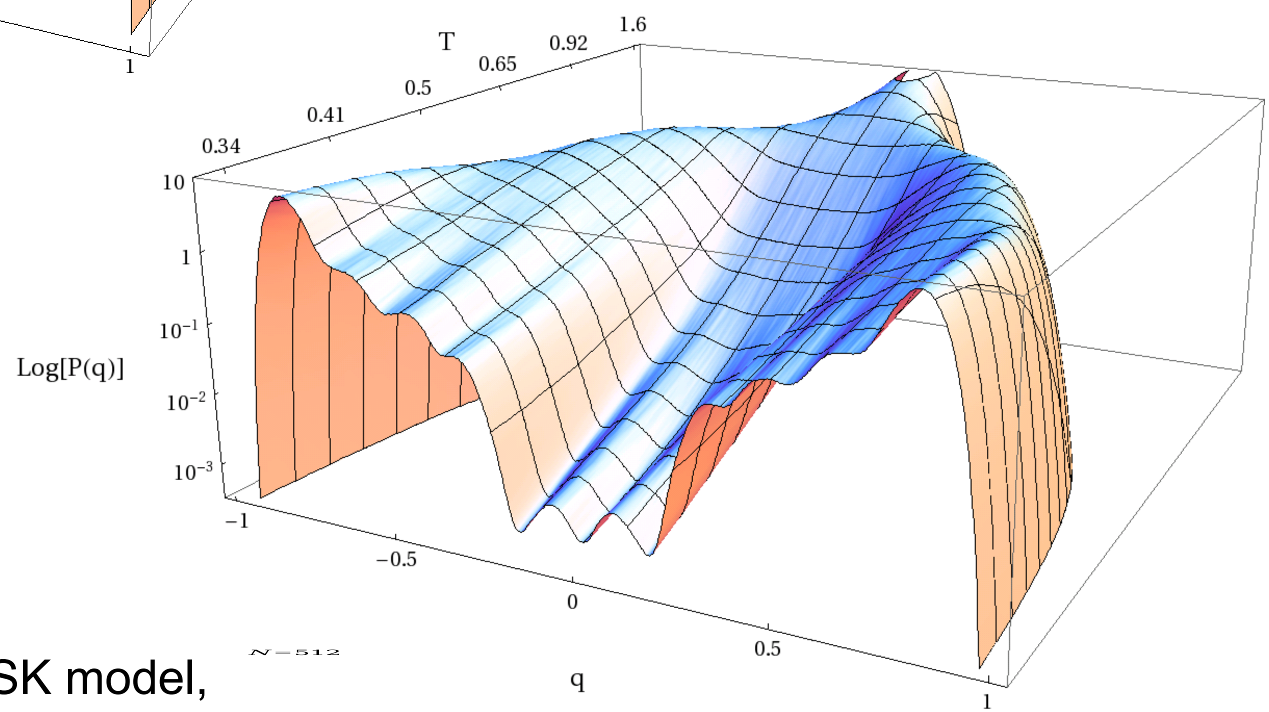
free energy barrier:

$$F_B\equiv\log\tau_B$$

Results 1a: Distribution $P_J(q,T)$ for ***ONE*** set of couplings



EA model, $V=8\times8\times8$



SK model, $N=512$

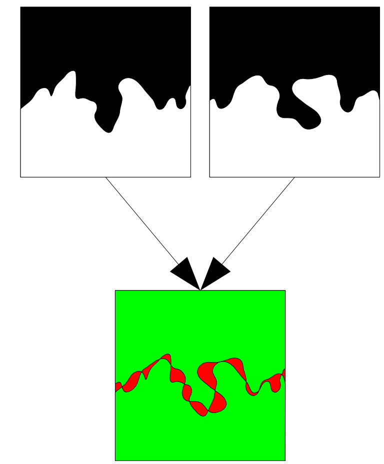
$$P(q)=\left[\sum_{ab} P_a \cdot P_b \cdot \delta(q-q_{ab})\right]_J$$

Result 1b: What does the ***average*** distribution of the EAI model look like?

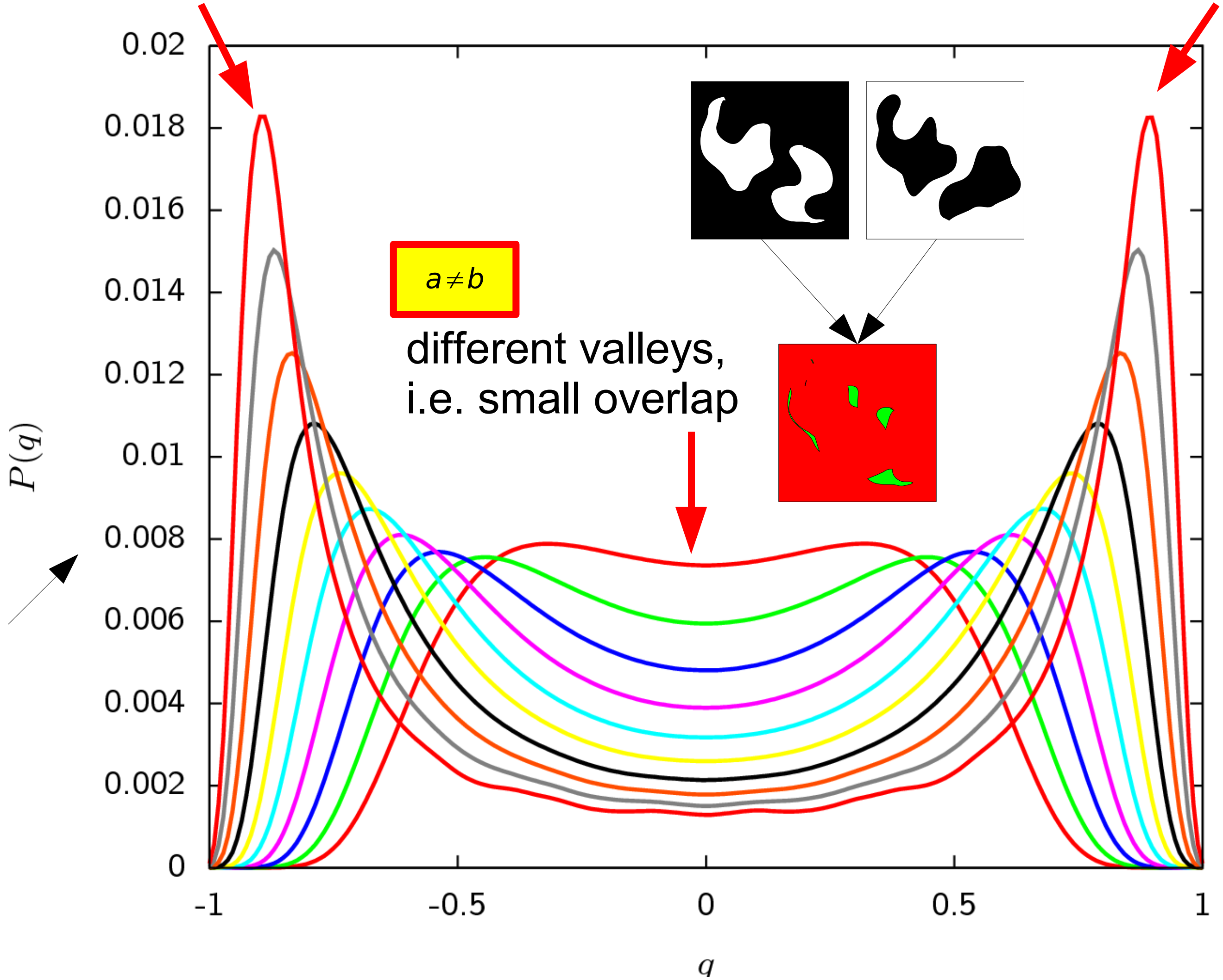
over the different couplings

$a=b$

same valley,
i.e. large overlap

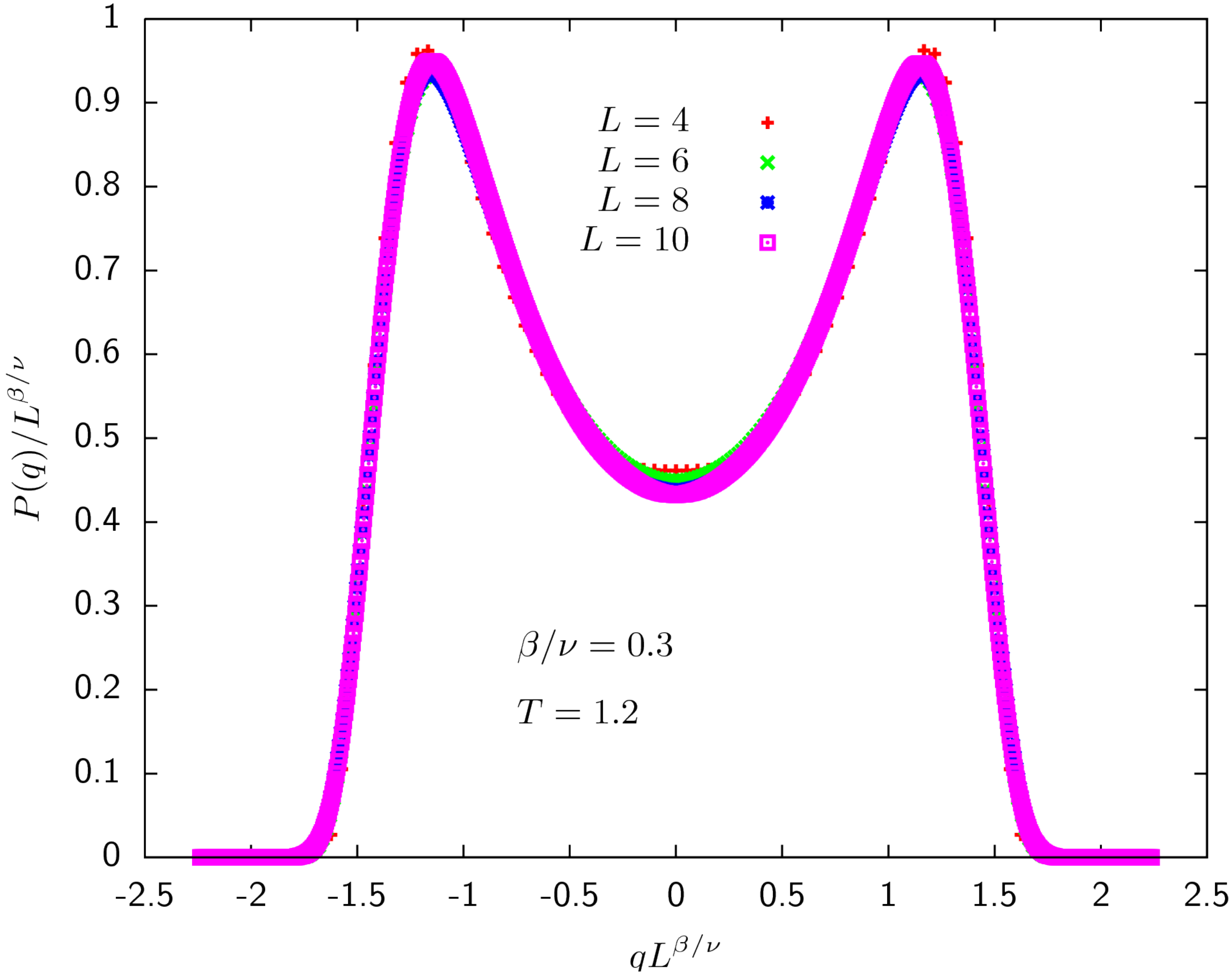


total inversion (of all spins)
of one system compared to right peak



<u>note the scale!</u>
$P(m)$ of Ising
model has
log-scale

Result 1c: FSS (just for fun & 'cause its free ...)

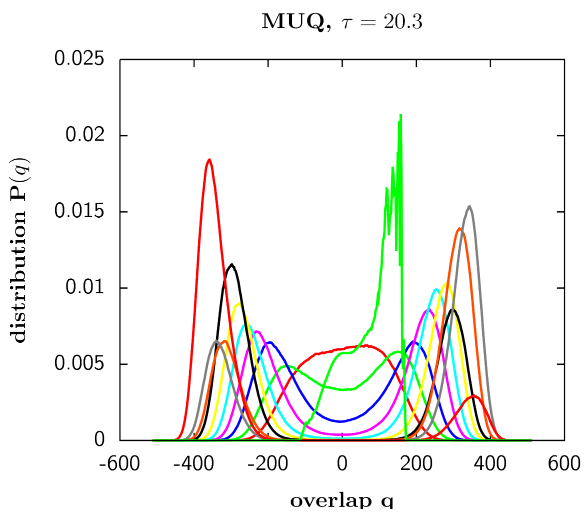


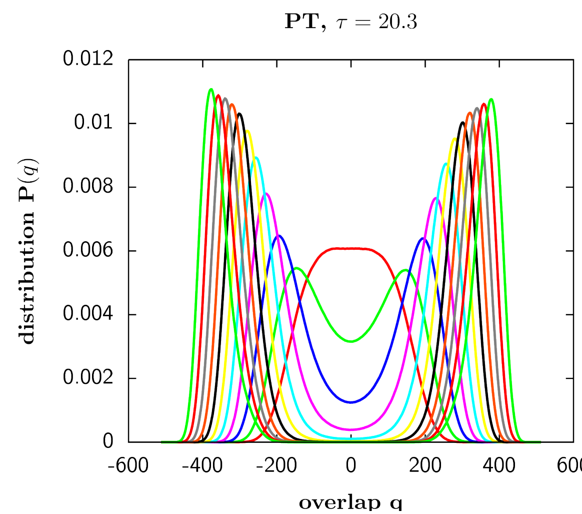
configuration (couplings) with large autocorrelation time

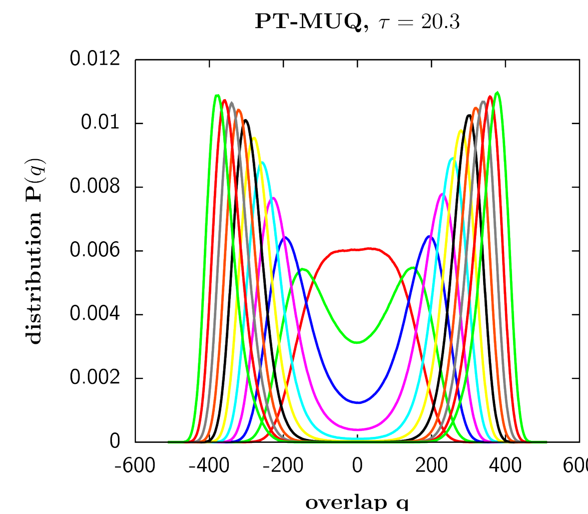
MUQ

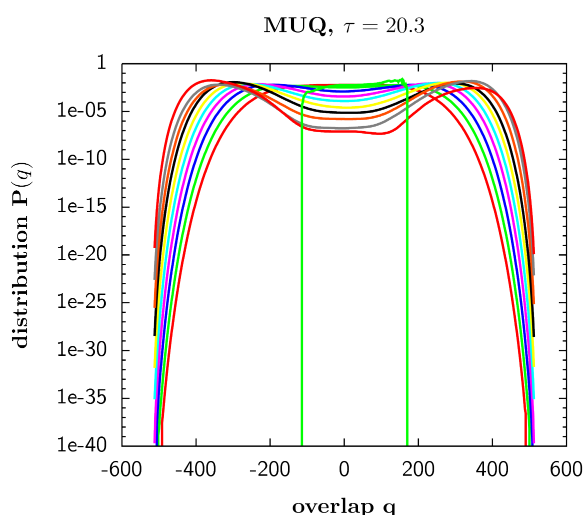
PT

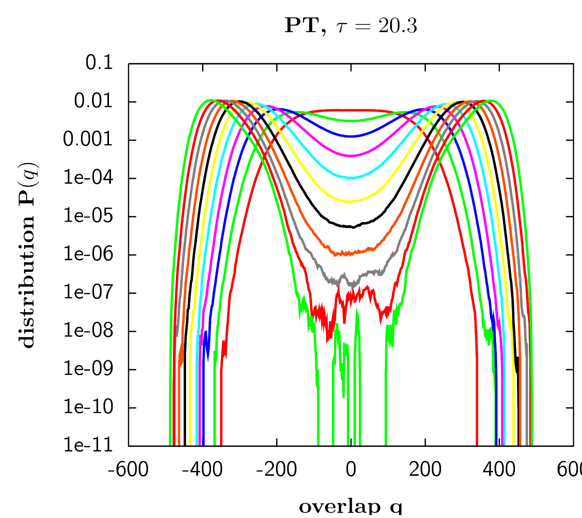
PT-MUQ

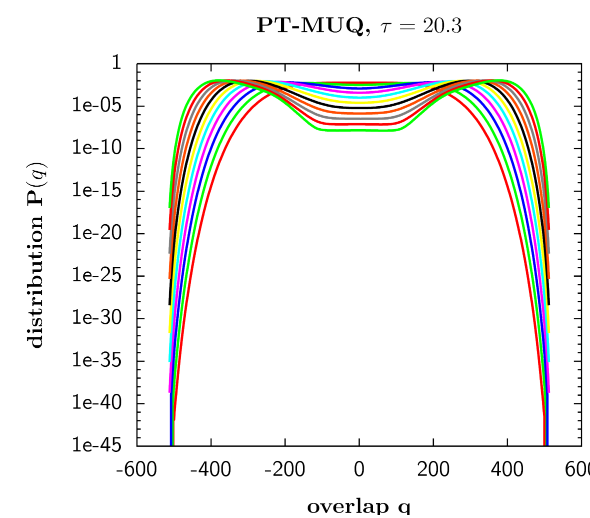










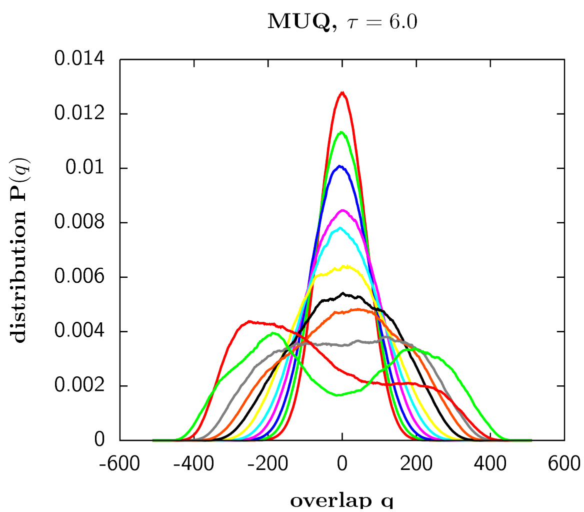


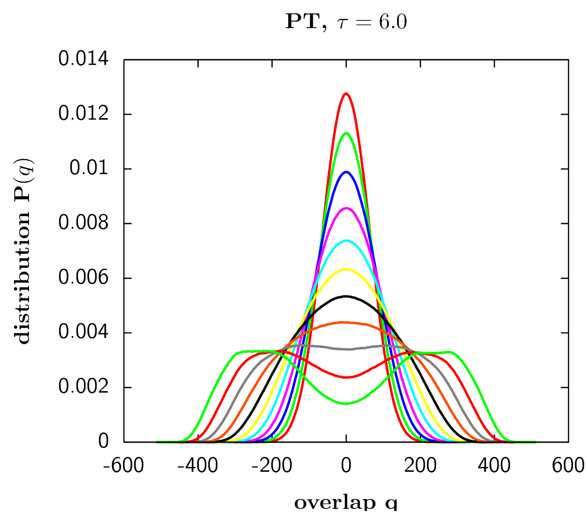
configuration (couplings) with large autocorrelation time

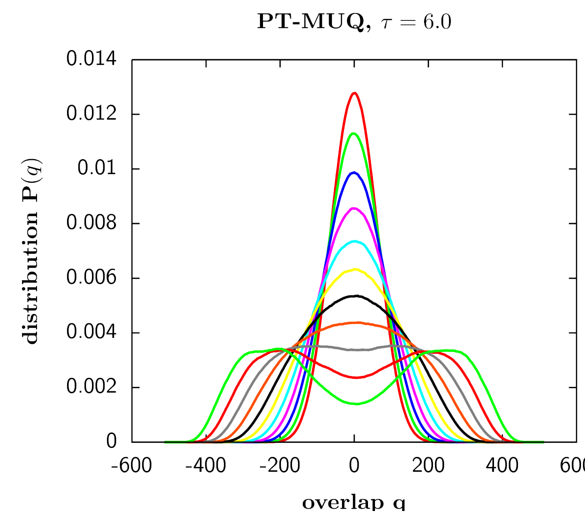
MUQ

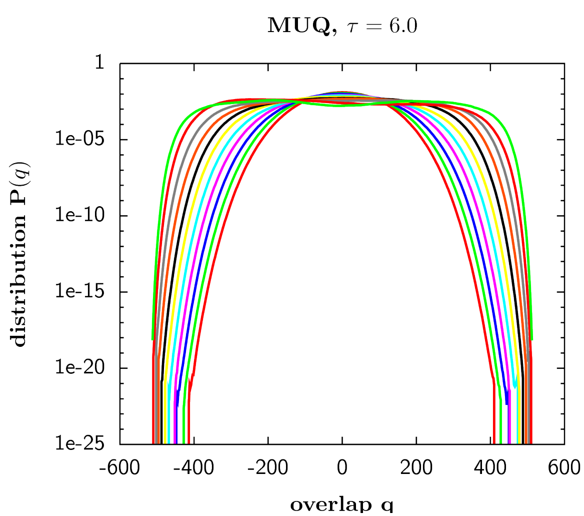
PT

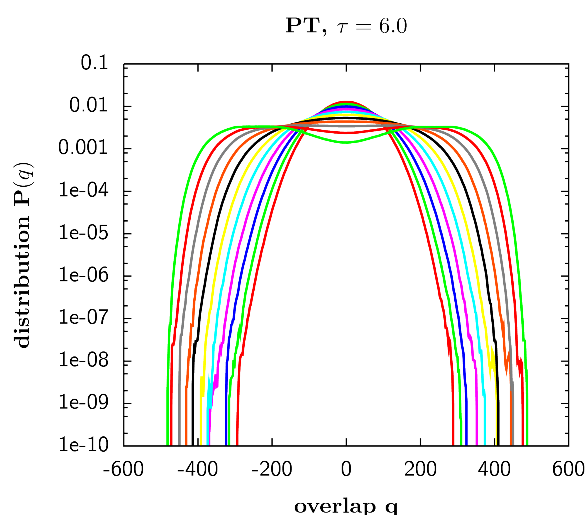
PT-MUQ

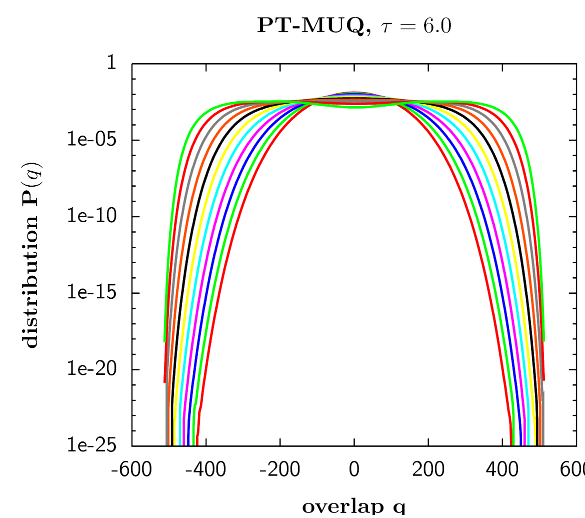






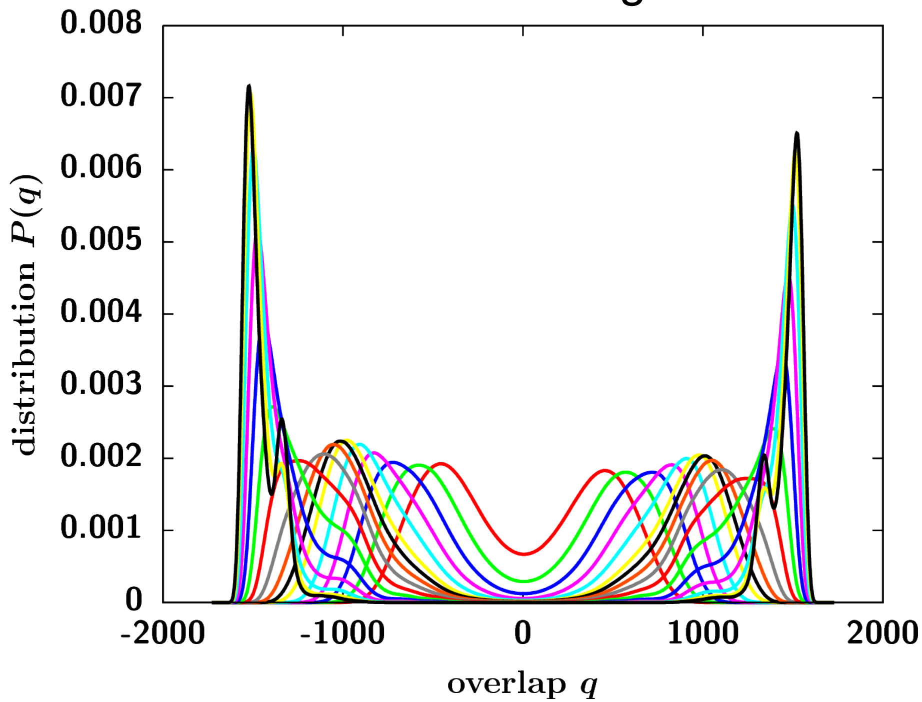




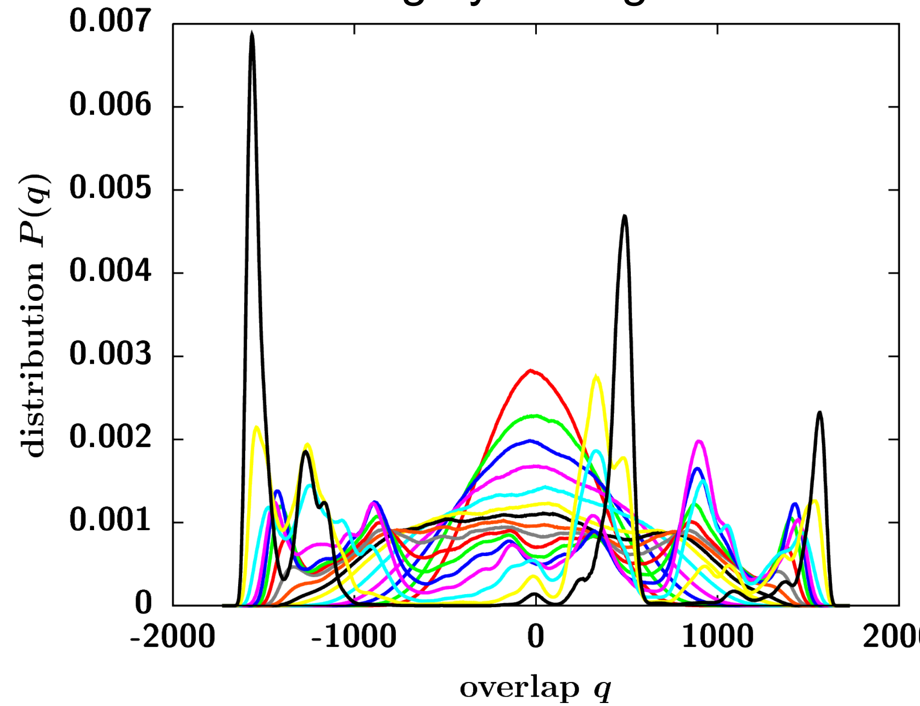


Resistance is futile?

“well behaved” configuration



“naughty” configuration



<u>Quality criterion:</u>

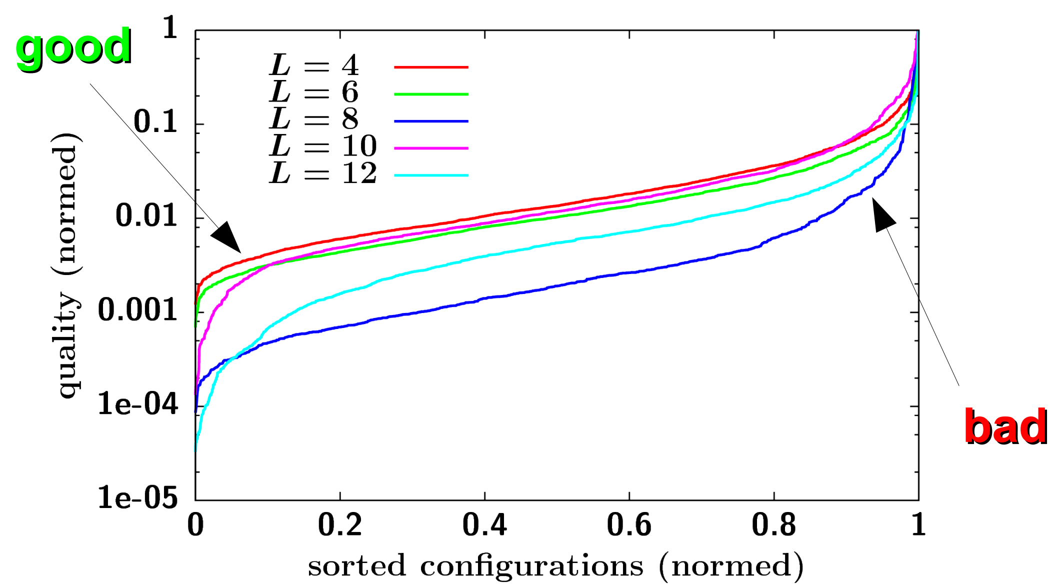
without PT: tunneling events
with PT: ?

<u>Idea: quadratic difference from the mean:</u>

$$\overline{P}(q) = \frac{P(q)+P(-q)}{2}$$

left: $$[P(q)-\overline{P}(q)]^2 = \frac{1}{4}[P(q)-P(-q)]^2$$

right: $$[P(-q)-\overline{P}(q)]^2 = \frac{1}{4}[P(q)-P(-q)]^2$$

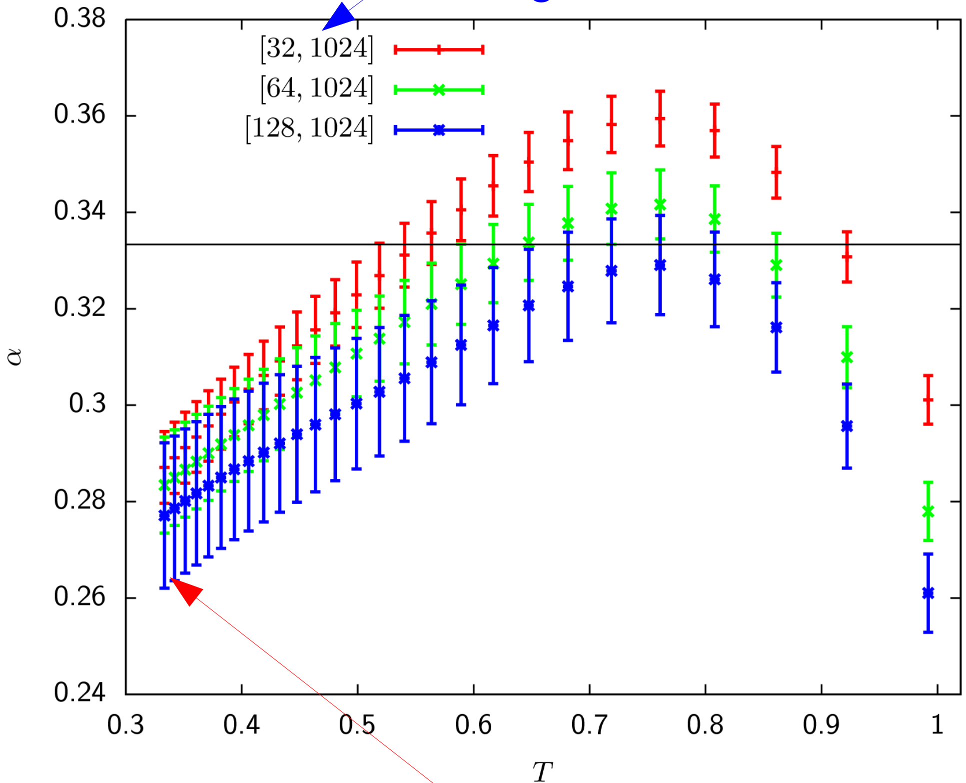


Results 2: FSS fit of $F_{\mathrm{B}} = \log \tau_{\mathrm{B}}$

A) SK model:

[E. Bittner, W. Janke, EPL 74 (2006) 195]

fit range



non-self-averaging (SK)

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

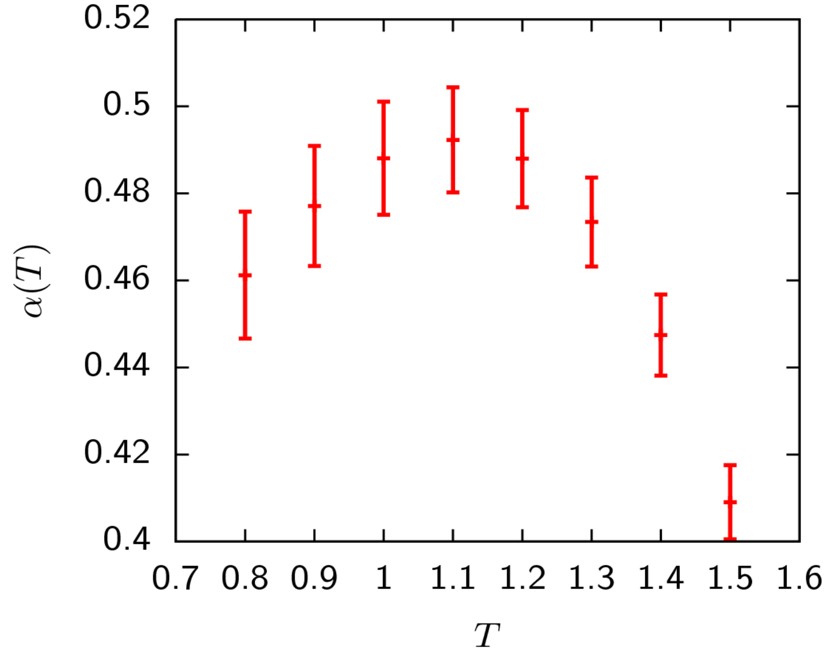
Analytic result:

[H. Kinzelbach and H. Horner, Z. Phys. B 84 (1991) 95]

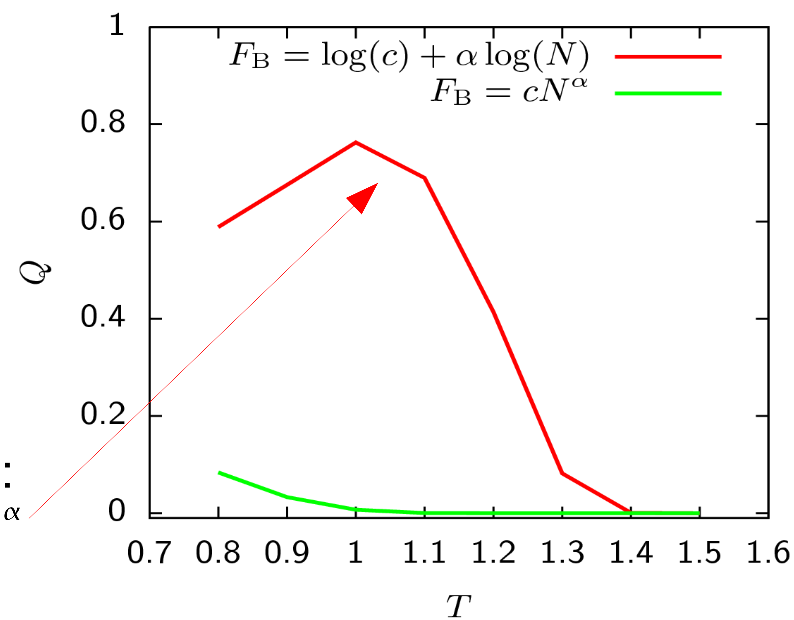
$$\tau_{\mathrm{B}} \propto \exp(cN^{\alpha})$$

$$\alpha = \frac{1}{3}$$

B) EAI model:



but goodness of fit ...

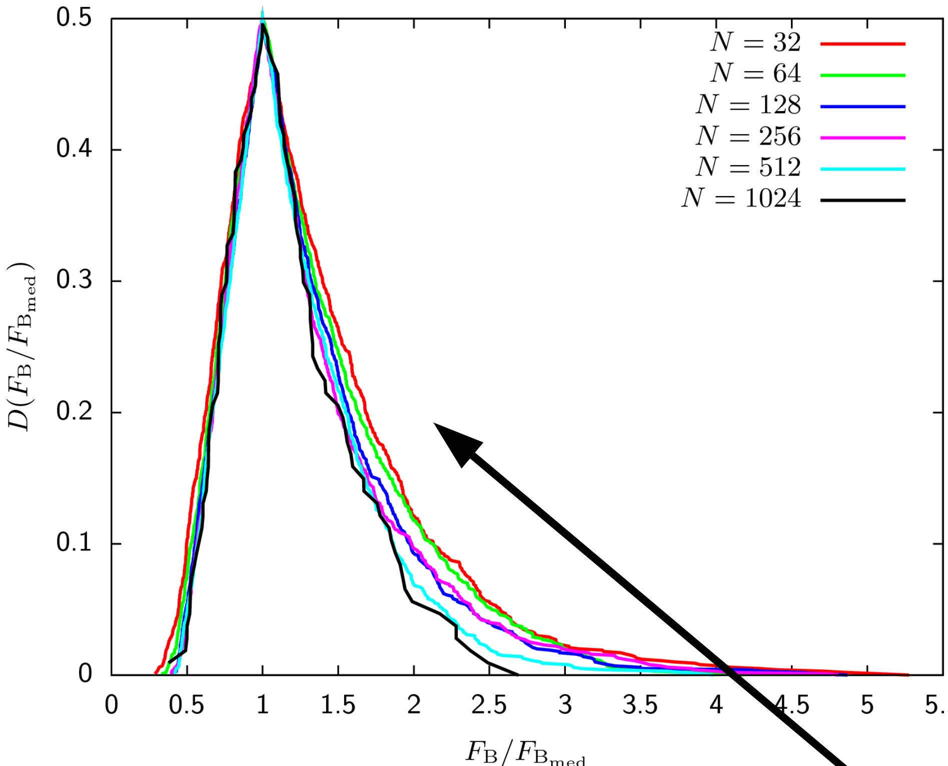


therefore, different fit:

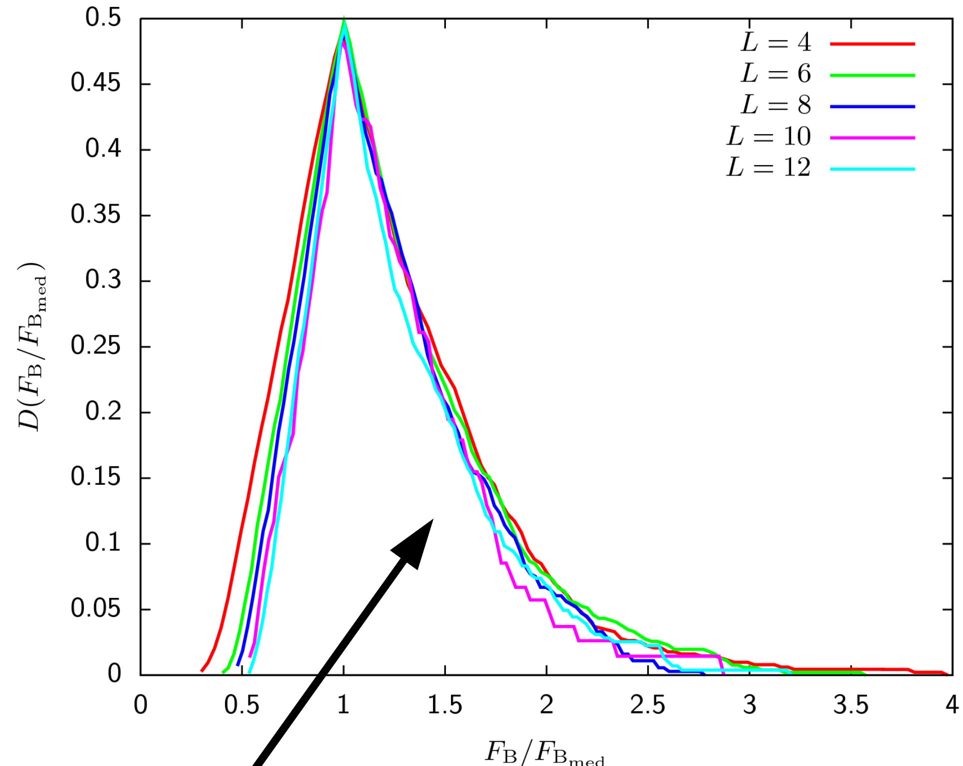
$$\tau_{\mathrm{B}} \propto cN^{\alpha}$$

Results 3: Peaked probability distribution $D(F_B/F_{B_{\mathrm{med}}})$

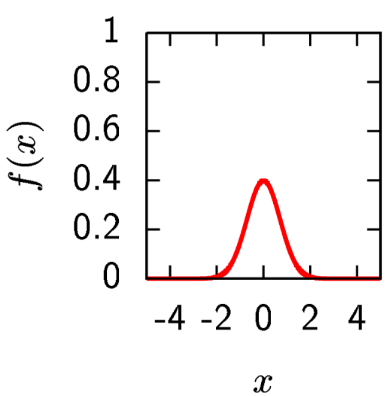
A) SK model



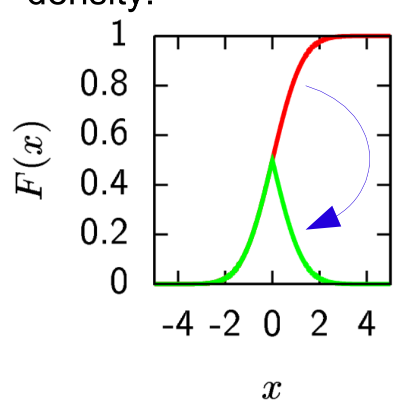
B) EA model



probability density:

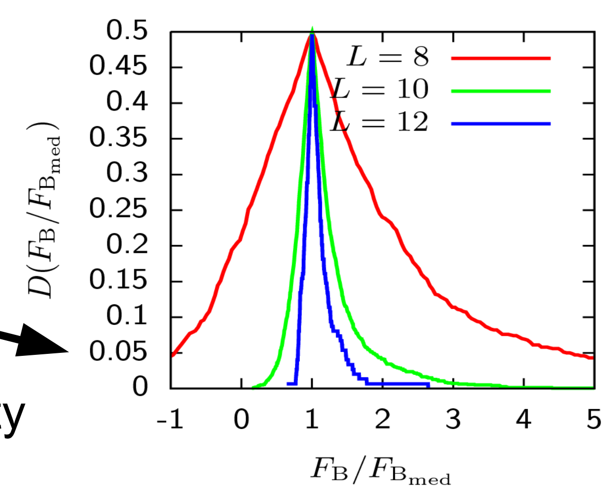


integrated probability density:



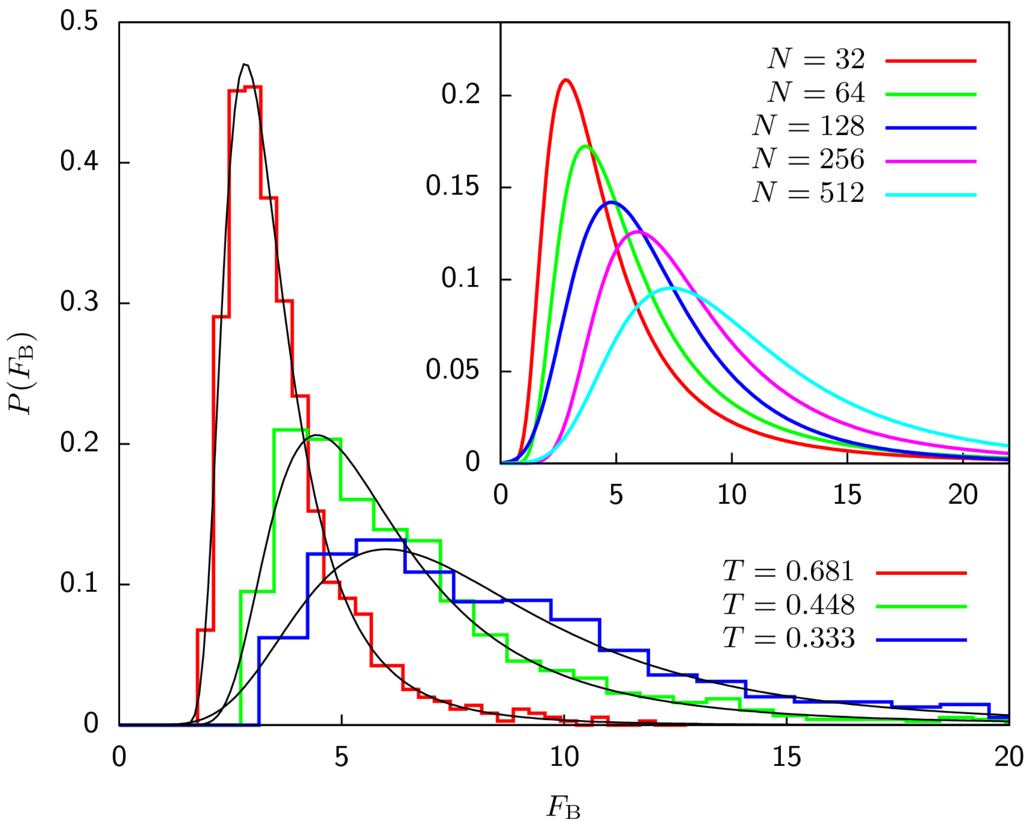
no scaling,
i.e. no selfaveraging!

in contrast:
barrier size
in energy **is**
selfaveraging quantity

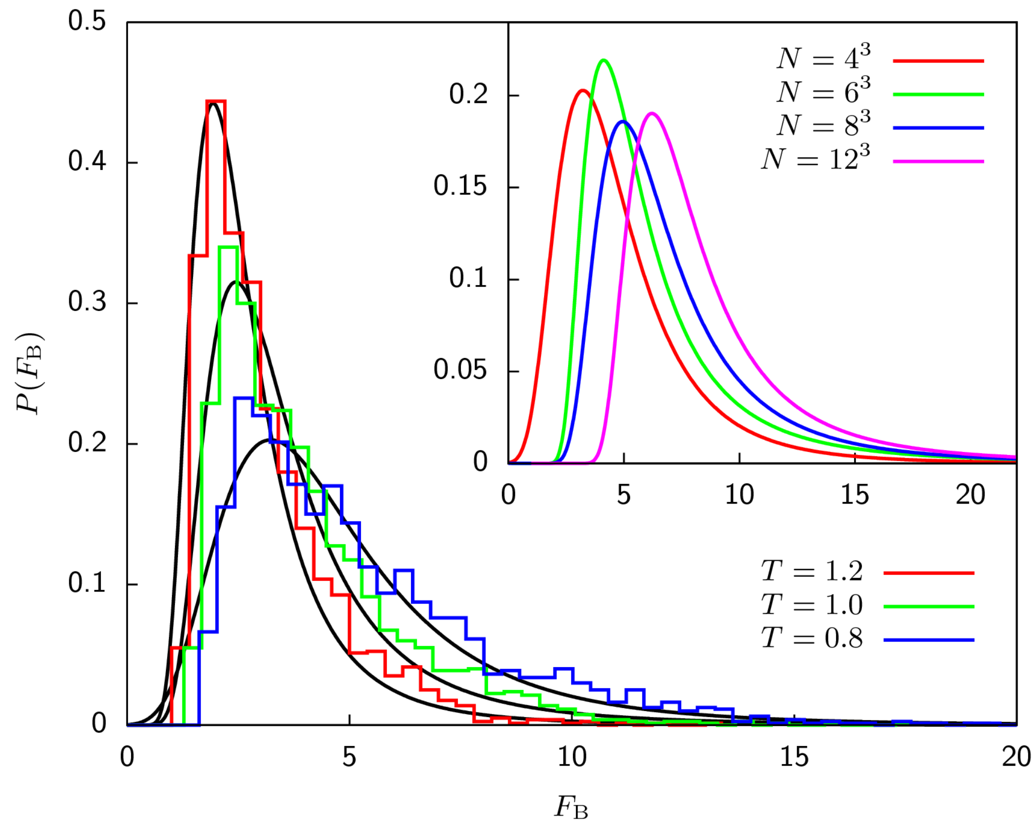


Results 4: Probability density distribution of the barrier sizes F_B

A) SK model



B) EA model



Fit integrated probability density:

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

$T < T_c \rightarrow \xi > 0$

$\rightarrow$ fat tailed (algebraic) Fréchet distribution

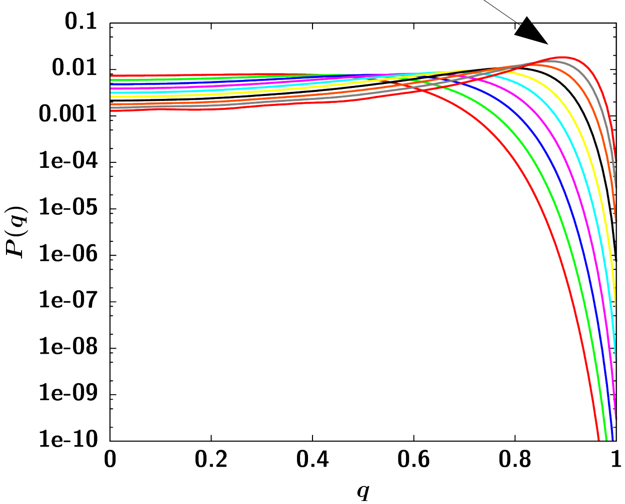
Results 5: Functional form of the overlap distribution

$P(q) = c_0 e^{-c_1 N (q - q_{max}^{\infty})^x}$

for $q > q_{max}^{\infty}$

mean-field (Parisi): $x = 3$

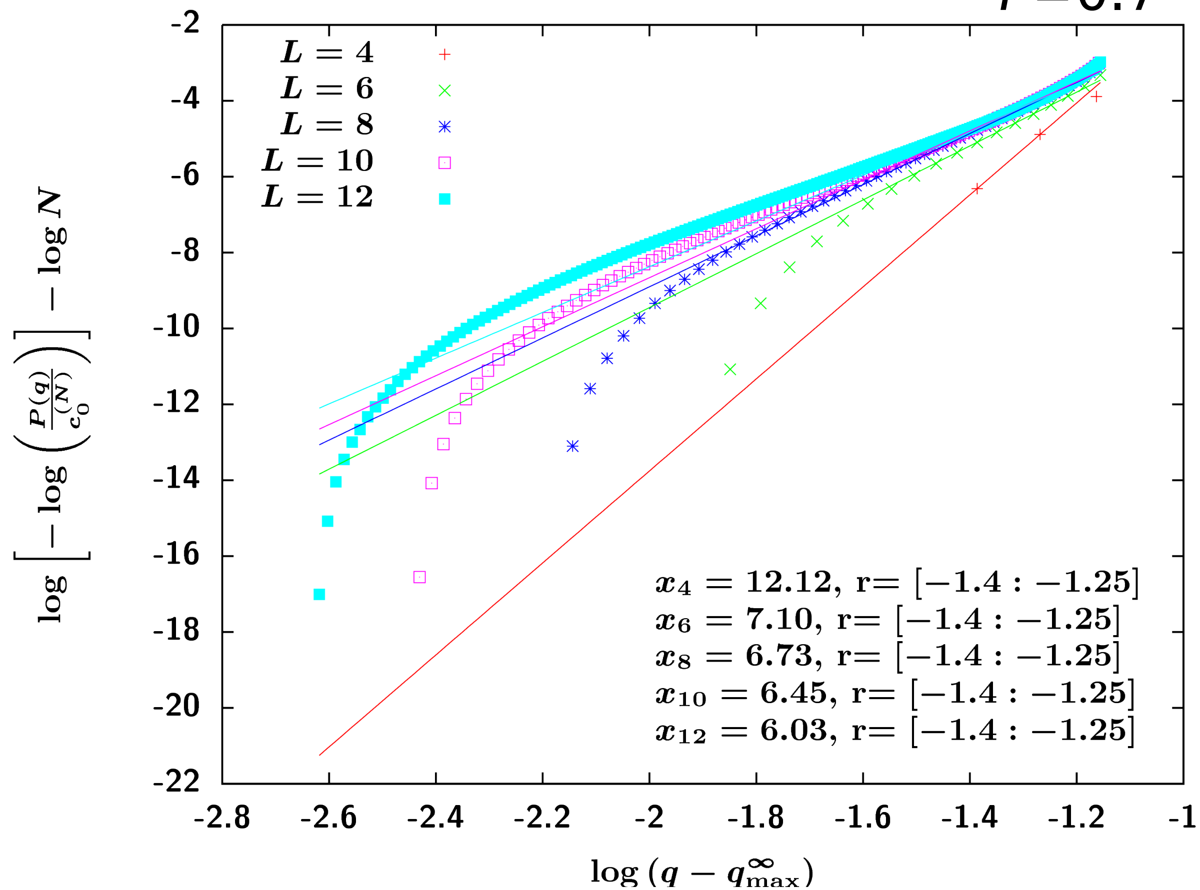
3D (Moore): $x = 6$ (?)



2xlog, then fit:

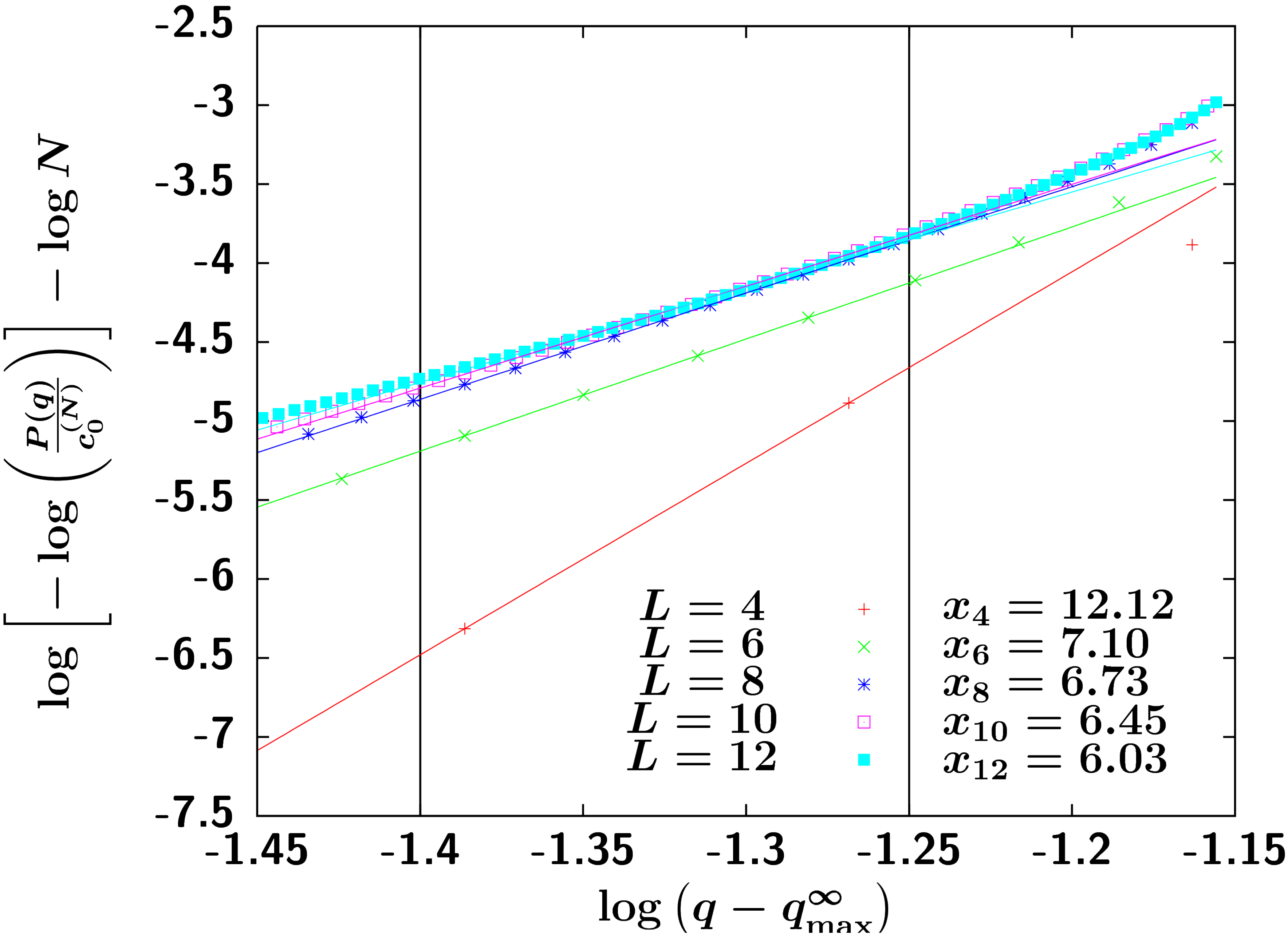
$$\ln\left[-\ln\left(\frac{P(q)}{c_0^{(N)}}\right)\right] - \ln(N) = \ln c_1 + x \ln\left(q - q_{max}^{\infty}\right)$$

$T = 0.7$



<u>quality of the fit:</u>
consistent fits can be only achieved over a "somewhat" restricted range

Zoom of the last plot:



Conclusions:

A) 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 $T \approx 0.5\, T_{\mathrm{c}}$

B) Physical

the free energy barriers of the <u>SK and EA</u> 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!

A) Thank you for your attention!

B) Publications:

B. Berg, A. Billoire and W. Janke
Phys. Rev. Lett., 80 (1998) 4771
B. Berg, A. Billoire and W. Janke
Phys. Rev. B., 61 (2001) 12143
E. Bittner, W. Janke,
"Free-energy barriers in the Sherrington-Kirckpatrick Model"
Europhys. Lett, 74 (2006) 195
E. Bittner, A. Nußbaumer and W. Janke
"Free-energy barriers of spin glasses"
in NIC Symposium 2008, edited by G. Münster, D. Wolf, M. Kremer,
NIC Series, Vol. 39, 221 (2008)

C) Work is supported by:

Deutsche Forschungsgemeinschaft
EU-RTN Network "ENRAGE"
Computer time: NIC, FZ-Jülich

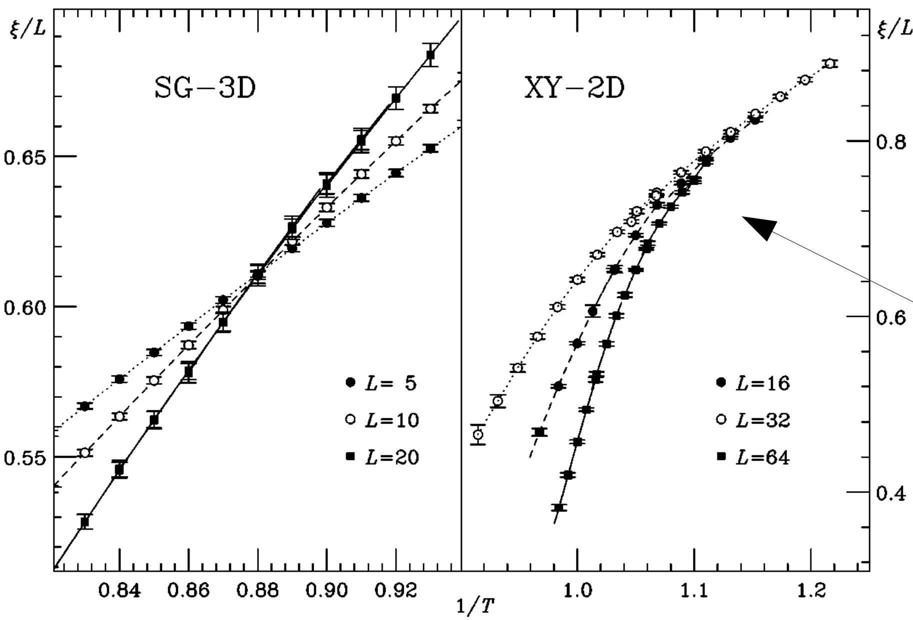
Supplement 1:

Finite temperature transition in 3D: Yes/No?

Yes $T \approx 1.1$ $g_{sg} \approx 0.75$

Universality class: 2nd order/BKT

Correlation length divided by system size:



[H. G. Ballesteros et al.,PRB 62 (2000) 14237]

Early MC [Bhatt and Young, PRL 54 (1985) 924]: line of critical points terminating at T=1.2 similar BKT in 2D XY

Berenzinskii-Kosterlitz-Thouless (BKT) transition

"simple" 2nd order transition

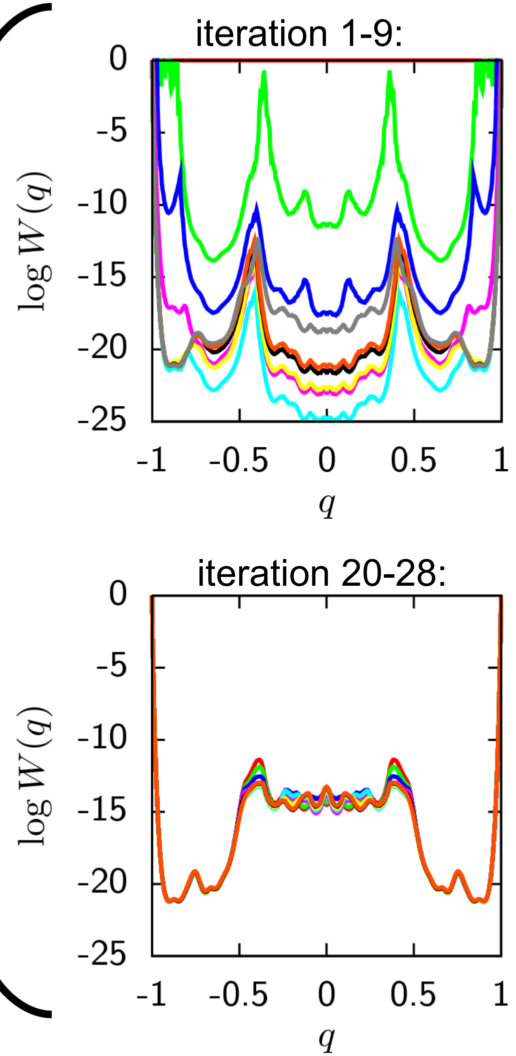
Four dimensions or higher?

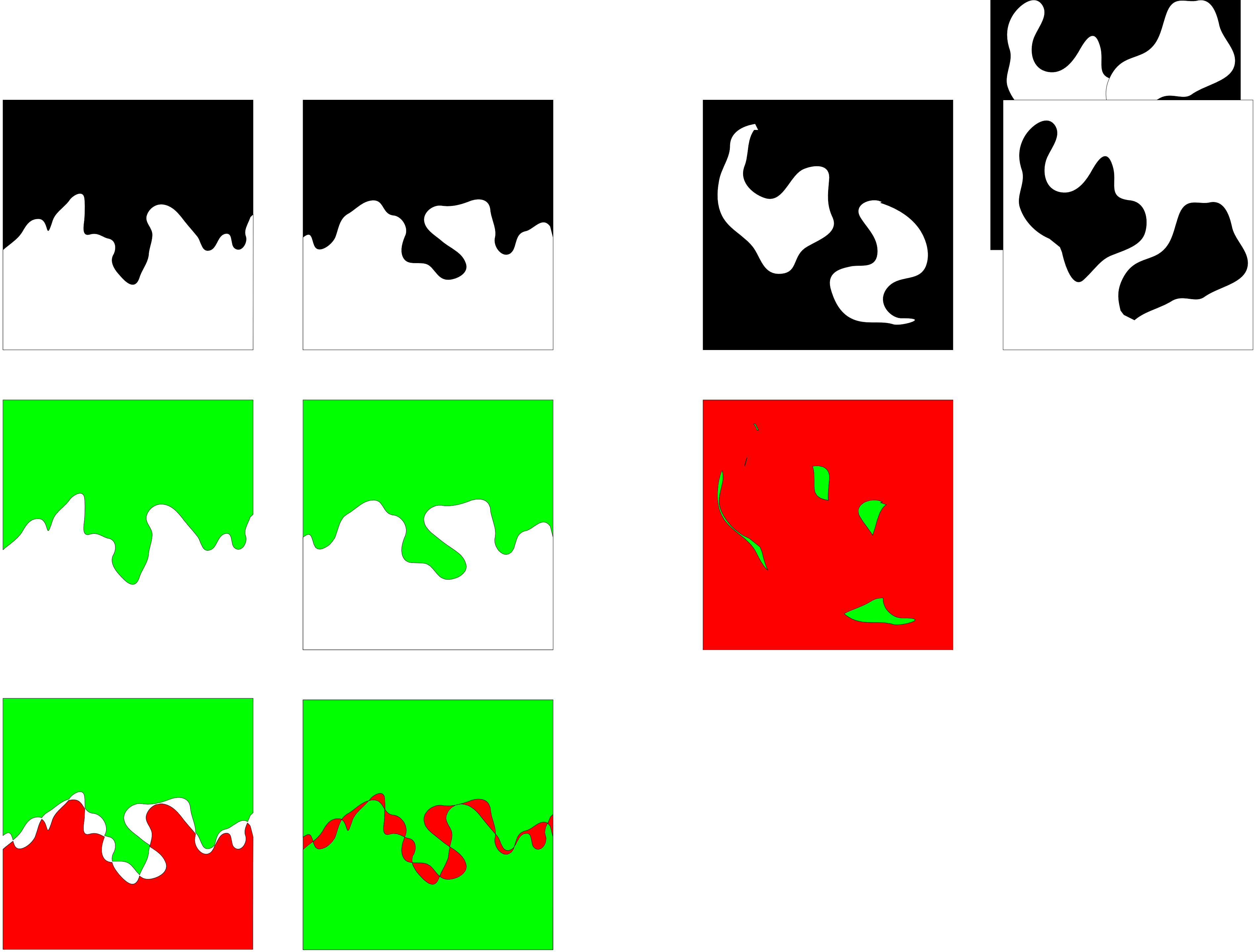
Simpler to simulate (well separated from the lower critical dimension)
Finite-temperature well established ($T_c \sim 1.75$) by Binder-parameter crossing

Supplement 2:

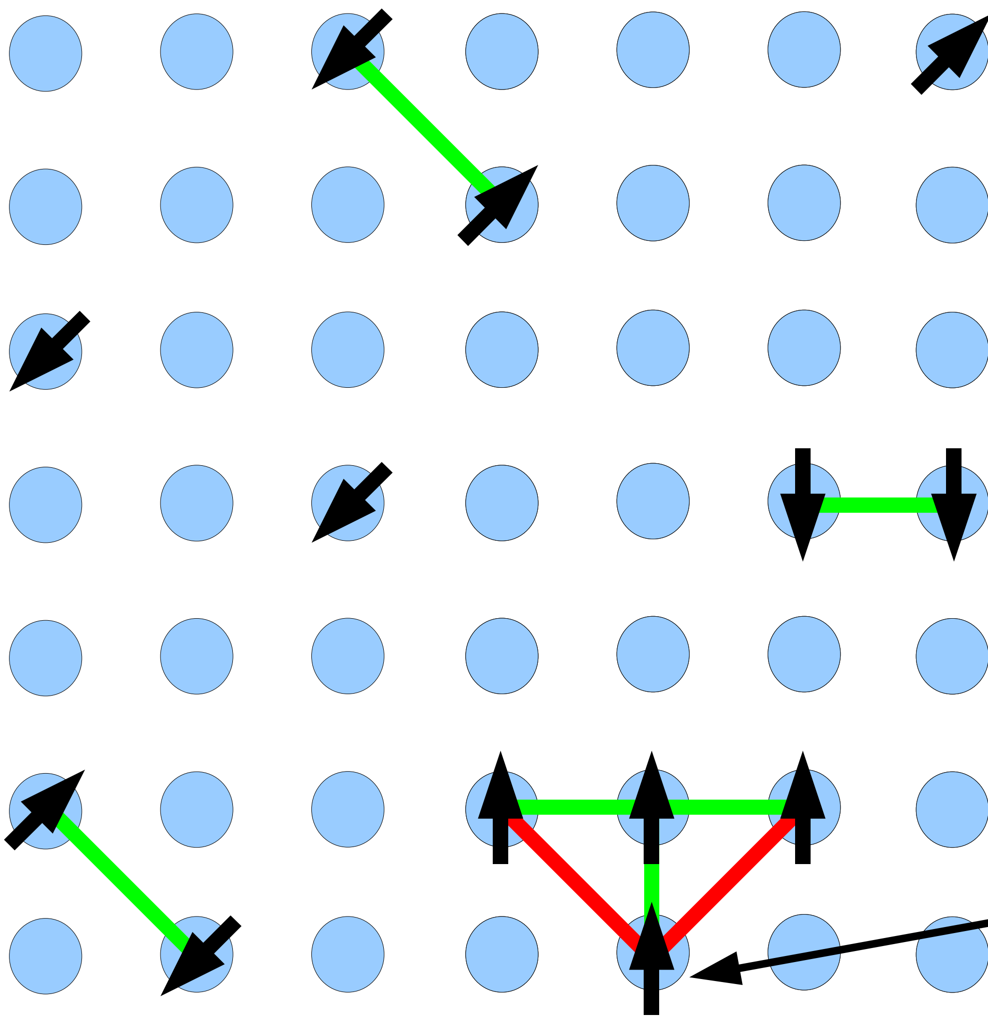
<u>Do the weihgts saturate?</u>

Yes





And the explanation?



T is very low,
doping around 30%,

n.n.: ferromagnetic $J_1 > 0$

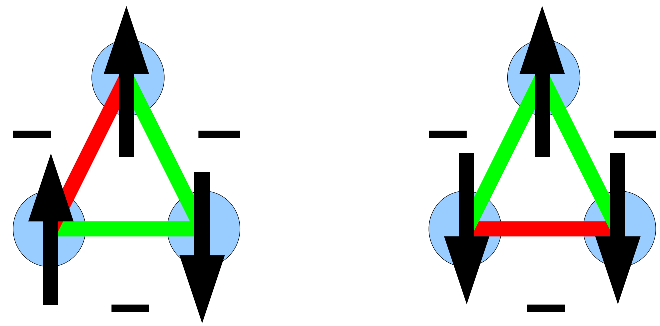
n.n.n: anitferromagnetic $J_2 < 0$

Sketch: $J_1 = 2|J_2|$

frustration of the lower spin:
cannot decide if he wants to satisfy
n.n. neighbour by ↓
or n.n.n. neighbours by ↑

Is frustration sufficient for a spin glass?

NO! Counter example:
antiferromagnetic triangular lattice



here:
4 other (symmetric configurations)

fully frustrated
no co-operative freezing transition (Mydosh: slow blocking to ground state with large mag. fluctuations)

⇒ Add: **mixed interactions**, i.e.
ferromagnetic (J>0) and antiferromagnetic (J<0)

Enough?

NO! Counter example:
Kagome lattice

Add: **randomness/disorder**, i.e.

site randomness = distribution of distances between spins

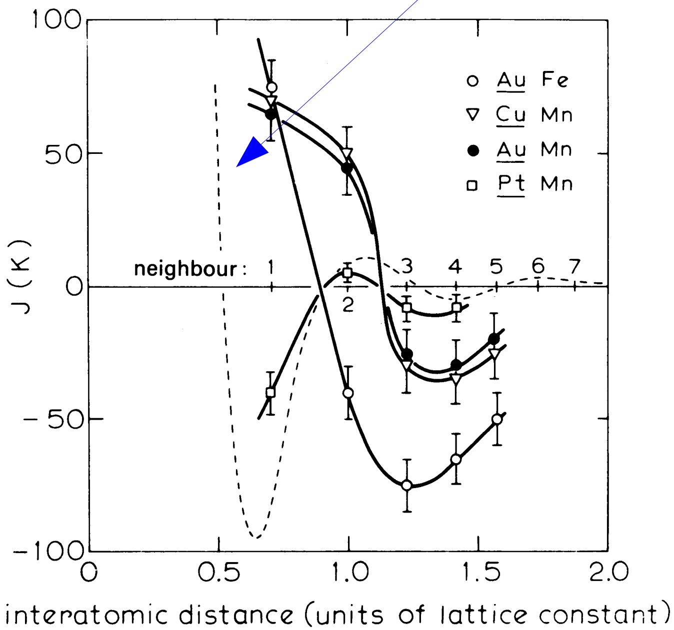
<u>bond randomness</u> = nearest-neighbour interaction varies (+/-J)

Finally: **randomness** + **mixed interaction**

can lead to **frustration** spin glass

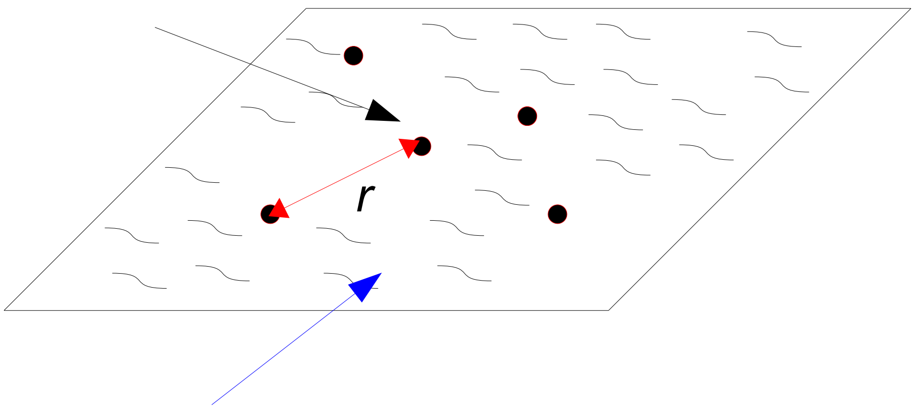
RKKY =Ruderman, Kittel, Kasuy, Yosida

Hamiltonian: $H = J(2k_F r)\sigma_i \sigma_j$ $\qquad J(x) = J_0 \frac{\cos(x)}{x^3}$



from: Morgownik and Mydosh (1983)

impurities, e.g. Fe, Mn, ...



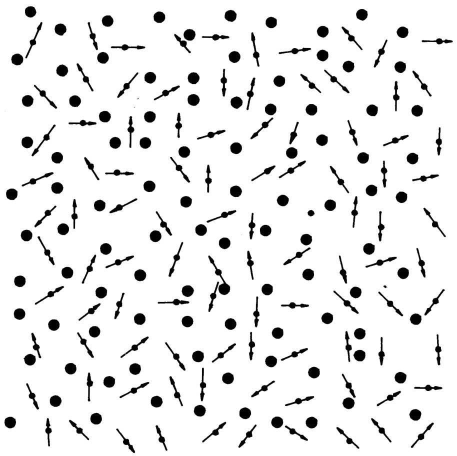
sea of conduction electrons from non-magnetic metal host-matrix, e.g. Au, Cu, Pt, ...

How to create randomness ?

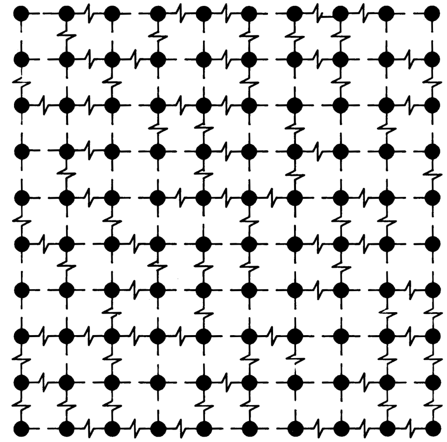
take non-magnetic metall (Au, Cu, Pt ...)
+ elements with magnetic moment (Mn, Fe, Gd, Eu, ...)

archetypes are noble metal alloys: (also called: canonical SG)

$Cu_{1-x}Mn_x$ $Au_{1-x}Fe_x$



random site SG
random bond SG



$Rb_2Cu_{1-x}Co_xF_4$ (2D)

$Fe_{1-x}Mn_xTiO_3$ (3D)

RSB picture for
finite dimensions
short range interactions

(a) there are ∞ many pure states with varying overlaps
(b) predictions derived from (a)

---

droplet picture (for
finite dimensions
short range interactions)

(a) there are 2 pure states mapped to each other (like ferromagnet)
(b) scaling of free energy of droplet
(c) predictions derived from (a) and (b)

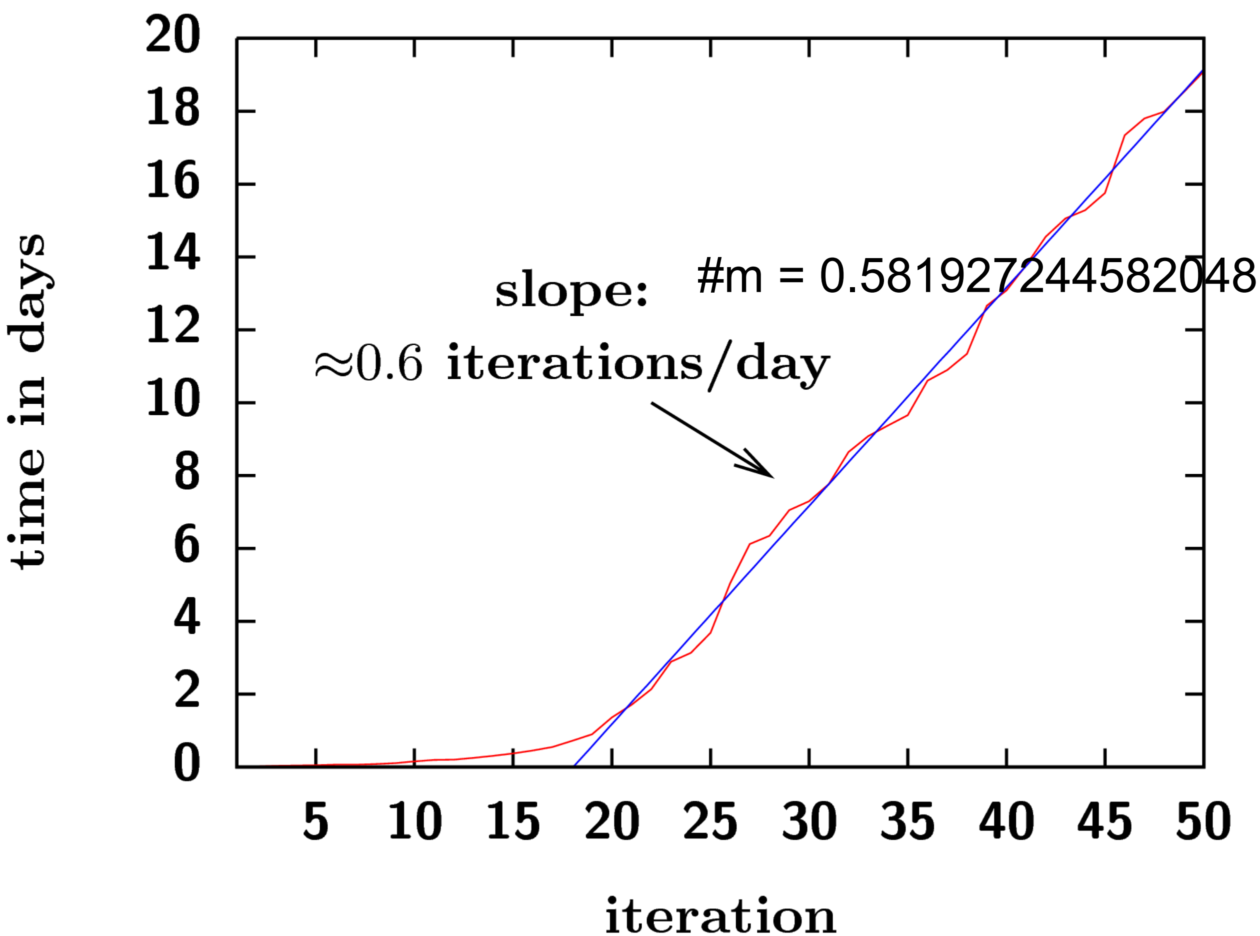
Detour (or cul-de-sac): e.g.: Wang-Landau

Update rule for state X_1 to X_2: $p(X_1 \rightarrow X_2) = min\left[\frac{g(X_1)}{g(X_2)}\right]$

$g(X_{1,2}) = frequency(X_{1,2}) \times f(iteration)$

gets somehow smaller

result of an (unbiased) 5x5x5 EAI SG:



criterion (e.g.):

$$\frac{h(min)}{h(max)} \approx c = 0.8$$

<u>gets worse for larger system!</u>