Exact Ground States of Finite Ising Spin Glasses Obtained by ”Branch-and-Bound”

S. Kobe

.

kobe@theory.phy.tu-dresden.de

http://www.physik.tu-dresden.de/itp/members/kobe.html

Technische Univ. Dresden, Inst. für Theor. Physik, D-01062 Dresden, Germany

Outline

- ISING model: A short history
- Exact ground states of finite ISING spin glasses
- Results:
  - Lattice models:

    Energy landscape

    Relaxation
  - Mean field models:

    Energy exponents and correction to scaling

    Ferromagnetic – spin-glass transition

Historical remarks

Letter of Wolfgang Pauli to H. B. G. Casimir:

Princeton, 11. Oktober 1945

" ... A few weeks will be sufficient for you and others to learn everything of
scientific interest which happened during these 'lost years'.
I am sending you today a package with reprints, please divide
them among persons who are interested.

There is a paper of Onsager included (...) of which I think
that it is a masterpiece of mathematical analysis.
It contains the rigorous solution of the Kramers - Wannier order-disorder problem
for the two dimensional model (unfortunately the method cannot be generalized
for three dimensional crystals). ... "

Ising Model: Phase transition, scaling behaviour

Zero field ISING model:

$$\mathcal{H} = - \sum_{1 \le i < j \le N} J_{ij} S_i S_j \qquad\qquad S_i = 1 \vee -1$$

– $J_{ij} > 0$ between nearest neighbours of a lattice; $J_{ij} = 0$ else

– Ground state is trivial

– Phase transition: (ferromagnetic) order - disorder a rough value of the current amplitude at resonance. We find for the current at resonance

$$I = -\left[2\pi c\left(\frac{\kappa}{\mu}\right)^{\frac{1}{2}} a\right] 0.04 \cos\left(\frac{3\pi}{2}\xi\right) \cos \omega\tau. \qquad \text{(III 25)}$$

The current is in phase with the impressed electromotive force in the two extreme thirds of the antenna, but out of phase in the middle third. As the current amplitude at the center of the antenna is only some 4 percent of that at first resonance, the second and higher order resonances are evidently of little importance as compared with the first resonance.

PHYSICAL REVIEW VOLUME 65, NUMBERS 3 AND 4 FEBRUARY 1 AND 15, 1944

Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition

LARS ONSAGER
Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut

(Received October 4, 1943)

The partition function of a two-dimensional "ferromagnetic" with scalar "spins" (Ising model) is computed rigorously for the case of vanishing field. The eigenwert problem involved in the corresponding computation for a long strip crystal of finite width (n atoms), joined straight to itself around a cylinder, is solved by direct product decomposition; in the special case $n=\infty$ an integral replaces a sum. The choice of different interaction energies $(\pm J, \pm J')$ in the (0 1) and (1 0) directions does not complicate the problem. The two-way infinite crystal has an order-disorder transition at a temperature $T=T_c$ given by the condition

$$\sinh(2J/kT_c)\sinh(2J'/kT_c)=1.$$

The energy is a continuous function of T; but the specific heat becomes infinite as $-\log|T-T_c|$. For strips of finite width, the maximum of the specific heat increases linearly with $\log n$. The order-converting dual transformation invented by Kramers and Wannier effects a simple automorphism of the basis of the quaternion algebra which is natural to the problem in hand. In addition to the thermodynamic properties of the massive crystal, the free energy of a (0 1) boundary between areas of opposite order is computed; on this basis the mean ordered length of a strip crystal is

$$(\exp(2J/kT)\tanh(2J'/kT))^n.$$

INTRODUCTION

THE statistical theory of phase changes in solids and liquids involves formidable mathematical problems.

In dealing with transitions of the first order, computation of the partition functions of both phases by successive approximation may be adequate. In such cases it is to be expected that both functions will be analytic functions of the temperature, capable of extension beyond the transition point, so that good methods of approximating the functions may be expected to yield good results for their derivatives as well, and the heat of transition can be obtained from the difference of the latter. In this case, allowing the continuation of at least one phase into its metastable range, the heat of transition, the most appropriate measure of the discontinuity, may be considered to exist over a range of temperatures.

It is quite otherwise with the more subtle transitions which take place without the release of latent heat. These transitions are usually marked by the vanishing of a physical variable, often an asymmetry, which ceases to exist beyond the transition point. By definition, the strongest possible discontinuity involves the specific heat. Experimentally, several types are known. In the $\alpha-\beta$ quartz transition,[1] the specific heat becomes infinite as $(T_c-T)^{-\frac{1}{2}}$; this may be the rule for a great many structural transformations in crystals. On the other hand, supraconductors exhibit a clear-cut finite discontinuity of the specific heat, and the normal state can be continued at will below the transition

[1] H. Moser, Physik. Zeits. 37, 737 (1936).

Ernst Ising 1925

Peoria 1996

Ising Spin Glass Models

Zero field ISING model:

$$\mathcal{H} = - \sum_{1 \le i < j \le N} J_{ij} S_i S_j \qquad\qquad S_i = 1 \vee -1$$

- J_{ij} arbitrary
- Ground state is not known!!!

Spin Glass Models (Lattice vs. Mean-Field Models)

- Lattice models:

$$J_{ij} = \pm 1 \quad or \quad G_{ij};$$

i.e. the couplings between spins beeing nearest neighbours in a (cubic) lattice are randomly distributed

- Mean-field models:
e.g SHERRINGTON-KIRKPATRICK (SK) model:

$$J_{ij} = \frac{G_{ij}}{\sqrt{N}}$$

$G_{ij} \longrightarrow$ independent identically distributed Gaussian random numbers with zero means and variance one.

A Related Mean-Field Model

SK model with non-symmetric distribution of Gauss couplings:

$$P(J_{ij}) = x\delta(J_{ij} + \frac{|G_{ij}|}{\sqrt{N}}) + (1-x)\delta(J_{ij} - \frac{|G_{ij}|}{\sqrt{N}})$$

i.e. the sign of interactions are inversed according the probability x

limiting cases:

$x = 0$ $\longrightarrow$ ferromagnetic system
$x = 0.5$ $\longrightarrow$ SK model
$x = 1$ $\longrightarrow$ antiferromagnetic system

No shift of the Gauss distribution !!!

How much states ?

N	2^N	notes
1	2	
2	4	
3	8	
4	16	
5	32	
...	...	
10	1024	
20	1048576	$\approx$ (Maximal-)number of ancestors in 20th generation (14th century)
...	...	
24	16 777 216	$\approx$ combinations in German Lotto
...	...	
47	$\approx$ 1.4 x 10^{14}	$\approx$ age of mankind in seconds (4 Mio. a)
...	...	
58	$\approx$ 3 x 10^{17}	$\approx$ time since "big bang" in seconds (13 Mrd. a)
...	...	
64	$\approx$ 2 x 10^{19}	"chessboard"-bet: fields vs. grains
...	...	
90	$\approx$ 2 x 10^{27}	$\approx$ time since "big bang" in ns
...	...	
10^{10}	unimaginable!	

Exact Ground States: Optimization

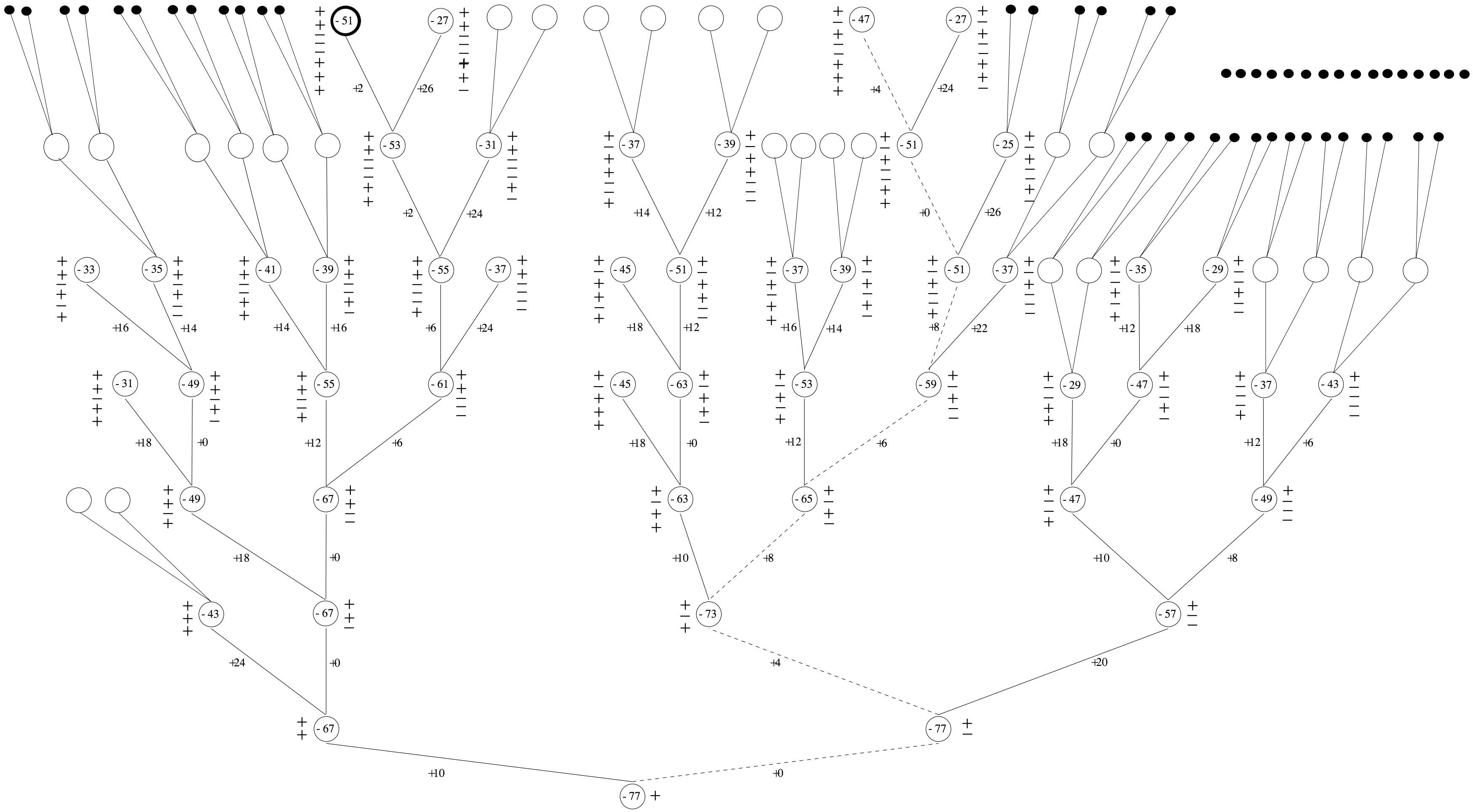
Complexity: NP-complete

Method: "branch-and-bound":
exact nonlinear discrete optimization
S. K., A. Hartwig, *Comp. Phys. Commun. 16 (1978) 1*

example: $N = 8$

$$\mathbf{J} = \begin{pmatrix} 0 & -5 & -2 & -5 & -6 & -1 & 0 & 0 \\ & 0 & -10 & -4 & 0 & -2 & -1 & 0 \\ & & 0 & 0 & 0 & -3 & 0 & -1 \\ & & & 0 & -3 & -5 & -7 & -4 \\ & & & & 0 & -4 & -5 & -8 \\ & & & & & 0 & 0 & -1 \\ & & & & & & 0 & 0 \\ & & & & & & & 0 \end{pmatrix}$$

Branch-and-Bound Tree



Branch-and-Bound Tree

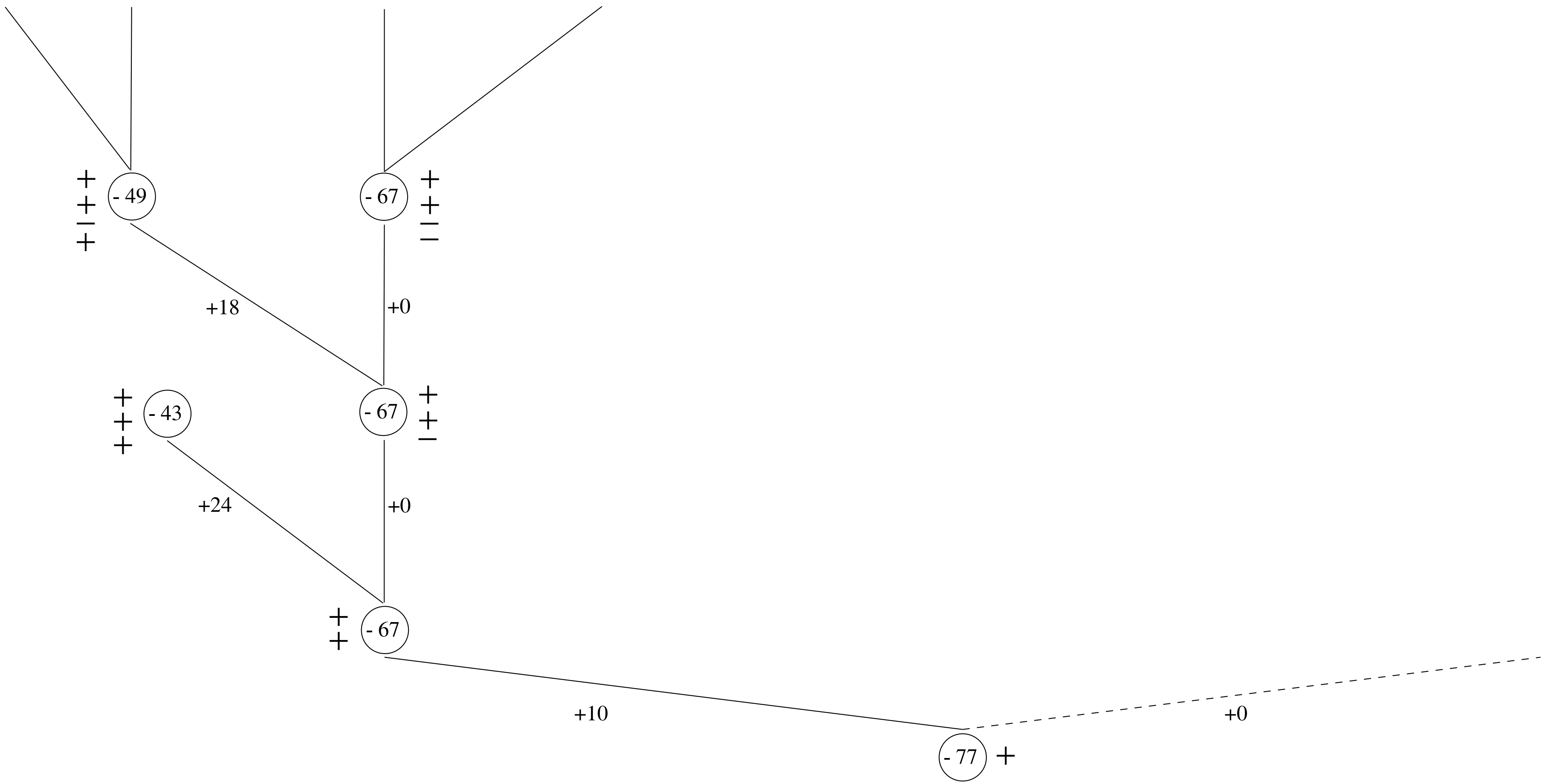
Energy of the branching level E_l (with $E_{l=N} = E_{states}$):

$$E_l = E_{l-1} + 2 \sum_{k(\|l)}^{l-1} |J_{kl}|$$

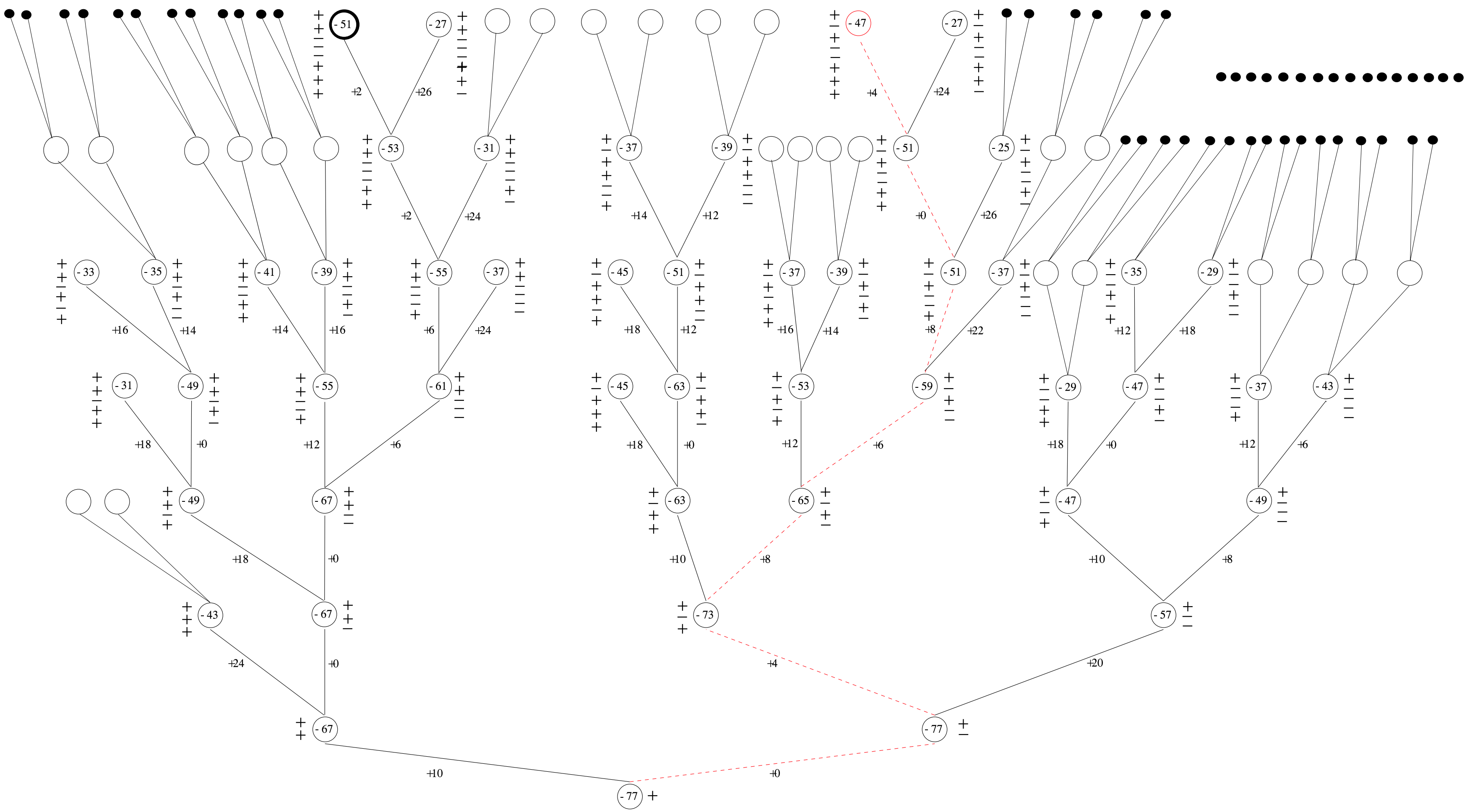
$$E_l \geq E_{l-1}$$

example: $N = 8$; $E_1 = E_{id} = -77$

Branch-and-Bound Tree: Part

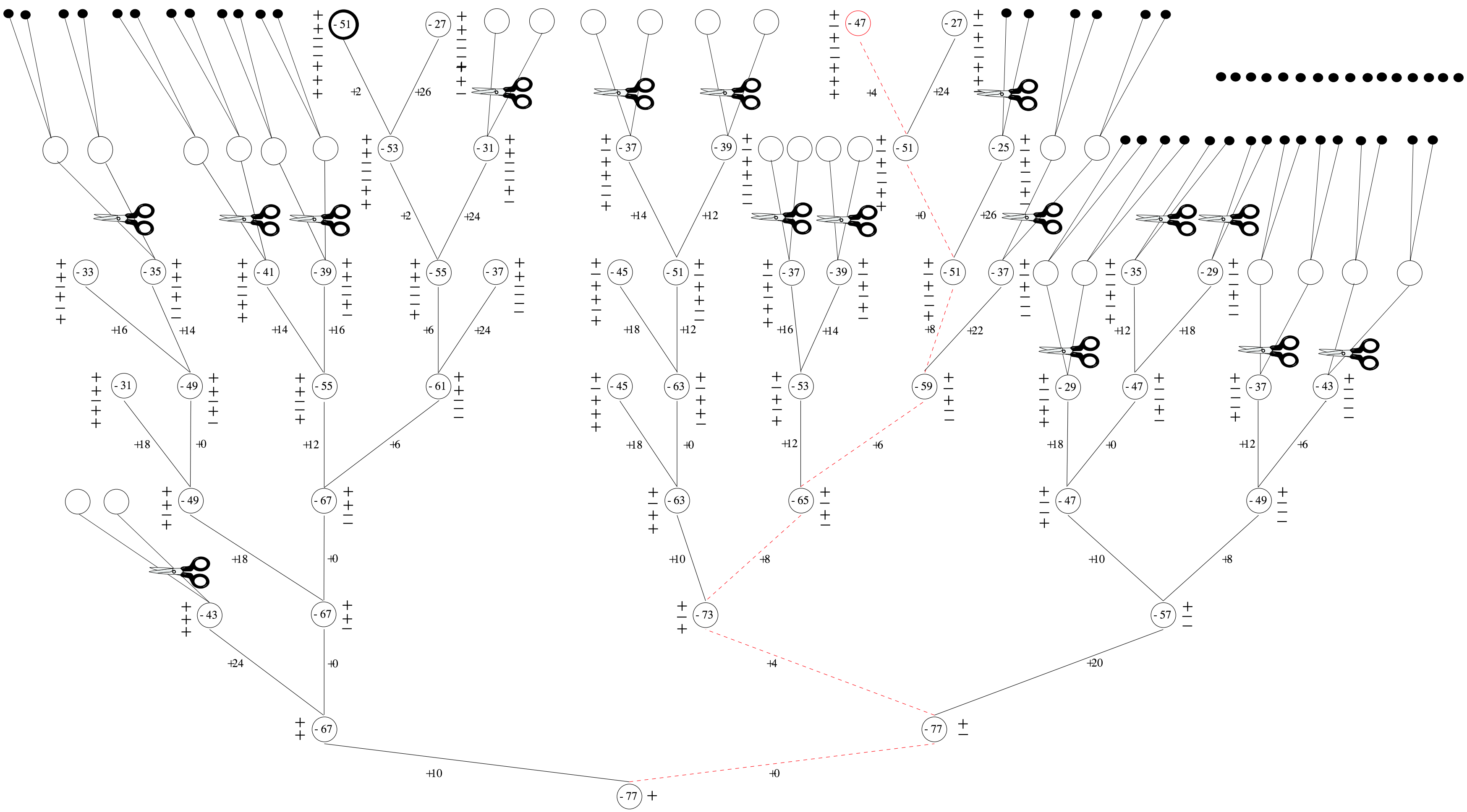


Branch-and-Bound Tree



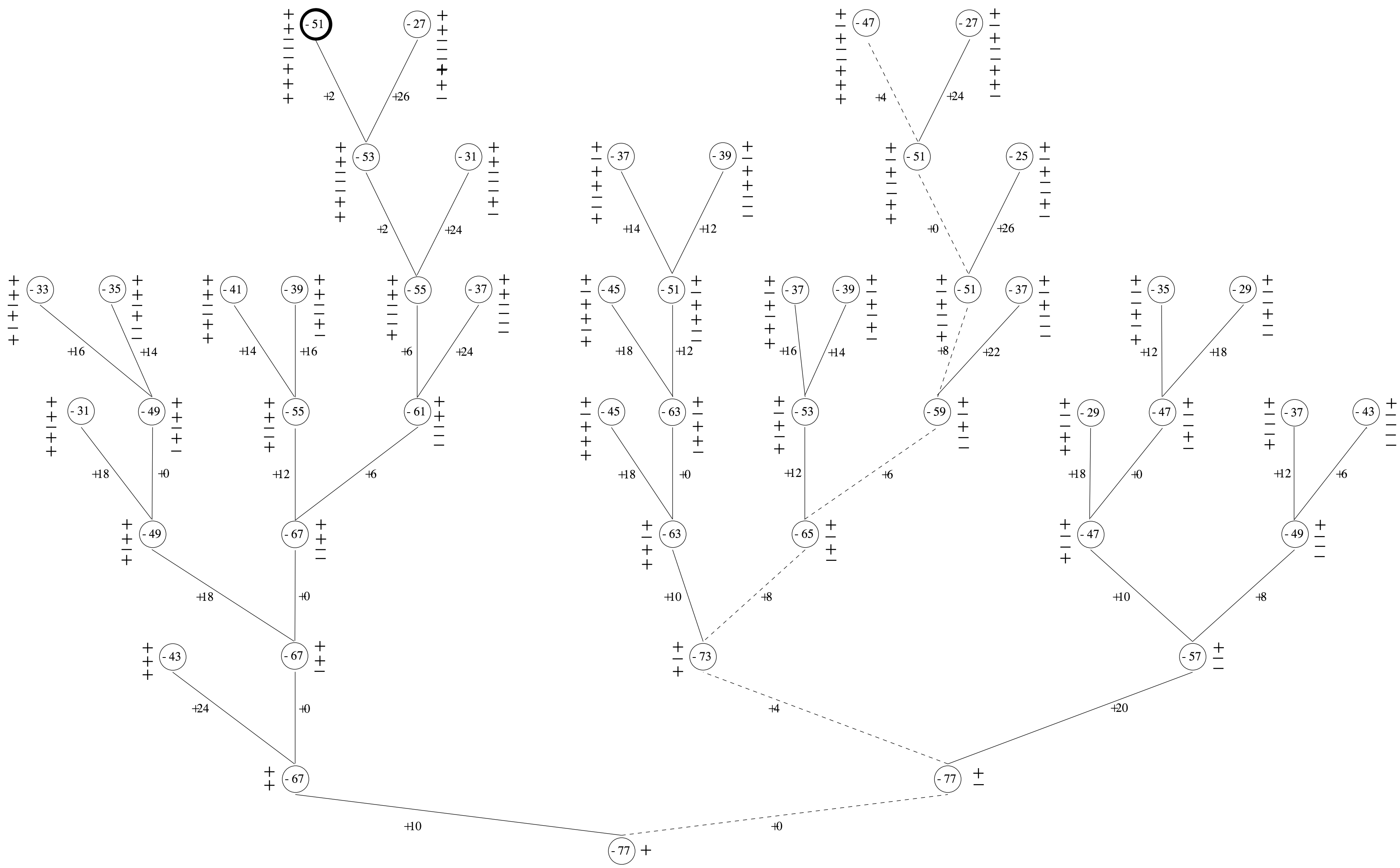
$N = 8$; $E_{id} = -77$; $E_{bound} = -47$ (heuristic solution: $- - -$)

Branch-and-Bound Tree



$N = 8$; $E_{id} = -77$; $E_{bound} = -47$ (heuristic solution: $- - -$)

Branch-and-Bound Tree



$N = 8$; $E_{id} = -77$; $E_{bound} = -47$ (heuristic solution: $- - -$);
exact solution: $E_0 = -51$.

Misfit parameter: A measure for frustration

- Misfit parameter $\longrightarrow$ a useful rescaling of the ground-state energy per spin
- Definition: $\mu_0 = \frac{1}{2}\left(1 - e_0/e_0^{id}\right)$
- with $e_0^{id} \longrightarrow$ reference energy of a related non-frustrated system:
  $J_{ij} = |J_{ij}|$ (lattice model)
  $J_{ij} = \frac{|G_{ij}|}{\sqrt{N}} \quad \longrightarrow \quad e_0^{id} = (N-1)/(2\pi N)^{1/2}$ (SK and related models)
- Properties:
  - μ_0 is the fraction of each bond of the system, which is on average not satisfied.
  - Example: Antiferromagnetic triangular lattice $\longrightarrow \mu_0 = \frac{1}{3}$,
    because one of three bonds of equal strength cannot be satisfied.
  - Maximum value: $\mu_0 = \frac{1}{2}$ for highly frustrated systems
    (e.g. high-dimensional hypercubic and fcc fully frustrated $\pm J$ systems).
  - SK and related models belongs also to the class of systems with maximum occurring frustration.

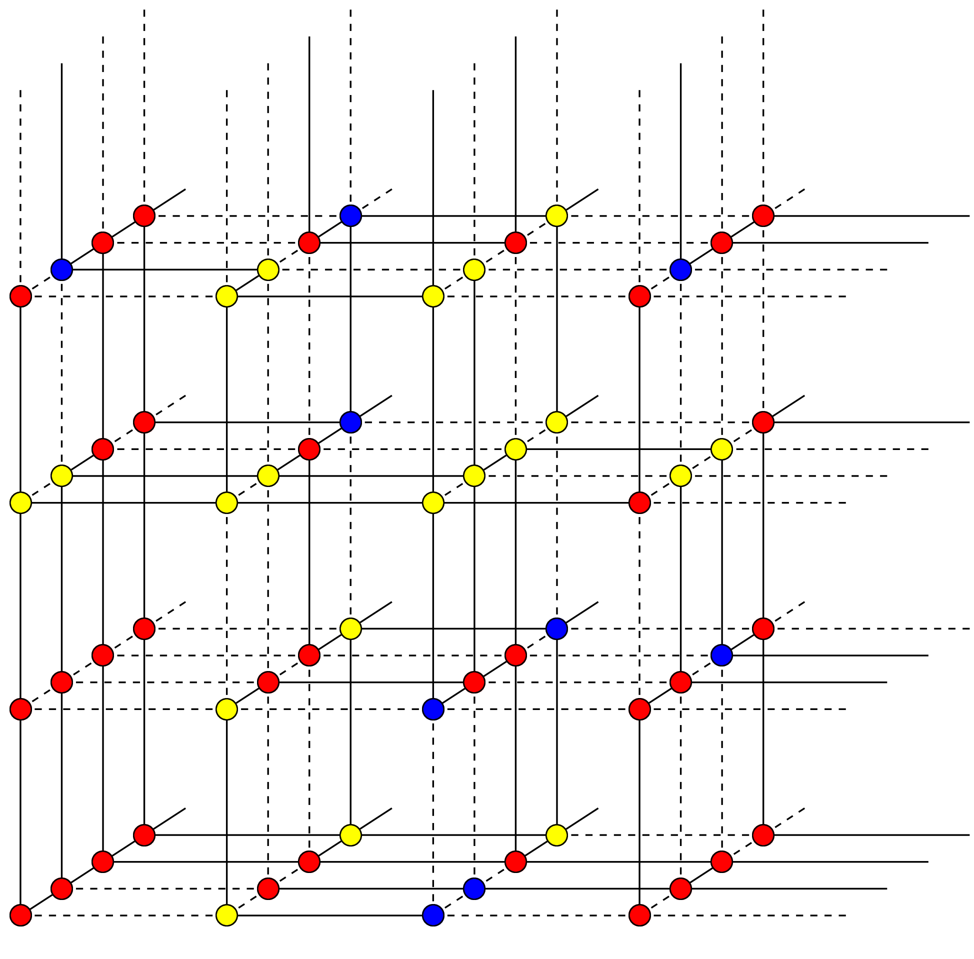
Lattice Models

Misfit parameter: Lattice models ($\pm J$ spin glass)

lattice type	D	μ_0	e_0 from
honeycomb	2	0.09	W. LEBRECHT, E.E. VOGEL *(1994)*
square	2	0.1495	I.A. CAMPBELL, A.K. HARTMANN, H.G. KATZGRABER *(2004)*
triangular	2	0.22	W. LEBRECHT, E.E. VOGEL *(1994)*
simple cubic	3	0.202	*various authors*
hypercubic	4	0.24	S. BÖTTCHER, A. G. PERCUS *(2001)*
hypercubic	5	0.26	S. BÖTTCHER, *private communication*

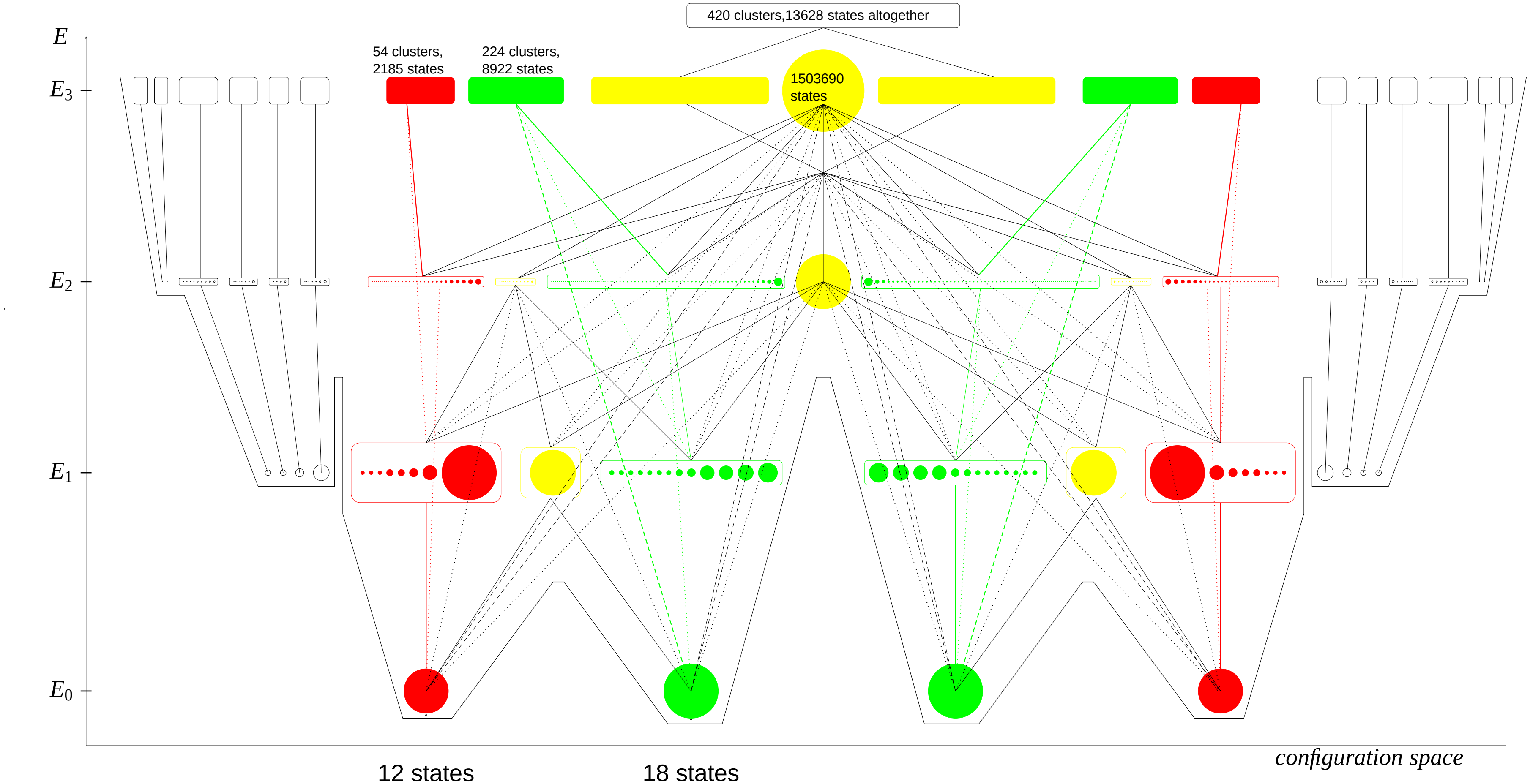
(S. KOBE, J. KRAWCZYK in: *Computational Complexity and Statistical Physics, in press*)

Ground state clusters: Configuration vs. real space



- two (fixed) spin clusters in the real space: "red" and "yellow" spin domains
- Reversal of one spin domain ⇒ another cluster in the configuration space
- "free" spins between the spin domains ⇒ degeneracy of ground state clusters

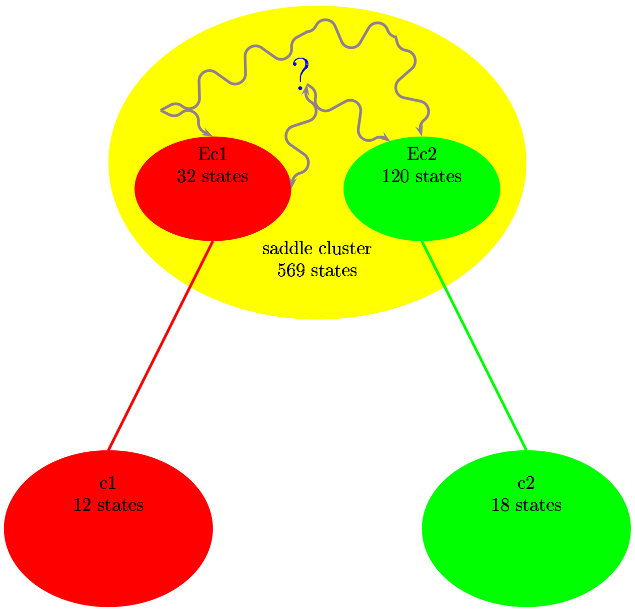
Exact Landscape

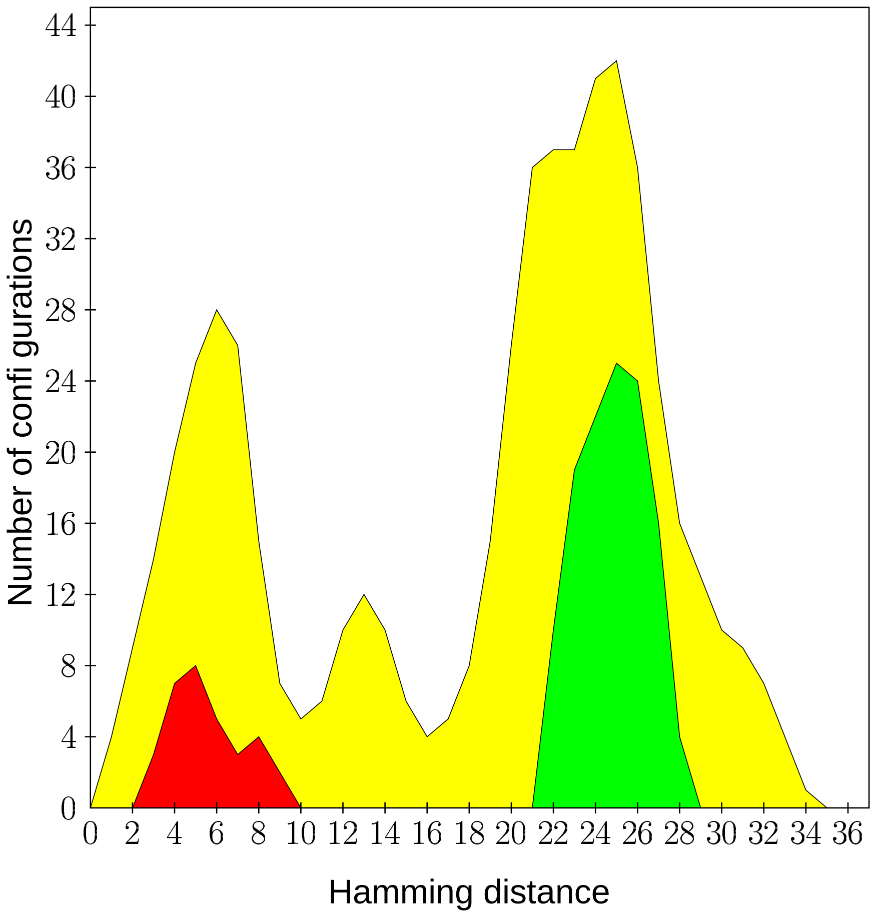


System $4 \times 4 \times 4$ the first excitation ○ - 50 states, the second excitation ◦ - 300 states

- 1.635.796 states up to E_3,
- clusters of states form valleys (#1, #2),
- valleys are connected via saddle clusters

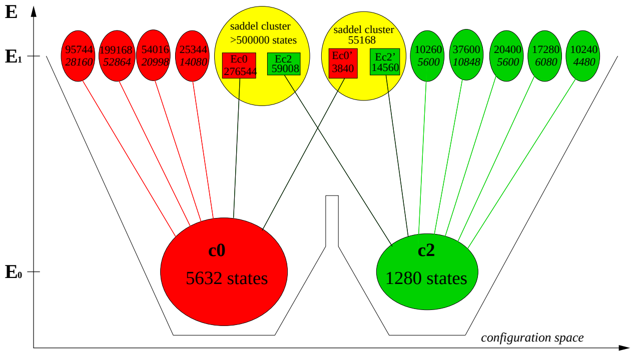
Landscape: Inner profile of the saddle cluster

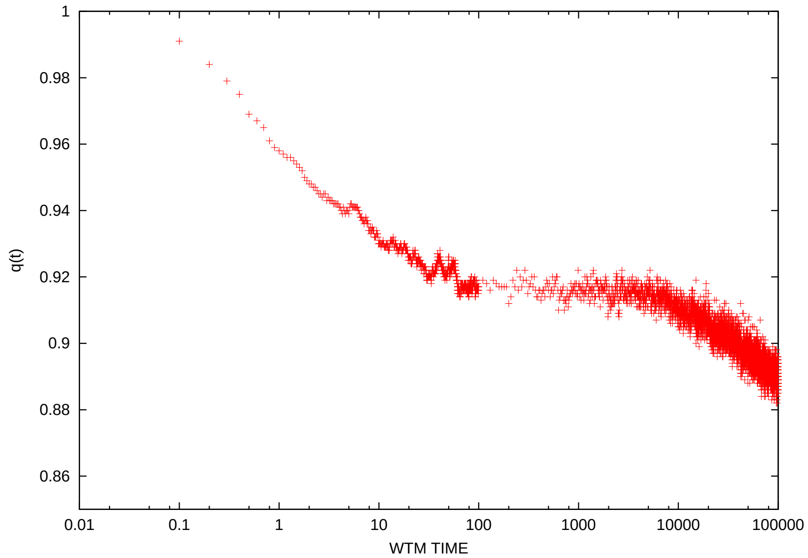




- Restriction of "transition" between clusters via saddle cluster
- Hamming distance of all pairs of states in the saddle cluster (right)
- "Bottleneck" has to be passed: "entropic barrier"

L = 12: Landscape and dynamics





- More complex saddle cluster structure (left)
- Dynamics: q vs. WTM time for 20 runs at $T = 0.37$ starting from one ground state (right) $q_{pl} = 0.915 \pm 0.02 \Rightarrow \overline{h_d} = 73 \pm 2 \Rightarrow$ "width of the valley"

Ground states from A.K. HARTMANN: Genetic Cluster-Exact Approximation

Mean – Field Models

Energy exponents (zero temperature)

Notation of

J.-P. BOUCHAUD, F. KRZAKLA, O.C. MARTIN, *Phys. Rev. B 68 (2003) 224404*

Lattice models: $N = L^d$

$$\overline{E_J(L)} = e_0 L^d + e_1 L^{\Theta_s} + \dots .$$

$$\overline{e_J(L)} = \overline{E_J(L)}/L^d = e_0 + e_1 L^{-\omega} + \dots .$$

Scaling of the energy fluctuations:

$$[\overline{E_J^2(L)} - \overline{E_J(L)}^2]^{1/2} = \sigma_0 L^{\Theta_f} + \dots .$$

Scaling exponents:

shift exponent $\Theta_s \rightarrow \omega = d - \Theta_s$
fluctuation exponent Θ_f

Energy exponents ctd.

$L \longrightarrow N^{1/d}$

$$\overline{e_J(N)} = e_0 + e_1 N^{-\omega'} + \dots .$$

$$\overline{\sigma_J(N)} = [\overline{e_J^2(N)} - \overline{e_J(N)}^2]^{1/2} = \sigma_0 N^{-\rho} + \dots .$$

with

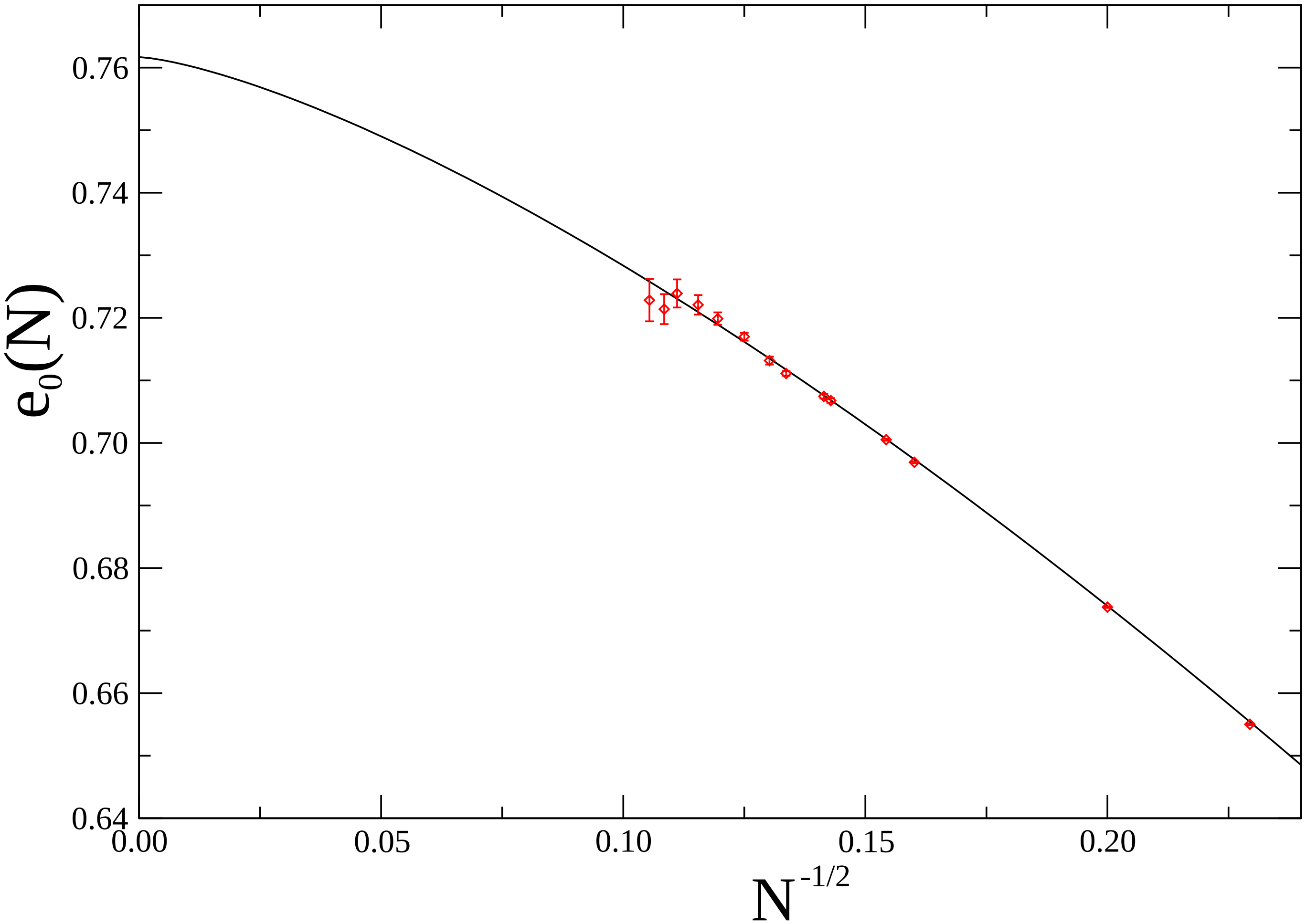
$$\omega' = \omega/d = 1 - \frac{\Theta_s}{d}$$

$$\rho = 1 - \frac{\Theta_f}{d}$$

System sizes and numbers of realizations

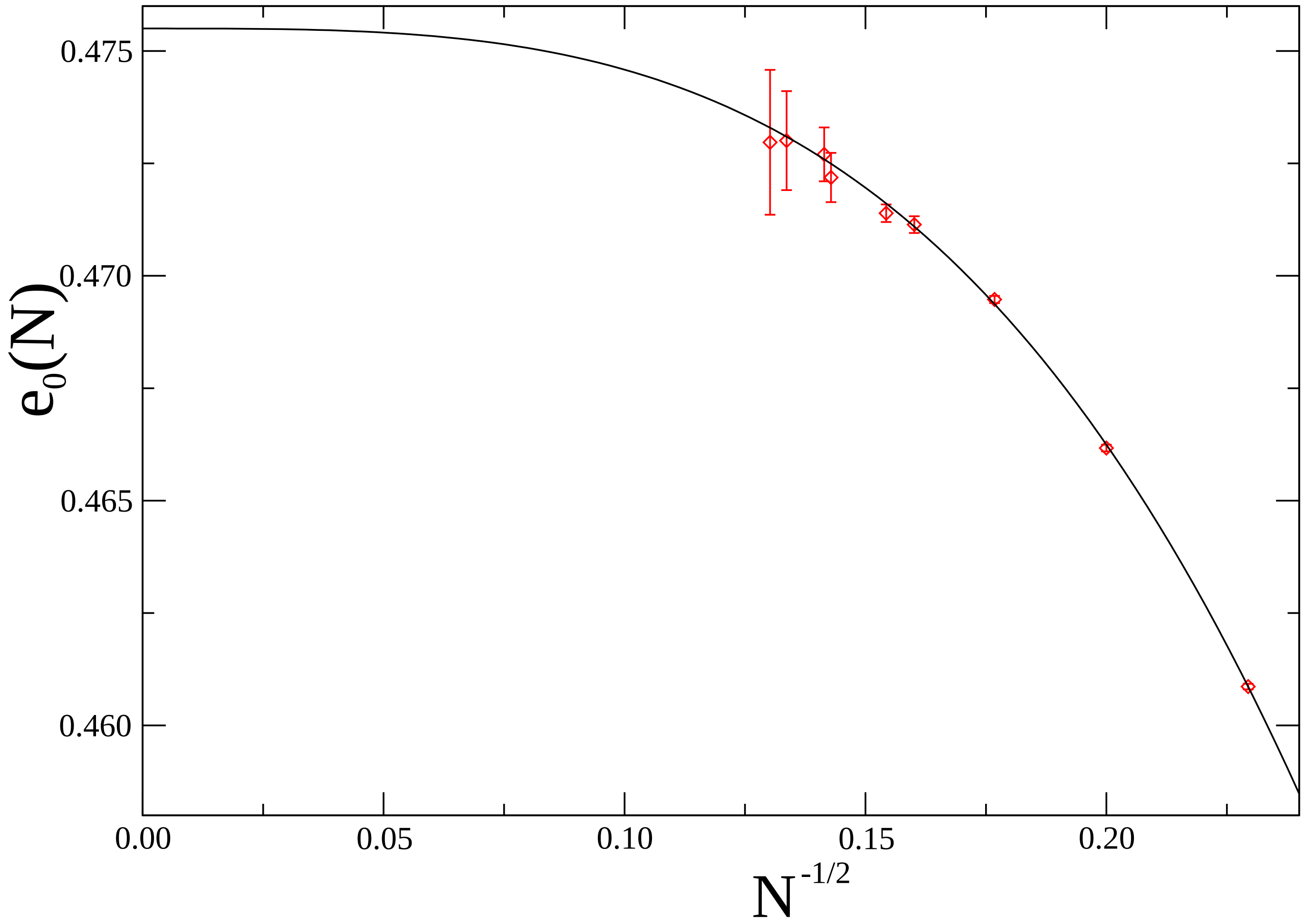
N	# of samples	
	$x = 0.5$ (SK)	$x = 1.0$
19	257909	438242
25	229086	207149
32		123220
39	74827	16519
42	50797	13828
49	7933	1486
50	7724	1181
56	6274	282
59	2082	136
64	1779	
70	634	
75	236	
81	126	
85	112	
90	42	

Results: Ground-state energy (SK model)

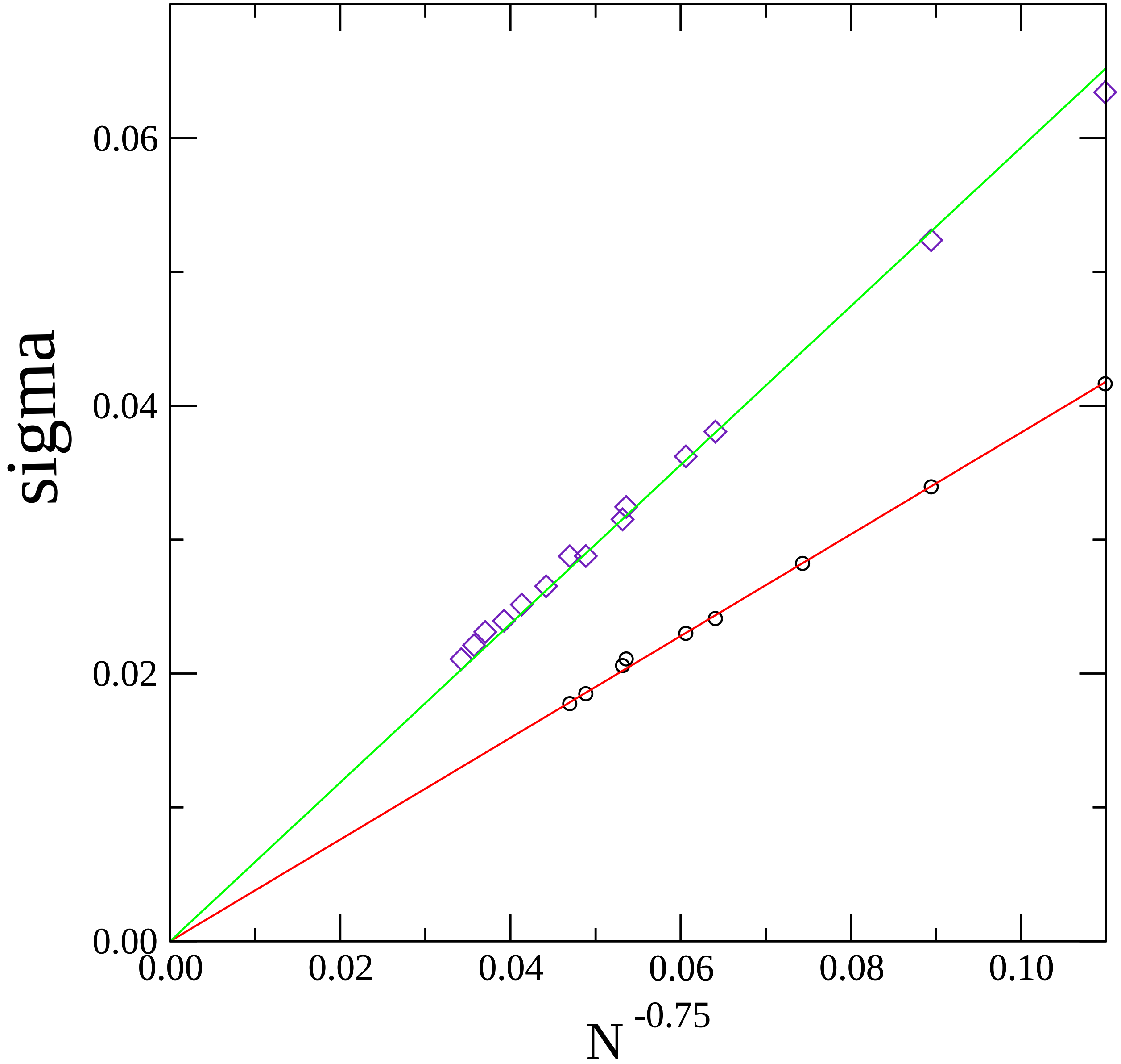


Results: Ground-state energy (x = 1: AFM model)

No analytical solution known!

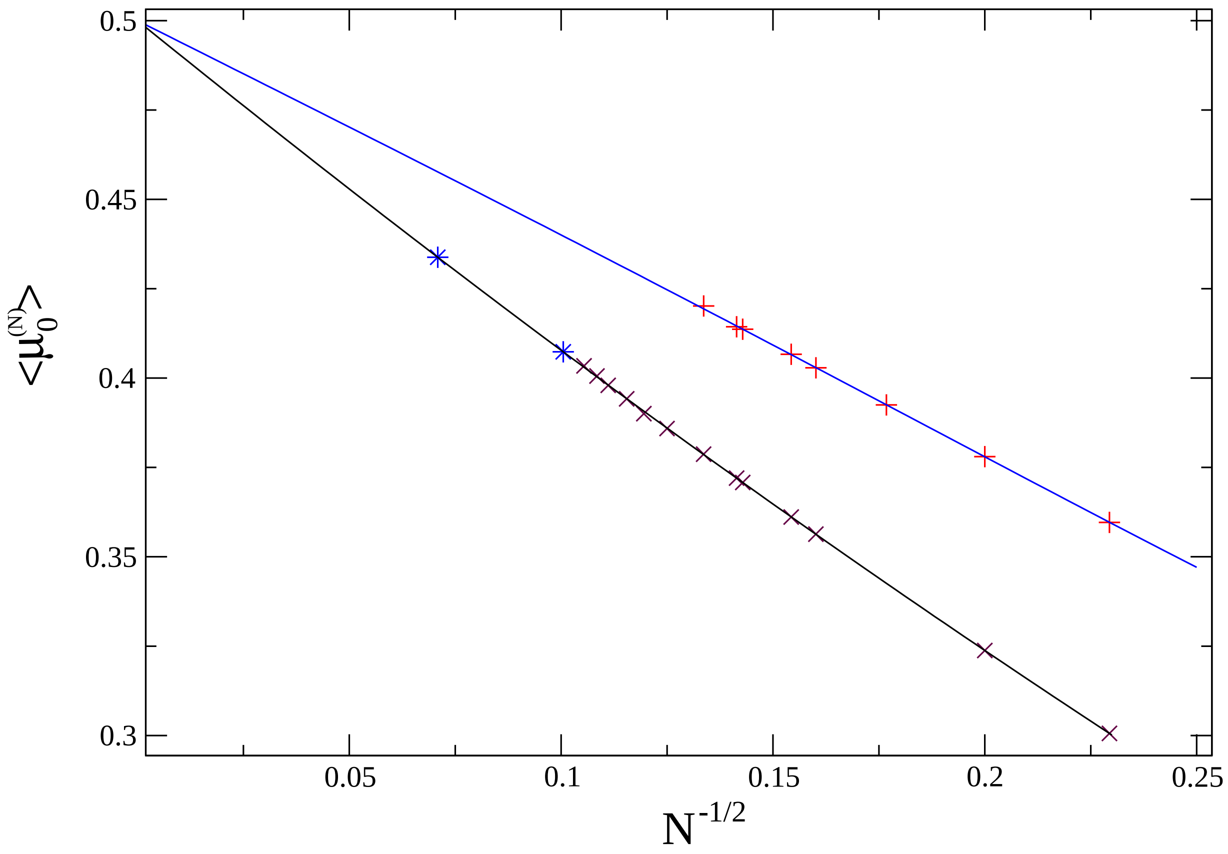


Results: Fluctuation exponent



upper curve: $x = 0.5$ (SK); lower curve: $x = 1$ (afm)

Results: Misfit parameter



upper curve: $x = 1$ (afm); lower curve: $x = 0.5$ (SK)

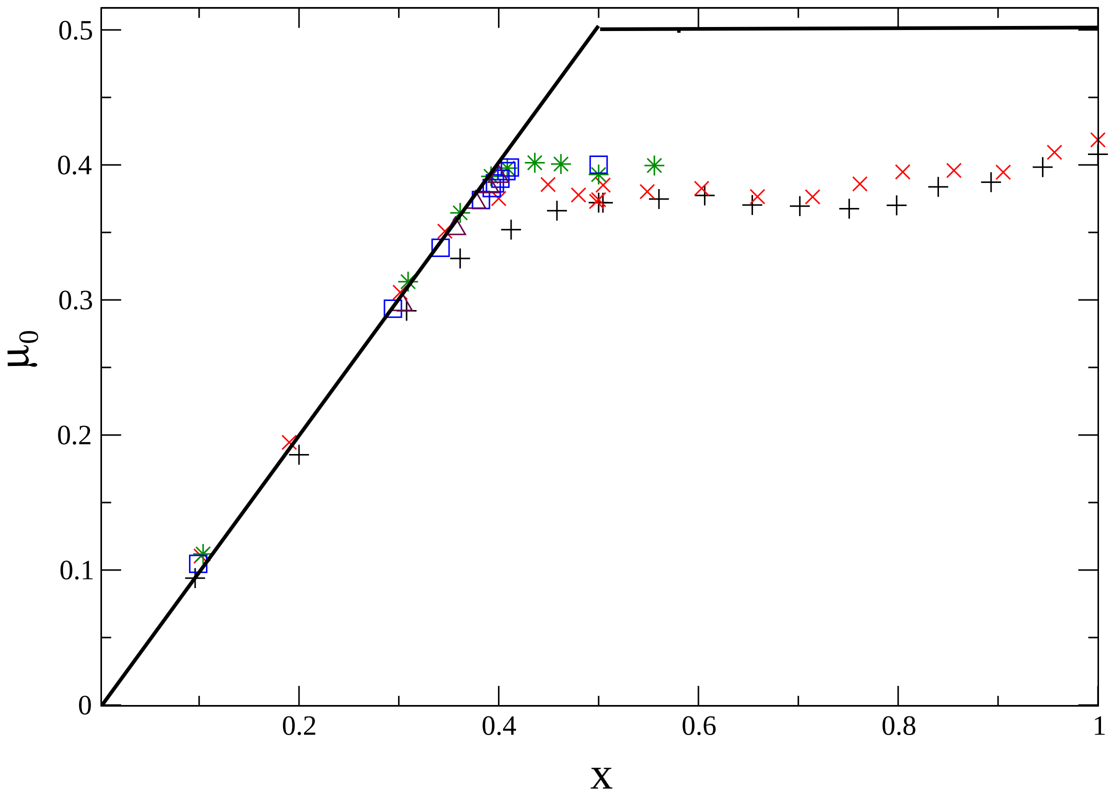
blue stars: M. PALASSINI, *cond-mat/0307713*: hybrid genetic algorithm

Results of fitting procedures

#	x = 0.5 (SK)			x = 1.0		
	e_0	ω'	ρ	e_0	ω'	ρ
$\overline{e_0(N)}$ 3-p	-0.7615(25)	0.698(23)		-0.4755(5)	1.66(9)	
item 2-p	*)	0.684(2)		-	-	
$\overline{\mu_0(N^{-1/2})}$ 3-p	-0.7655(38)	0.652(31)		-0.4756(4)	1.63(8)	
item 2-p	*)	0.671(3)		-	-	
$\overline{\sigma_J(N)}$ 2-p			0.710(5)			0.736(9)

*) The analytical value $e_0^{RSB} = -0.76321(3)$ is used for the 2-parameter fit
(M. A. CRISANTI, T. ROSSI, *Phys. Rev. E 65, 046137 (2002)*)

Phase transition



Summary

- Optimization algorithms $\rightarrow$ exact results for finite spin glass models
- Semi-quantitative understanding of dynamics (relaxation) in lattice models
- For mean-field models: SK ground states for small N are consistent with RSB solution and other numerical results.
- Related models are introduced: AFM model is "higher" frustrated for finite N.
- Ground-state energy $e_{0,\text{afm}}$ is estimated.
- Predictions from energy scaling:
  - SK and AFM model have the same fluctuation exponent: $\Theta_f/d \simeq 1/4$.
  - The shift exponent is different: $\Theta_s/d \simeq 1/3$ (SK) and -2/3 (AFM).
- Outlook:
  - Phase transition between ferromagnetic and spin-glass ground state near $x = 1/2$?
  - Another related model: A fully connected $\pm J$ model

Acknowledgement

KLAUS HANDRICH

ANDREAS HARTWIG
FRANK DASKE

THOMAS KLOTZ
GÜNTER MILDE

PAWEL POLASZEK
MARIUSZ NOGALA
JAROSŁAW KŁOS
JAROSŁAW KRAWCZYK

EUGENIO VOGEL, JAIME CARTES, PATRICIO VARGAS, DORA ALTBIR