2D SG Partition Functions

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Work in collaboration with A. Galluccio, J. Lukic, O. C. Martin and G. Rinaldi (`cond-mat 0309238`, in print on PRL). Compute (many) exact partition functions of (large) 2D Ising SG, $J = \pm 1$ with PBC. Galluccio, Löbl and Vondrák: Pfaffians, modular arithmetics, Chinese remainder theorem. Results:

- Solve dispute. Physical scaling as $\beta \longrightarrow \infty$ $c_V \sim \beta^2 e^{-2\beta}$ (anomalous, see $1D$ Ising).
- $\xi \sim e^{\beta}$, and hyperscaling works.
- Ground state properties ($\theta^E = \theta_{DW} = 0$ etc...).
- Number of excitations (possible mechanism for anomalous scaling).
- MKA anomalous scaling (to be published).

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Summary

- Spin glasses, $2D$ Ising spin glasses. The quenched physics.
- $T = 0$ and low T physics. Choice of couplings and "universality".
- Monte Carlo versus ground states computations. Computations of Z_β.
- The dispute: Swendsen and Wang with (optimized) Monte Carlo versus Kardar-Saul with exact transfer matrix.
- The Galluccio-Löbl-Vondrák algorithm.
- Our findings. The anomalous scenario.

SG: frustration + disorder (complexity)

Quenched averages

$$H = -\sum_{\text{nn } i,j} J_{ij}\sigma_i\sigma_j$$

couplings J_{ij} are random quenched.

Huge interest:

1. Parisi solution of mean field SK theory.
2. paradigmatic role (boring as materials, as such).

Open debate on behavior in finite D.

"For sure": $D_c^L \geq 2$, no transition in $2D$ for $T > 0$.

As $T \longrightarrow 0$: scaling theory. Coarse graining and scaling Ansatz.

$$\tilde{J}(l) \sim l^\theta$$

effective coupling among (block) spins at large distance.

$2D$: $\theta < 0$ (and/or zero, see later). Coupling becomes weaker at large scale, and the ordered state is unstable and breaks down.

Typical choices for the probability distribution of quenched couplings: $P(J) \sim \exp(-J^2/2)$ or $J = \pm 1$ with uniform probabilities, or many other possibilities (but equivalent, see later).

In $2D$ this can play (and does play) a role in deciding the "critical behavior" as $T \longrightarrow 0$ (see C. Amoruso, EM, O. Martin and A. Pagnani, PRL **91** (2003) 087201).

Starting point is

$$\delta E \equiv E_{GS}^{(P)} - E_{GS}^{(AP)}$$

and as $L \longrightarrow \infty$

$$\overline{\left(\delta E - \overline{\delta E}\right)^2} \sim L^{2\theta}$$

While for Gaussian J one has $\theta = -0.28$ for binary couplings one finds clearly (Hartmann and Young) $\theta = 0$.

We find that all $P(J)$ which can only produce quantized energies give $\theta = 0$, while all distribution that can generate continuous energies without a gap give $\theta \simeq -0.28$ (even if for example are built on only two coupling values, but with an irrational ratio).

1. $D \leq D_c^L \Longrightarrow$ small δE values are relevant for the large distance behavior of the system $\Longrightarrow$ gap in coupling distribution can play a role.
2. $\theta_{(D)} = 0$ does only mean $D \leq D_c^L$, not $D = D_C^L$.

Monte Carlo versus Ground State computations.

1. MC for Spin Glasses is very difficult.

   "Naive" MC is basically of no use. High free energy barriers make impossible exploring the full phase space.

   Optimized Monte Carlo (multicanonical, replica MC, parallel tempering) helps.

   Still: it is difficult to go at low T. You are never sure you thermalized...

2. Computing GS you study directly T=0 physics. No problems with thermalization.

   Main problem: what do you learn, say, about finite T physics? (it seems it works...).

3. A third approach: compute directly the full partition function. "Best of both worlds" (but: depending on the algorithm only reach some observables) (but: can only do it in some models, see later...).

The dispute

Saul and Swendsen (PRL **38** (1988) 4840) after a very accurate optimized MC simulation claimed to detect an anomalous scaling behavior.

2D Ising Spin Glass, $J = \pm 1$, Periodic Boundary Conditions. V=128^2

$$c_V \sim \beta^2 e^{-A\beta} \quad , \qquad A = 2 \ .$$

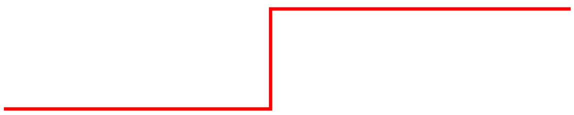
Would expect $A = 4$, since minimal excitation costs $4J$.

Periodic Boundary Conditions 1D Ising model analogy. Minimal excitation is $4J$, since $\Downarrow \Uparrow \Downarrow$

kink − antikink

Still, an easy computation gives $c_V \sim \beta^2 e^{-2\beta}$.

Now. With fixed boundary conditions minimal excitation only costs $2J$.



kink

But infinite volume limit does not depend on boundary conditions... Answer: kink-antikink excitation is no elementary. Notice that there are too many of them, $O(V^2)$.

$T \longrightarrow 0$, V fixed: eventually find $e^{-4\beta}$. But scaling limit, small T and large V: $e^{-2\beta}$.

Kardar and Saul, NP B **432** (1994) 641. They reanalyzed the problem by computing exactly the full partition function. $2D$ Ising Spin Glass with PBC, $J = \pm 1$.

They follow Kac and Ward:

1. From high T expansion, in terms of closed graphs on the square lattice (including graphs wrapping around the lattice).

$$Z = 2^V \left(\cosh\left(\beta J\right)\right)^{2V} \sum_{c:B} A_B \tanh\left(\beta J\right)^B$$

where the sum is on closed graphs with B bonds.

2. Kac-Ward $\longrightarrow$ the problem is rephrased in a local random walk with non-trivial weights. $4V \times 4V$ hopping matrix.

PBC: need four matrices (see later Galluccio-Löbl theorem for graphs of bounded genus). In this case one finds (Potts-Ward, 1955):

$$Z = \frac{1}{2}\left(-Z_1 + Z_2 + Z_3 + Z_4\right)$$

$$Z_\lambda = 2^V \left(\cosh\left(\beta J\right)\right)^V \sqrt{\det\left(1 - U_\lambda \tanh\left(\beta J\right)\right)}$$

U_λ: 4 different hopping matrices, of size $4V \times 4V$.

So: $\{J_{ij}\} \longrightarrow$ four matrices $U_\lambda \longrightarrow$ traces of U_λ^W for $W \leq V \longrightarrow$ polynomial in $e^{-\beta}$, density of states $\longrightarrow$ $Z = \sum_E N(E) e^{-\beta E}$.

Lot of precautions to deal with large numbers (Kardar and Saul also compute zeroes of Z).

Polynomial time estimated roughly as $\sim V^{3.2}$.

They have basically:

L	S
4-8	8000
10-14	2000
16-18	800

and few samples for larger lattices.

This turns out to be too small...

So, they disagree with Swendsen-Wang, and claim

$$c_V \sim \beta^3 e^{-4\beta}$$

(note the anomalous power, see fully frustrated Ising model in $2D$).

Number of excitations looks smaller than in $1D$ Ising. Claim is here that

$$\log V < S_1 - S_0 < \log V^2$$

But, again, the authors notice (as a sign of severe warning) that they cannot clearly detect the asymptotic behavior.

Our approach (Galluccio, Löbl and Vondrák PRL **84** (2000) 5924)

Similar to Kardar-Saul, but many further:

1. theoretical results
2. technical improvements

Summary:

$Z_{\beta}^{ISG2D} \longrightarrow$ generating function of cuts

Galluccio-Löbl: it is possible to solve the Max Cut problem in polynomial time for any graph of genus bounded by a constant. The method provides directly the generating function of cuts.

$\longrightarrow$ Eulerian subgraphs

$\longrightarrow$ perfect matching

$\longrightarrow$ (on graphs of bounded genus) Pfaffian computation (square root of the determinant of an antisymmetric matrix). Need 4^g Pfaffians.

$\longrightarrow$ compute Pfaffian by using modular arithmetics (no need for infinite precision).

$\longrightarrow$ use the Chinese Remainder Theorem to reconstruct the exact partition function.

Cut of a graph $G = (V, E)$ (vertices, edges) is a partition of its vertices into two disjoint subsets $V_1, V_2 \subset V$ and the implied set of edges between the two parts (each edge can carry a weight w_e, and the total weight of the cut is $w(C)$).

Max Cut (min Cut): divide vertices in two parts so that total weight of edges between the two parts is max (min).

Generating function of cuts: polynomial

$$\sum_{\text{over all cuts}} x^{w(C)} \, .$$

Eulerian subgraph: set of edges U such that each vertex of V is incident with an even number of edges from U.

Perfect matching: set of edges P such that each vertex of V is incident with exactly one edge from P.

From Ising to Cuts

Assign spins to $+1$ or -1. $V_+ = \{i \in V | \sigma_i = +1\}$ $V_- = \{i \in V | \sigma_i = -1\}$. Let $C(V_+, V_-)$ be the cut of spins $+1$ and -1. $W \equiv \sum_{\{i,j\}\in E} J_{ij}$ is the sum of all edge weights in G.

$$H = \sum_{\{i,j\}\in C} J_{ij} - \sum_{\{i,j\}\in(E-C)} J_{ij} = 2w(C) - W$$

Let the generating function of cuts be

$$\mathcal{C}(G,x) = \sum_{\text{cuts in G}} c_k x^{W(C)} \ ,$$

where c_k is the number of cuts with weight k.

$$Z(\beta) = \sum_{\{\sigma\}} e^{-\beta H} \simeq \sum_{\text{cuts}} e^{-2\beta w(C)+\beta V} \simeq e^{\beta V}\mathcal{C}(G, e^{-2\beta})$$

From cuts to Eulerian subgraphs

$$\mathcal{C}(G, e^{-2\beta}) \sim x^{\frac{V}{2}} \prod_{\{i,j\}\in E} \left(\frac{x^{\frac{w_{ij}}{2}} + x^{-\frac{w_{ij}}{2}}}{2} \right)$$

$$\mathcal{E} \left(G, \frac{x^{\frac{w_{ij}}{2}} - x^{-\frac{w_{ij}}{2}}}{x^{\frac{w_{ij}}{2}} + x^{-\frac{w_{ij}}{2}}} \right)$$

E: generating function of Eulerian subgraphs.

By the Fischer construction Eulerian subgraphs can be rewritten as a perfect matching problem.

- Kasteleyn for planar graphs
  Galluccio-Löbl for graphs of bounded genus
  Perfect matching can be translated to a Pfaffian computation (of 4^g Pfaffian).

- Modular arithmetics. Work modulo some given prime number.
  Theorem: Let $P(x)$ be a polynomial of degree n with integer coefficients, $\Phi(p)$ a finite field of size $p > n$, and x_0, x_1, ... x_n distinct elements of $\Phi(p)$. Then there exists a unique polynomial of degree n over $\Phi(p)$ such that

  $$Q(x_i) = P(x_i) \bmod p, \quad i = 0, \ldots, n \ .$$

  The coefficients of $Q(x)$ are equal to the coefficients of $P(x)$ mod p.

- The Chinese Remainder Theorem.
  If we work in a number large enough of fields, i.e. p_1, p_2, ..., p_k such that

  $$\prod_{i=1}^{k} p_i > 2^n$$

  we can reconstruct the exact polynomial, i.e. the exact partition function. Great!

Summary of the Algorithm

1. Find prime numbers p_i such that

$$\prod_{i=1}^{k} p_i > 2^V \ .$$

   For each of them repeat steps 2, 3, 4 performing all operations in $\Phi(p_i)$.

2. Select $(m+1)$ distinct elements x_j of $\Phi(p_i)$. For each of them repeat step 3.

3. Write the 4^g matrices encoding the relevant orientations of the modified graph. This gives Z_β (in the point $e_\beta = x_j$).

4. From these values of $Z_\beta (\bmod p_i)$ in given points interpolate in $\Phi(p_i)$ and get the coefficients of the polynomial.

5. Apply the Chinese Remainder Theorem: compose the results from each $\Phi(p_i)$ to get the full Z_β.

Complexity: $O(V)$ finite fields, $O(V)$ evaluations in each field (for edge weights bounded by a constant), $O(V^{\frac{3}{2}})$ operations for a single evaluation of a polynomial $\Longrightarrow$ Total $O(V^{\frac{7}{2}})$.

Technically this approach and implementation by GLR looks to a “naive beginner” like me full of very brilliant ideas.

Main features:

- parallel;
- no problems with precision;
- basically only bound by CPU time, not by memory or word length;
- scaling $V^{\frac{7}{2}}$.

Our work. J. Lukic, A. Galluccio, EM, O. Martin, G. Rinaldi.

$2D$ Ising Spin Glass, PBC, $J = \pm 1$.

For example:

L	S
6	400000
10	100000
30	10000
40	1000
50	300

(and similar values for different L values).

$$F_J(\beta) = -\frac{1}{\beta} \log Z_J(\beta) \quad , \quad U_J(\beta) = \langle H_J \rangle \quad ,$$

$$c_V = L^{-2} \frac{dU_J}{dT} \quad ,$$

and average over samples. We mainly look at c_V (irrelevant constants are already subtracted).

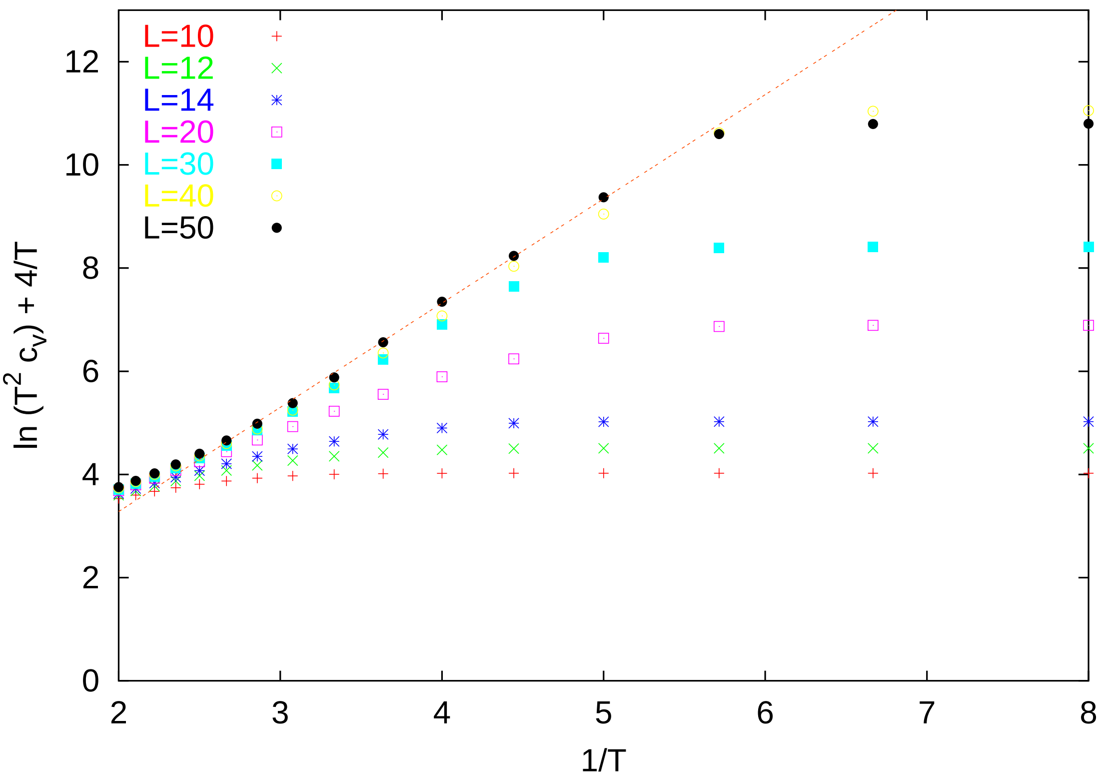
$$c_V \sim \beta^2 e^{-A\beta}$$

(we have checked that $p = 2$ is the best available choice for power corrections).

$$\log \frac{c_V}{\beta^2} \sim -A\beta$$

$$y \equiv \left(\log \frac{c_V}{\beta^2} + 4\beta\right) = (4 - A)\,\beta$$

So if we have naive scaling $y \sim$ constant in the scaling regime. If not: slope is $(4 - A)$.



Small T: saturation at constant value.

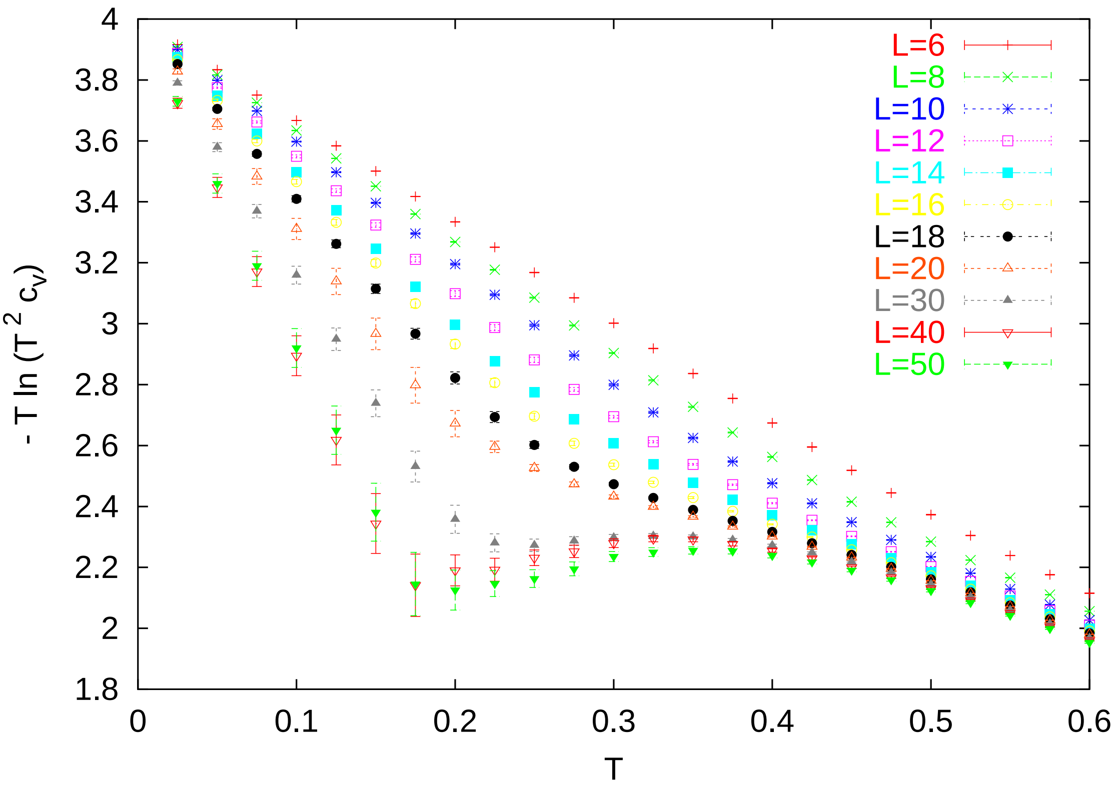
Intermediate T: $A \sim 2$.

Straight line: best fit $\beta \in [2.5, 5.5]$ gives $A = 2.02 \pm 0.03$.

$$-T \log\left(T^2 c_V\right) \sim A$$

So look at limit $T \longrightarrow 0$.

Very interesting scaling pattern.



Three regions:

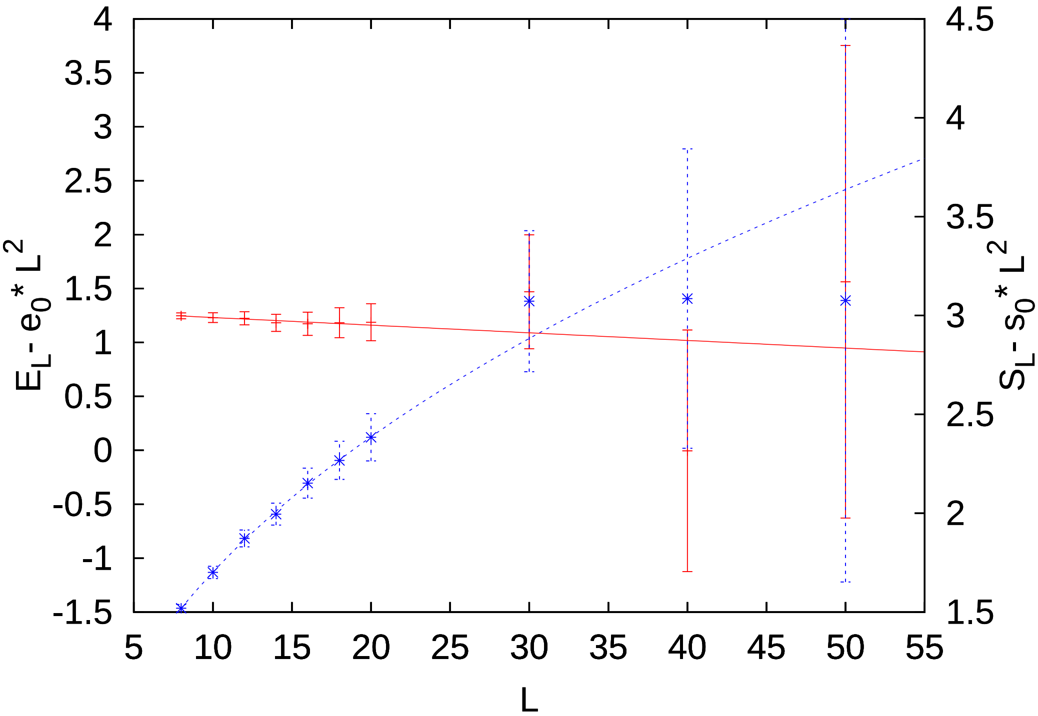
- high T "no scaling";
- low T $A = 4$ naive behavior;
- intermediate T, large lattices: $A = 2$.

$T = 0$ properties.

Lines in the plot are best fits.

$$e_0(L) = e_0^* + aL^{-2+\theta^e}$$

$e_0^* = -1.4017(3)$, $\theta^e = -0.08(7)$. We see that as good evidence that $\theta^e = \theta_{DW} = 0$ (Hartmann-Young).



$$s_0(L) = s_0^* + aL^{-2+\theta^s}$$

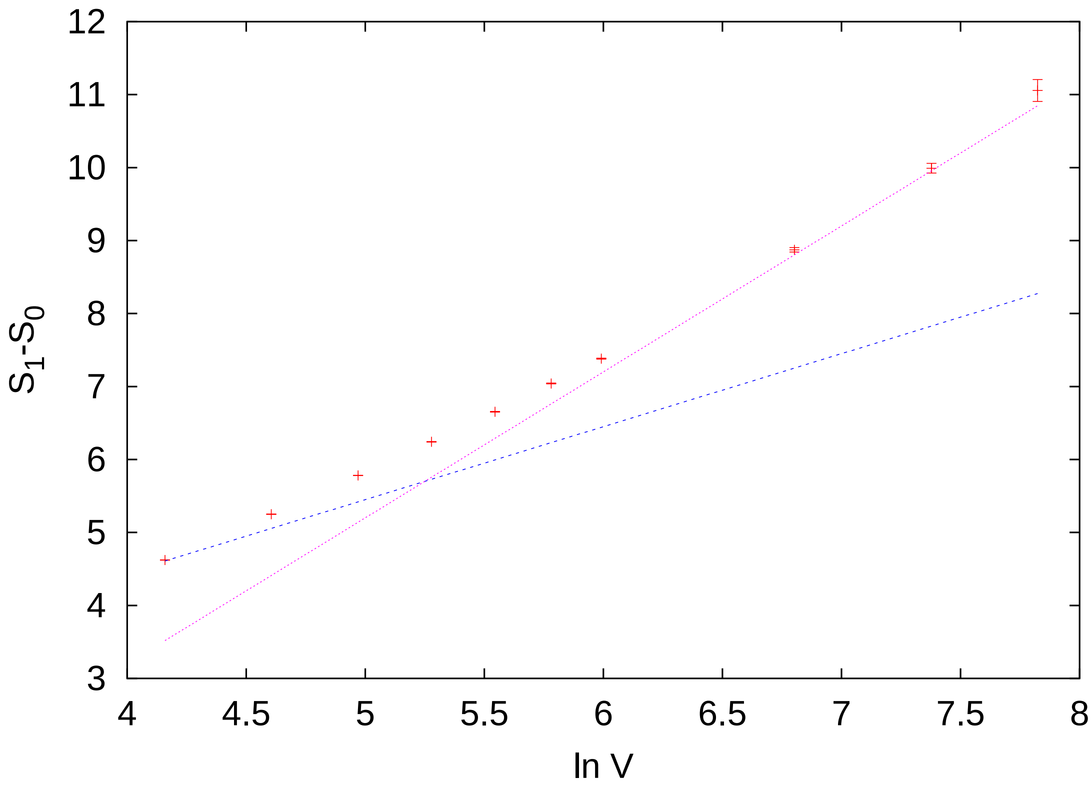
$s_0^* = 0.0714(2)$ (most precise estimate available), $\theta^s = 0.42(2)$. Could be that $\theta^s = 0.5$.

Anomalous density of excitations.

$$S_1 - S_0 = S(E_0 + 4J) - S(E_0)$$

Straight lines: $\log V$, $2 \log V$.

On large lattices: $2 \log V$ (Kardar-Saul could only see the transient behavior on smaller lattices).



$4J$ excitations “not elementary” (following the $1D$ Ising model terminology)?

Finite Size Scaling.

Difficult to fit from the numerical data the exact scaling law. We use two approaches.

1. For each L value we determine $T^*(L)$ as the temperature where "something happens" (where the data separate from the envelope).

   Scaling of such $\xi(T)$ obtained by inverting $T^*(L)$ prefers

   $$\xi \sim e^{\beta}$$

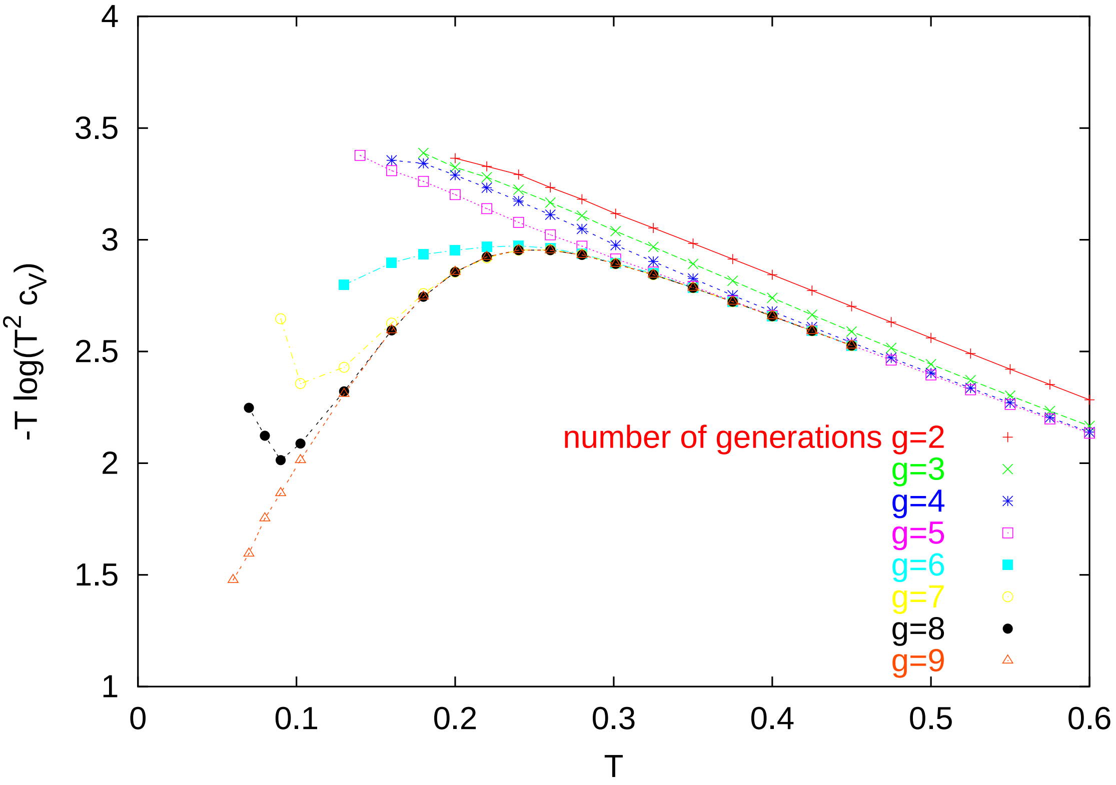
   far over $\xi \sim e^{2\beta}$. Hyperscaling works.

2. We can use a simple scaling argument based on the finding $S_1 - S_0 \sim 2 \log V$ to find the same behavior.

MKA approximation (to be published).

Very similar scaling pattern!

But $A = 1$? Here: MKA, $b = 3$ branches, $s = 3$ segments.



10^4 samples for 3 generations. 200 samples for 9 generations.

Here we know that $\theta = 0$ (Amoruso et al.).

Gaussian couplings: $c_V \sim T^{\alpha}$ as $T \longrightarrow 0$.

$J = \pm 1$: figure here. Very similar to $2D$ EA spin glass.