

Random quantum magnets in $d \geq 2$ dimensions: Critical behavior and entanglement entropy

Ferenc Iglói (Budapest)

in collaboration with

István Kovács

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AGENDA

- Introduction
 - quantum phase transitions
 - experimental examples
 - quantum spin glass
- Model and the RG method
 - random quantum Ising model
 - strong disorder RG method
 - exact results in 1D
 - concept of infinite disorder fixed point
 - Numerical implementation of the RG method for $D > 1$
- Bulk critical behavior
 - Finite-size critical points
 - Scaling at the critical point
 - Erdős-Rényi random graph
- Boundary critical behavior
 - slab, wedge, pyramid geometries
 - magnetization profiles
 - surface, edge, corner critical behavior
- Entanglement entropy
 - strong disorder RG calculation
 - slab, column and cube geometries
 - universal corner contribution at the critical point
- Conclusions

Introduction

- Quantum phase transitions
 - takes place at $T = 0$
 - due to quantum fluctuation
 - by varying a quantum control parameter
- Examples
 - rare-earth magnetic insulators
 - heavy-fermion compounds
 - high-temperature superconductors
 - two-dimensional electron gases
 - quantum magnets: LiHoF_4
- Disorder often play an important rôle
 - Anderson localization
 - many-body localization
 - quantum spin glasses: $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$
- Paradigmatic model: random transverse Ising model (RTIM)
 - in 1d exact results, also through strong disorder RG method
 - * infinite disorder scaling at the critical point
 - * dynamical (Griffiths-McCoy) singularities outside the critical point
 - in 2d numerical implementation of the SDRG method
 - * infinite disorder scaling
 - * but contradictory results through the quantum cavity approach

Aim of the present talk

- Improve the numerical algorithm of the SDRG method
- Study the critical behavior of the RTIM for $d > 2$
- Study Erdős-Rényi random graphs ($d \rightarrow \infty$)
- Study the boundary critical behavior at surfaces, corners, edges
- Study the entanglement entropy and its singularity at the critical point

Random transverse Ising model

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x$$

- J_{ij} couplings
 - independent random numbers from the distribution $p(J)$
 - h_i transverse fields
 - independent random numbers from the distribution $q(h)$
- box-h disorder
 - $p(J) = \Theta(J)\Theta(1-J)$ ($\Theta(x)$: Heaviside step-function)
 - $q(h) = \frac{1}{h_b} \Theta(h)\Theta(h_b - h)$
 - fix-h disorder
 - $p(J) = \Theta(J)\Theta(1-J)$
 - $q(h) = \delta(h - h_f)$

Quantum control parameter: $\theta = \log(h_b)$ or $\theta = \log(h_f)$.

Strong disorder RG approach

(Ma, Dasgupta, Hu 1979, D.S. Fisher 1992, F.I. & Monthus 2005)

- sort the couplings and transverse fields, $\Omega = \max(J_i, h_i)$
- eliminate the largest parameter - reduce the number of spins by one
- generate new effective parameters between the remaining spins
 - $\Omega = J_{ij}$ i and j form a ferromagnetic cluster - **aggregation**
in an effective field: $\tilde{h}_{ij} = \frac{h_i h_j}{J_{ij}}$
having a moment: $\tilde{\mu}_{ij} = \mu_i + \mu_j$
 - $\Omega = h_i$ site i is decimated out - **annihilation**
new effective couplings between sites j and k : $\tilde{J}_{jk} = \frac{J_{ij} J_{ik}}{h_i}$
- repeat the transformation
- at the fixed point Ω is reduced to $\Omega^* = 0$.
- **final result**: set of **connected clusters** with different **masses**, μ ,
decimated at different **energies**, Ω .

Exact results in 1D

Infinite disorder fixed point (IDFP)

- Critical point: $\overline{\log(J)} = \overline{\log(h)}$
 - distribution of the effective parameters is logarithmically broad
 - asymptotically exact decimation steps
 - strongly anisotropic scaling
 $\ln \Omega_L \sim L^\psi$, $\psi = 1/2$
 - large effective spin clusters
size: $\xi \sim |\theta - \theta_c|^{-\nu}$ $\nu = 2$

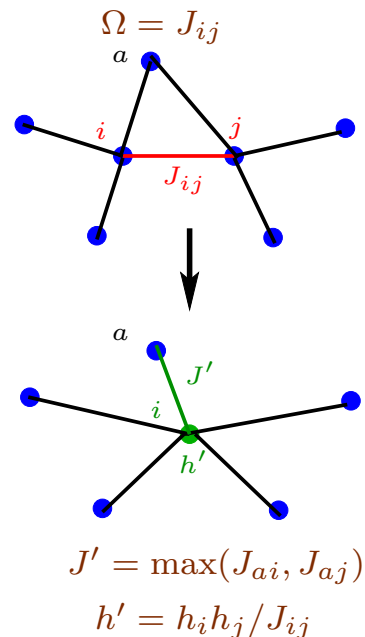
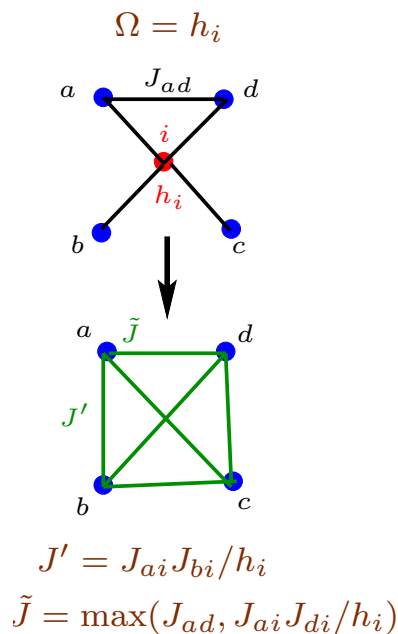
moment: $\mu \sim [\ln(\Omega_0/\Omega)]^\phi \sim L^{d_f}$

$$d_f = \phi \psi = d - x, \quad \phi = \frac{\sqrt{5}+1}{2}, \quad x = \frac{3-\sqrt{5}}{4}$$

- In the Griffiths phase: $\theta - \theta_c > 0$
 - non-singular static behaviour: $\xi < \infty$
 - singular dynamical behaviour:
 $\Omega \sim L^{-z}$ dynamical exponent: $z = z(\theta)$
 $\chi(T) \sim T^{-1+d/z}$, $C_v(T) \sim T^{d/z}$

Numerical implementation of the RG procedure for $D > 1$

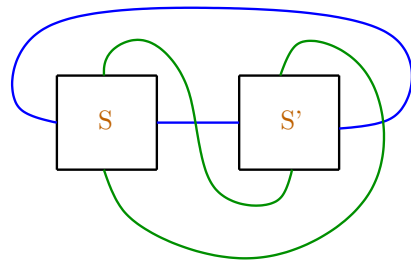
- differences with the 1D procedure
 - change in the topology
 - application of the maximum rule (valid at IDFP)



- problems with the naïve implementation
 - h -decimations induce several new bonds
 - the lattice transforms to a fully connected cluster
 - slow algorithm: for N sites works in $\mathcal{O}(N^3)$ time
- improved algorithm
 - concept of local maxima - which can be decimated independently
 - concept of optimal RG trajectory - along which the time is minimal
 - filtering out irrelevant bonds - getting rid of latent couplings
 - improved algorithm works in $\mathcal{O}(N \log N)$ time

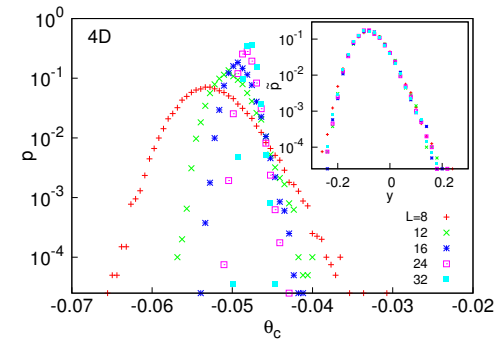
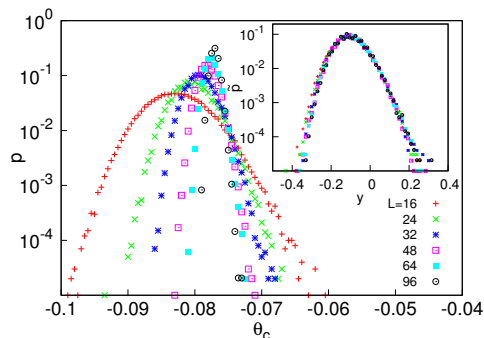
Bulk critical behavior

- Finite-size critical points - $\theta_c(S,L)$
 - two-copies of the same sample (S and S') are coupled together



- continuously increase θ and monitor the clusters, which are built of identical sites in the copies
- at $\theta_c(S,L)$ the last correlated cluster disappears, thus for $\theta > \theta_c(S,L)$ we are in the paramagnetic phase

- Distribution of pseudocritical points



- Finite-size scaling

- shift of the mean:

$$|\theta_c - \bar{\theta}_c(L)| \sim L^{-1/\nu_s}$$

- width of the distribution:

$$\Delta\theta_c(L) \sim L^{-1/\nu_w}$$

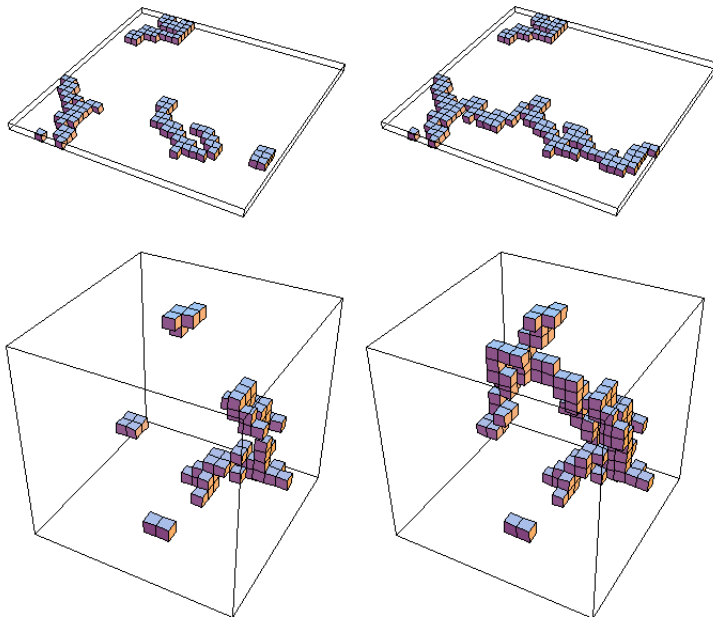
- numerical estimates:

$$\nu_s = \nu_w$$

like in a conventional random fixed point

Scaling at the critical point

- Cluster structure



correlation (left) and energy (right) clusters

- Correlation clusters \rightarrow magnetization

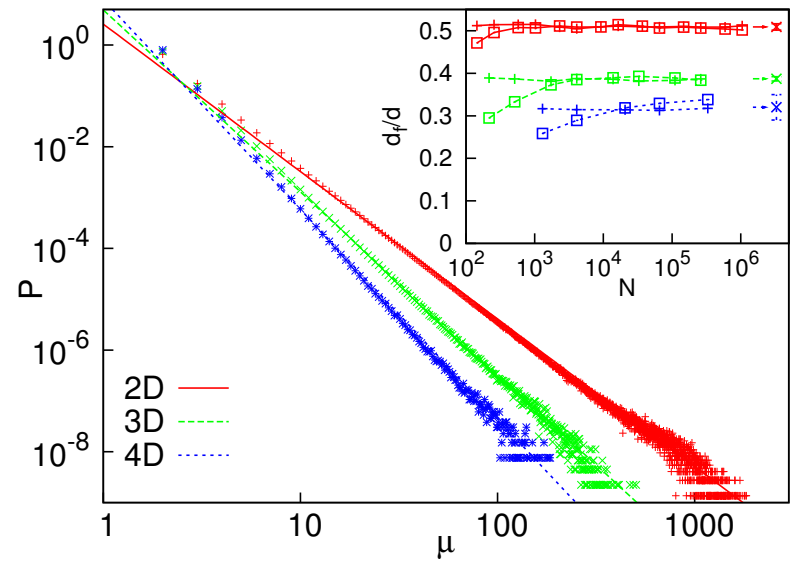
- mass: $\mu = N^\#$ of connected sites
- typical mass: $\mu \sim L^{d_f}$

– distribution function:

$$P_L(\mu) = L^{d_f} \tilde{P}(\mu L^{-d_f})$$

– power-law tail for large $\mu L^{-d_f} = u$

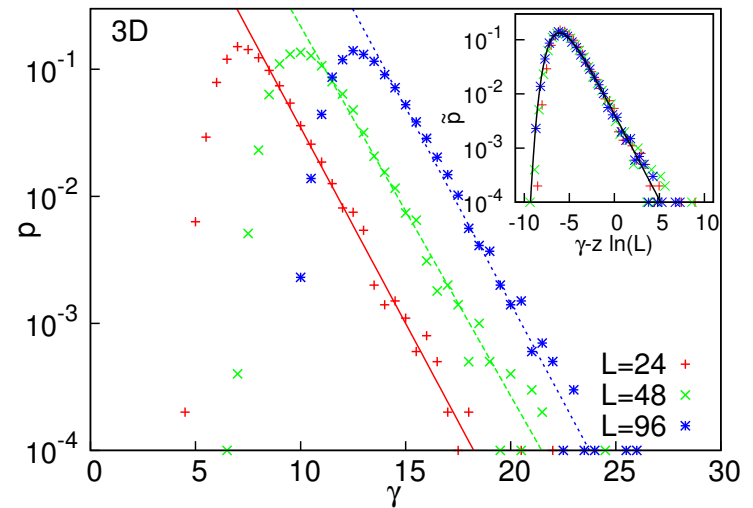
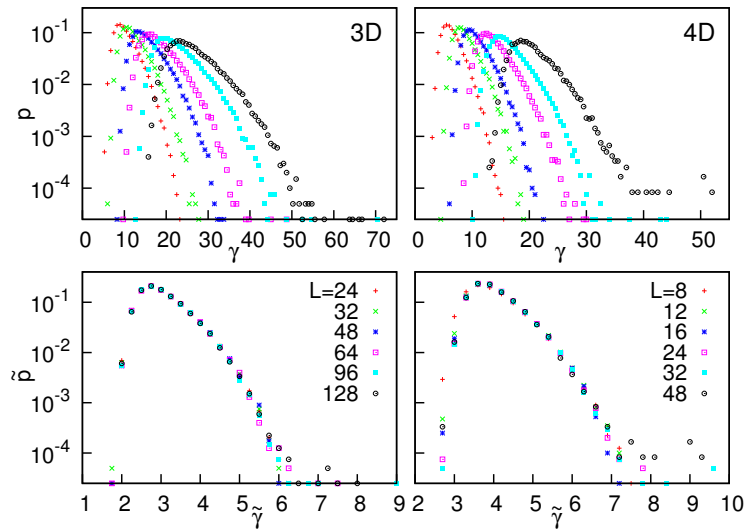
$$\tilde{P}(u) \sim u^{-\tau}, \text{ with } \tau = 1 + \frac{d}{d_f}$$



Energy clusters \rightarrow dynamical scaling

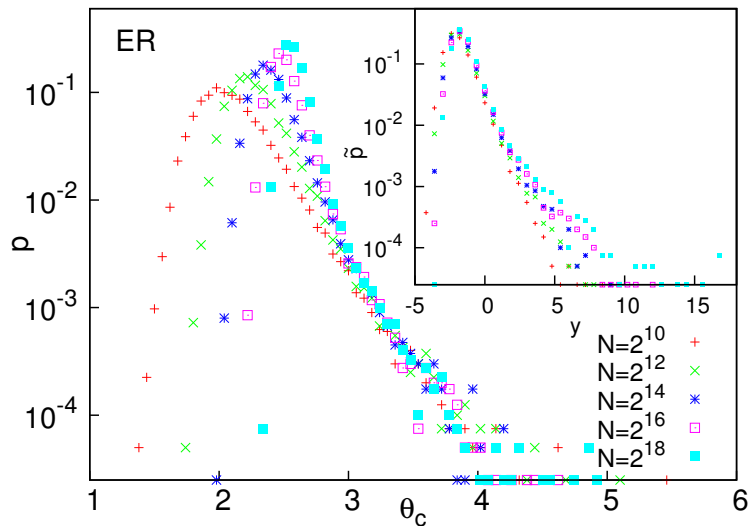
- **energy scale:** ε_L smallest gap associated with the energy cluster
- Critical point
 - typical value: $\gamma_L \sim L^\psi$
 - scaling combination $\tilde{\gamma} = (\gamma_L - \gamma_0)L^{-\psi}$
 - **Infinite disorder scaling**

- We use: $\gamma_L = \log \varepsilon_L$
- (disordered) Griffiths phase
 - typical value: $\gamma_L \sim z \log(L)$ [$\varepsilon_L \sim L^{-z}$]
 - distr.: $\log p(\gamma) \approx -(d/z)\gamma$, ($\gamma \gg 1$)
 - scaling comb.: $\tilde{\gamma} = (\gamma_L - z \ln(L) - \gamma_0)$

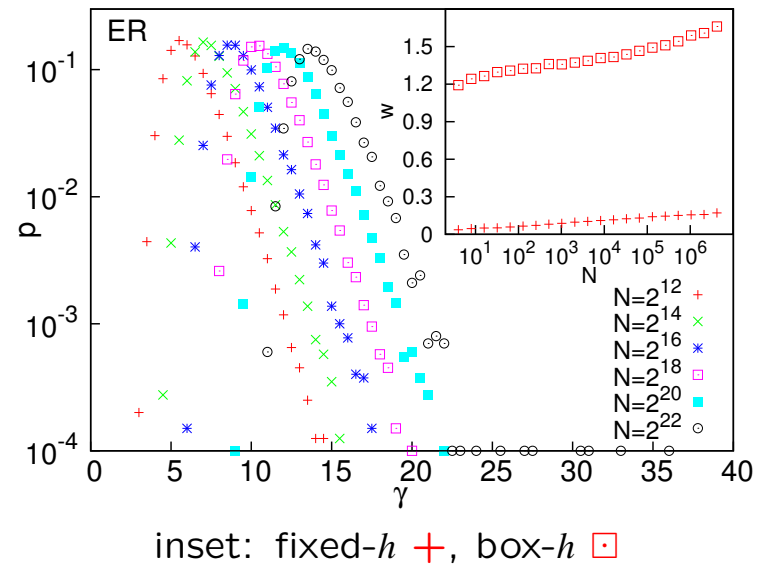


Erdős-Rényi (ER) random graphs $D \rightarrow \infty$

- Construction
 - N sites
 - $kN/2$ edges in random positions
 - $k > 1$ random graph is percolating
- Distribution of the pseudocritical points



- log-energy scaling

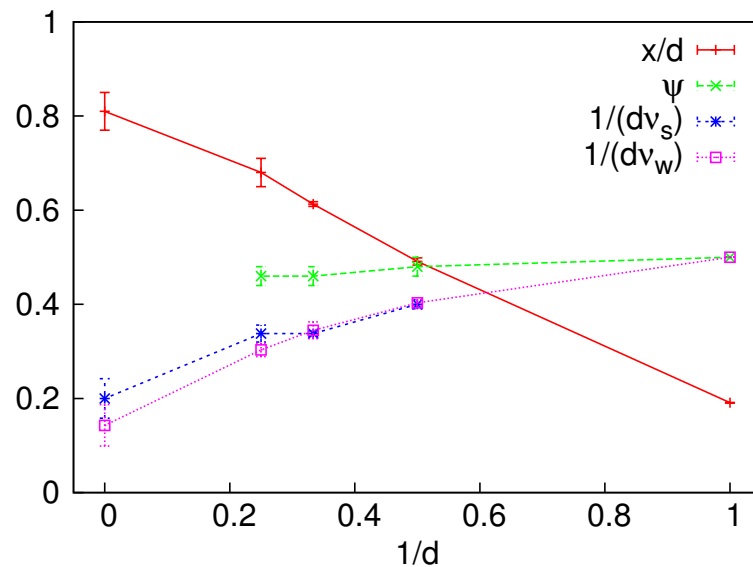


- logarithmically infinite disorder scaling
- width of the distribution:
 $W \approx W_0 + W_1 \log^\varepsilon N$
 $\varepsilon = 1.3(2)$

Bulk critical parameters

	1D	2D	3D	4D	ER
L_{max}		2048	128	48	
N_{max}		4.2×10^6	2.1×10^6	5.3×10^6	4.2×10^6
$\theta_c^{(b)}$	0	1.6784(1)	2.5305(10)	3.110(5)	2.775(2)
$\theta_c^{(f)}$	-1.	-0.17034(2)	-0.07627(2)	-0.04698(10)	-0.093(1)
dv_w	2.	2.48(6)	2.90(15)	3.3(1)	7.(2)
dv_s		2.50(6)	2.96(5)	2.96(10)	5.(1)
x/d	$\frac{3-\sqrt{5}}{4}$	0.491(8)	0.613(3)	0.68(3)	0.81(2)
ψ/d	1/2	0.24(1)	0.15(2)	0.11(2)	0. (log)

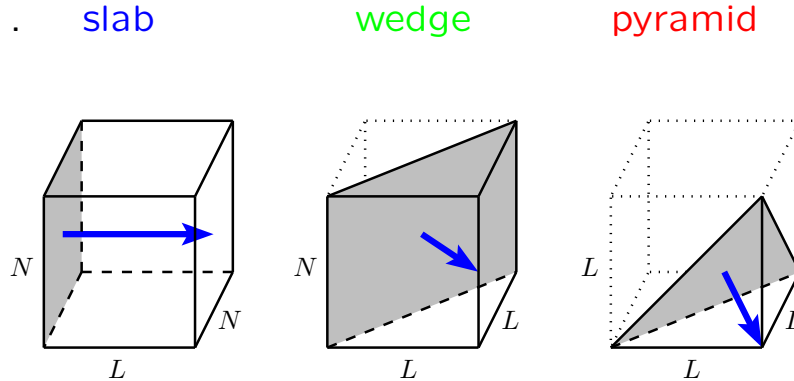
Conclusions at this point



- Infinite disorder fixed point at any dimensions
- Strong disorder RG approach is asymptotically exact
- Spin glass and random ferromagnet are in the same universality class

Boundary critical behavior

- Different finite geometries



- Different local exponents



- magnetization profiles

- from the fixed boundary:
(Fisher-de Gennes)

$$m_l \sim l^{-x_b}, \quad x = x_b, \quad l \ll L$$

- from the free part

$$m_{l'} \sim (l')^{x_{\alpha b}}, \quad l' = L_{\alpha} - l + 1 \ll L_{\alpha}$$

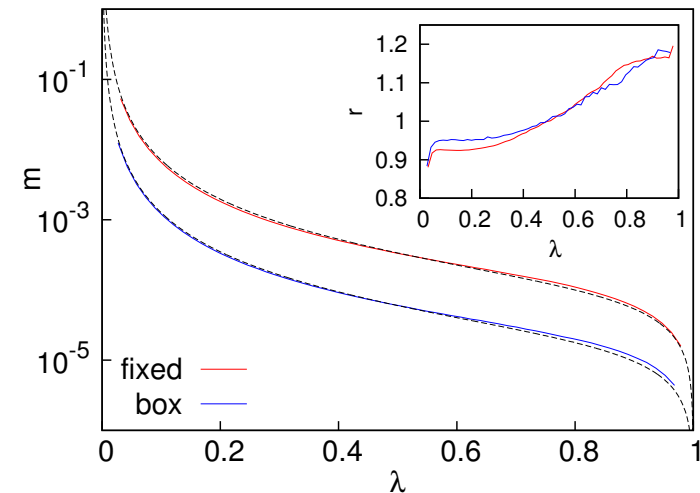
$$x_{\alpha b} = x_{\alpha} - x, \quad \alpha : s, c, e$$

- interpolation formula

$$m_l = \frac{A}{L^x} [\sin(\pi\lambda)]^x [\cos(\pi\lambda/2)]^{x_{\alpha}}$$

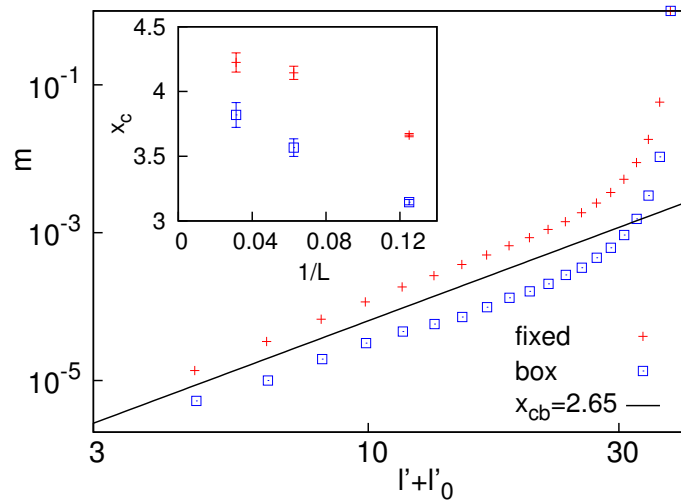
$$\lambda = l/L_{\alpha}$$

- results in 3D



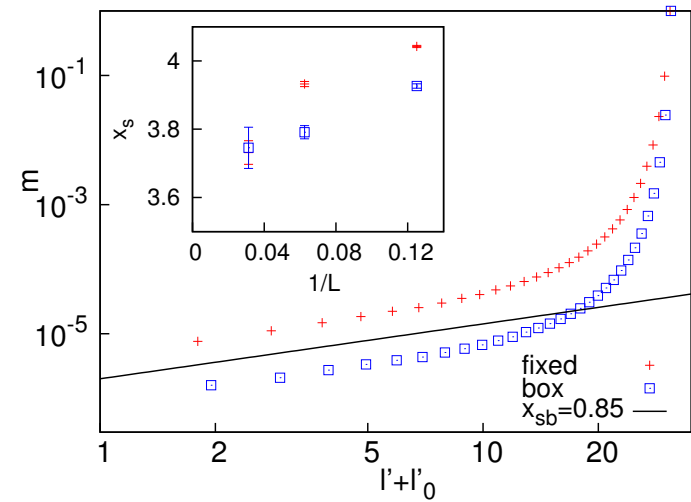
slab geometry, inset: ratio with the interpolation formula

- results in 3D



pyramid geometry, inset: corner exp.

- results in 4D



slab geometry, inset: surface exp.

Boundary critical exponents - summary

	bulk		surface		corner		edge	
	x	x_b	x_s	x_{sb}	x_c	x_{cb}	x_e	x_{eb}
1D	$(3 - \sqrt{5})/4$		0.5					
2D	0.982(15)	0.98(1)	1.60(2)	0.65(2)	2.3(1)	1.35(10)		
3D	1.840(15)	1.855(20)	2.65(15)	0.84(7)	4.2(2)	2.65(25)	3.50(15)	1.75(15)
4D	2.72(12)	2.72(10)	3.7(1)	0.85(15)				

Entanglement entropy

- entanglement entropy between a subsystem: A and the environment: B :

$$\mathcal{S}_A = -\text{Tr}(\rho_A \log_2 \rho_A)$$

- $\rho_A = \text{Tr}_B |0\rangle\langle 0|$: reduced density matrix with $|0\rangle$ the ground state of the complete system: which is a set of independent clusters
- each connected cluster with c number of spins is in a GHZ-state:

$$\frac{1}{\sqrt{2}} (|\underbrace{\uparrow\uparrow\cdots\uparrow}_{c \text{ times}}\rangle + |\underbrace{\downarrow\downarrow\cdots\downarrow}_{c \text{ times}}\rangle)$$

- for the GHZ-state

$$- \rho_A = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$- \mathcal{S}_{\text{GHZ}} = 1$$

- each cluster contained both in A and B gives 1 contribution to \mathcal{S}_A

- $\boxed{\mathcal{S}_A \sim L^{d-1}}$: area law

- **corrections at the critical point?**

- are they singular?

- form: $\sim L^{d-1} \ln \ln L$ or $\sim L^{d-1} + b \ln L$?

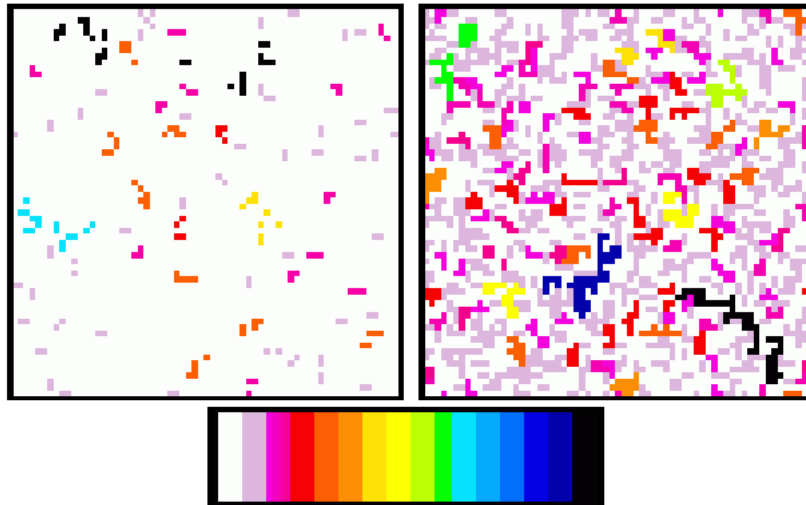
- origin: corner and/or bulk?

- are they universal?

- related to a diverging ξ ?

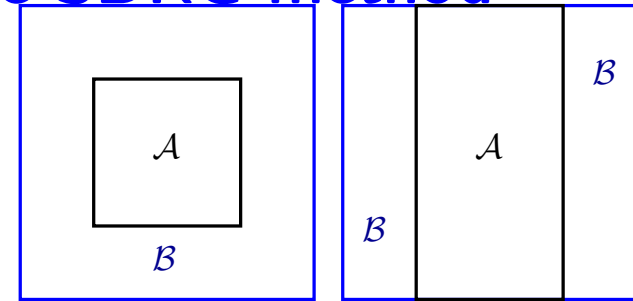
Numerical calculation by the SDRG method

- for a sample obtain the clusters through renormalization



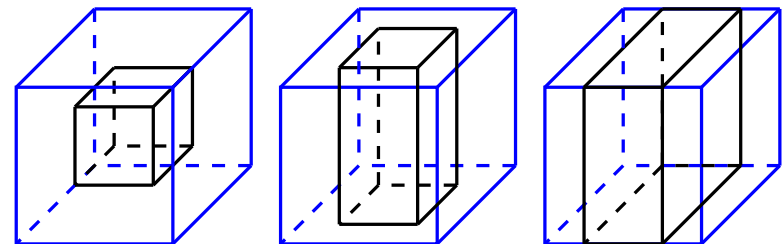
$L = 64$ box-h (left) fixed-h (right)

- Calculation in different geometries



square (cube)

strip (slab)



s_0^3

s_1^3

s_2^3

cube

column

slab

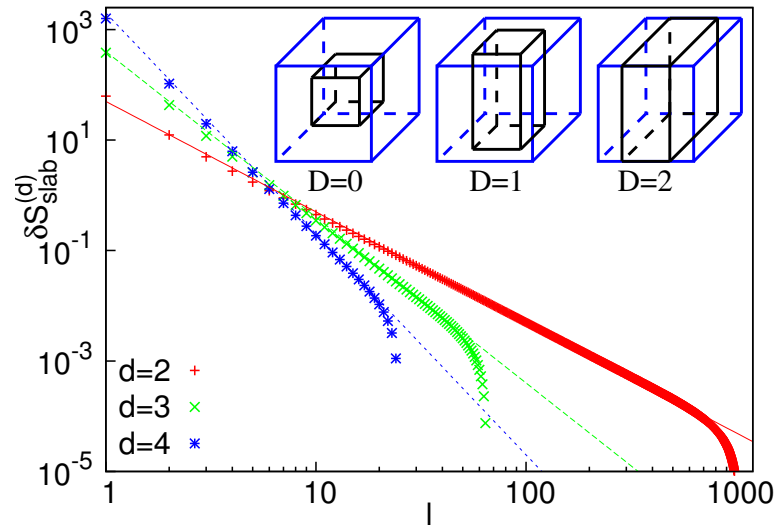
Slab geometry

- the same area (term) for different ℓ :

$$\mathcal{S}_{\text{slab}}^{(d)}(L, \ell) = a_{d-1} f_{d-1} + \text{corr}(\ell), \quad f_{d-1} = L^{d-1}$$

- the finite difference is related to the correction

$$\delta \mathcal{S}_{\text{slab}}^{(d)}(L, \ell) = \mathcal{S}_{\text{slab}}^{(d)}(L, \ell + 1) - \mathcal{S}_{\text{slab}}^{(d)}(L, \ell)$$



- numerical data at the critical point:

$$\delta \mathcal{S}_{\text{slab}}^{(d)}(L, \ell) \sim \ell^{-d}$$

- no singular corrections!

- phenomenological explanation

- domains which contribute to the entropy are of size $\xi \leq \ell$

- finite-size corrections are for $\xi \approx \ell$

- number of these blobs are $n_{bl} \sim (L/\ell)^{d-1}$

- each blob has the same $\mathcal{O}(1)$ correction

- total correction:

$$\mathcal{S}_{\text{slab}}^{(d)}(L, \ell) - a_{d-1} f_{d-1} \sim n_{bl} \sim \ell^{d-1}$$

- singular contributions are due to corners!

Cube (square) geometry in 2d

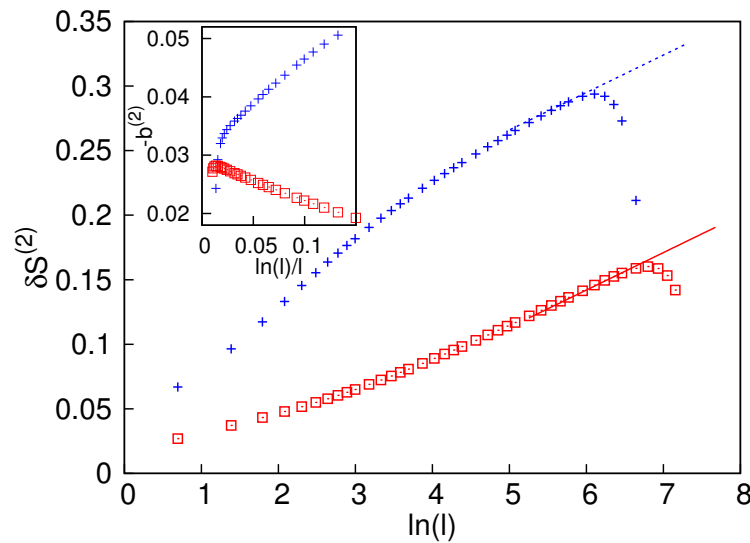
- corner correction to the area-law:

$$\mathcal{S}_{\text{cube}}^{(2)}(\ell) = a_1 f_1 + \mathcal{S}_{\text{cr}}^{(2)}(\ell)$$

- calculate the difference:

$$\delta \mathcal{S}^{(2)}(\ell) \equiv \mathcal{S}^{(2)}(\ell) - 2\mathcal{S}^{(2)}(\ell/2)$$

$$\approx \mathcal{S}_{\text{cr}}^{(2)}(\ell) - 2\mathcal{S}_{\text{cr}}^{(2)}(\ell/2)$$



fixed- h (+) and box- h (□)

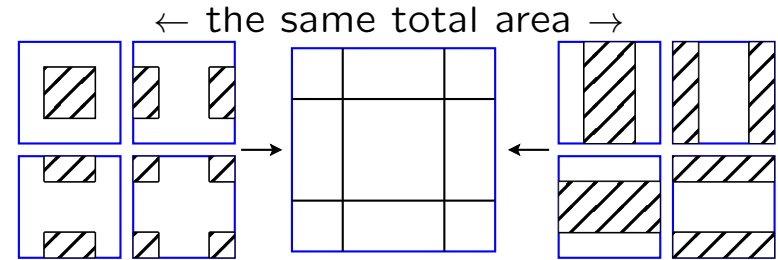
- numerical data:

$$\delta \mathcal{S}^{(2)}(\ell) \simeq \mathcal{S}_{\text{cr}}^{(2)}(\ell) + cst \simeq -b^{(2)} \ln \ell + cst$$

- universal logarithmic correction:

$$b^{(2)} = -0.029(1)$$

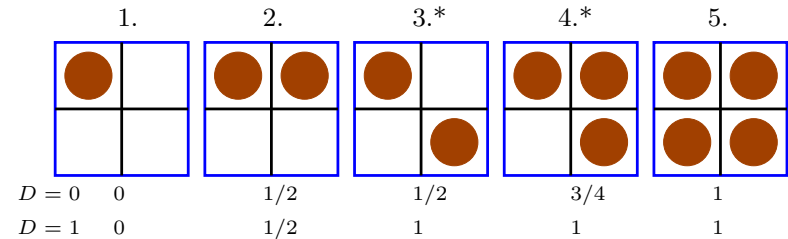
- direct calculation of the corner contribution for $\ell = L/2$**



corners

no corners!

- relation with the cluster geometry



Cube geometry in $d > 2$

- edge and corner corrections to the area-law:

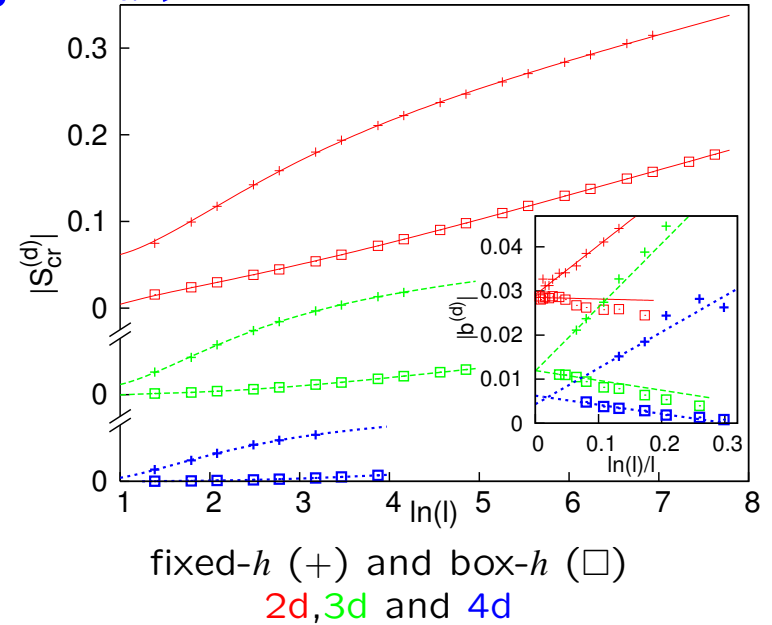
$$\mathcal{S}_{\text{cube}}^{(2)}(\ell) = a_{d-1}f_{d-1} + \sum_{E=1}^{d-2} a_E f_E + \mathcal{S}_{\text{cr}}^{(2)}(\ell)$$

- $1 \leq E < d - 1$: dimension of the edge, $f_E \sim L^E$

- $a_E - a_E(\ell) \sim \ell^{-E}$, as for the surface term

- **direct calculation of the corner contribution for $\ell = L/2$**

$$\mathcal{S}_{\text{cr}}^{(d)} = \sum_{D=0}^{d-1} \left(-\frac{1}{2}\right)^D \binom{d}{D} \mathcal{S}_D^{(d)}$$



- numerical data:

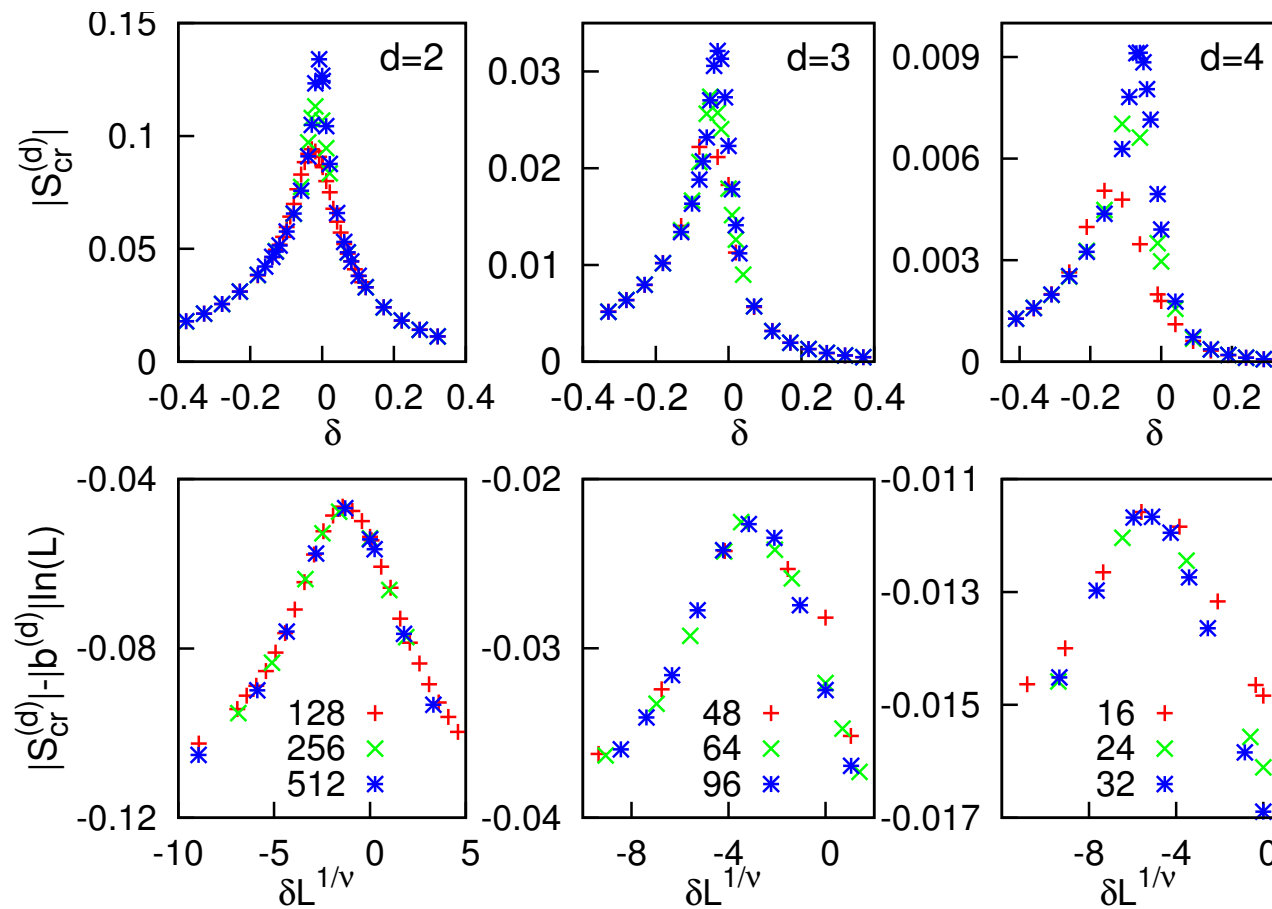
$$\mathcal{S}_{\text{cr}}^{(d)}(\ell) \simeq -b^{(d)} \ln \ell + cst$$

- universal logarithmic correction:
 $b^{(2)} = -0.029(1)$, $b^{(3)} = 0.012(2)$ and $b^{(4)} = -0.006(2)$

Phenomenological explanation

- consider 2-site clusters (at the end of the RG)
- “corner clusters” have points at hypercubes connected by the main diagonal
- relative coordinates of the 2-site clusters:
 $0 \leq x_j \leq L/2, j = 1, 2, \dots, d$ (periodic b.c.)
- the corner entropy (averaging over all positions):
 $-2 \prod_{j=1}^d (-x_j/L)$
- probability of a 2-site cluster of length r is:
 the average pair-correlation function:
 $C_{av}(r) \approx n_r^2$
 $n_r \sim r^{-d}$: the density of non-decimated sites
- average contribution:
 $\mathcal{S}_{cr}^{(d)}(\ell) \sim - \int_1^\ell dx_1 \dots \int_1^\ell dx_d \prod_{j=1}^d (-x_j/r^2)$
 $\sim (-1)^{d+1} \int_1^\ell (r^{d-1} r^d) / r^{2d} dr$
 $\sim (-1)^{d+1} \ln \ell$

Corner correction outside the critical point



The singularity is related to a diverging correlation length!

Experimental realization - LiHoF₄

(Rosenbaum, Aeppli *et al*)

classical system

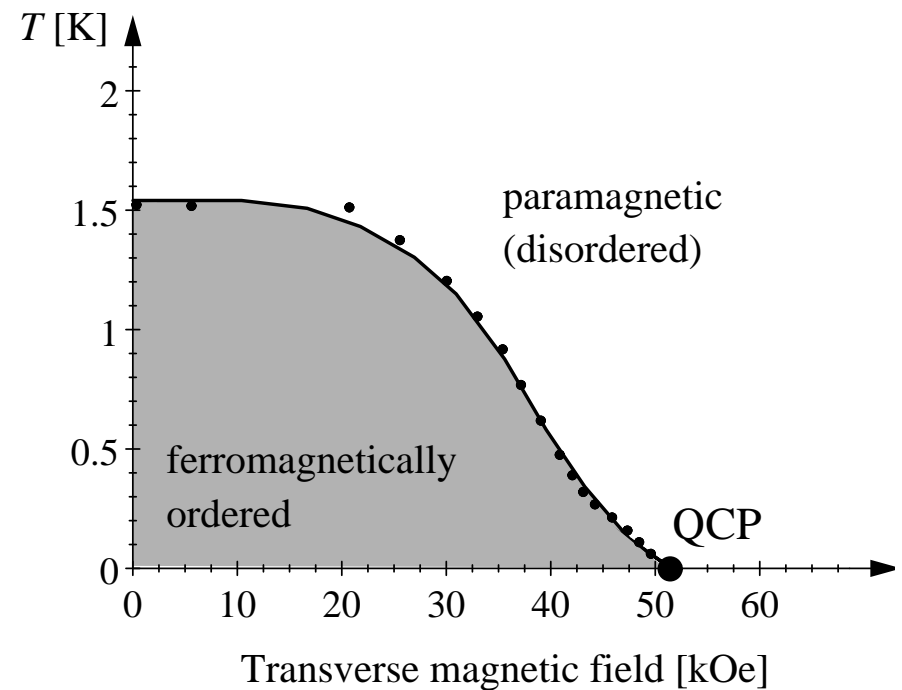
dipole coupled Ising ferromagnet with Curie

temperature $T_c = 1.53K$

quantum fluctuations

applying magnetic field H_t transverse to the

Ising axis splits the up-down states by $h \sim H_t^2$



Quantum spin glass - $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$

(Rosenbaum, Aeppli *et al*)

- magnetic **Ho** is substituted by nonmagnetic **Y**
- a spin glass (SG) phase enters in the classical phase diagram (b)
- SG phase in the presence of quantum fluctuations (c)
- the SG phase stays at $T = 0$: quantum spin glass (d)

