

Ising and Potts models in a random field: results from (quasi-)exact algorithms

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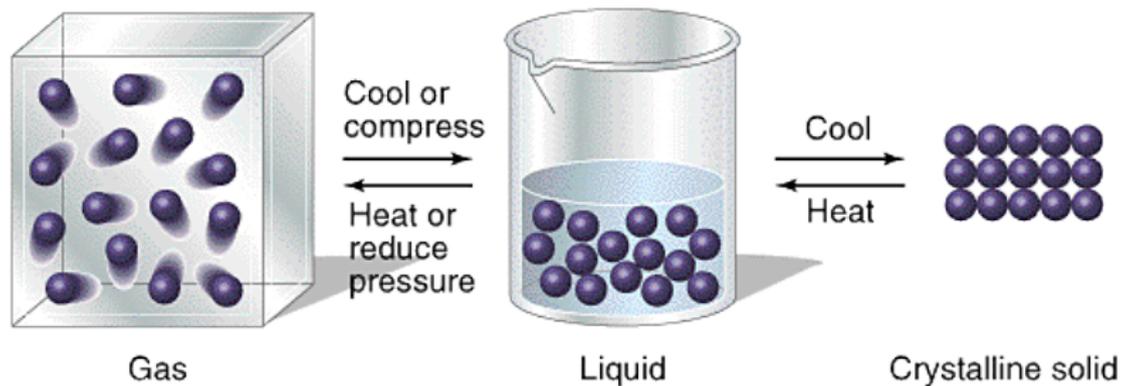
Kolloquium Theoretische Physik
Carl von Ossietzky-Universität Oldenburg, January 12, 2023



TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

Phases of matter

Classical physics



Starting point: the (2D) Ising model

Simple model for liquid-gas or magnetic transition, the Ising model.



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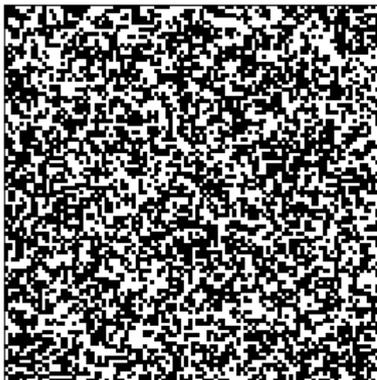
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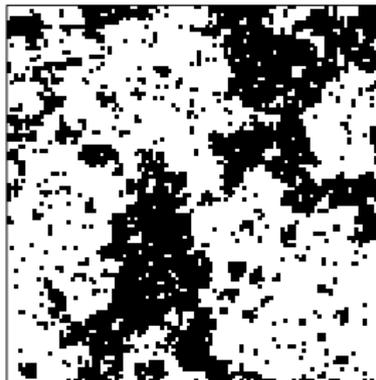
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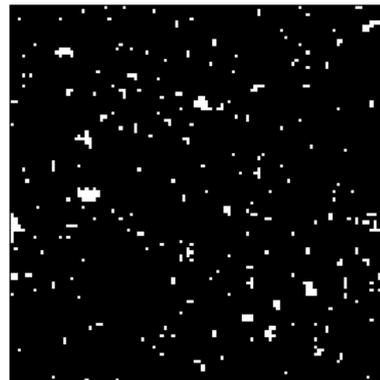
$T \gg T_c$



$T \approx T_c$

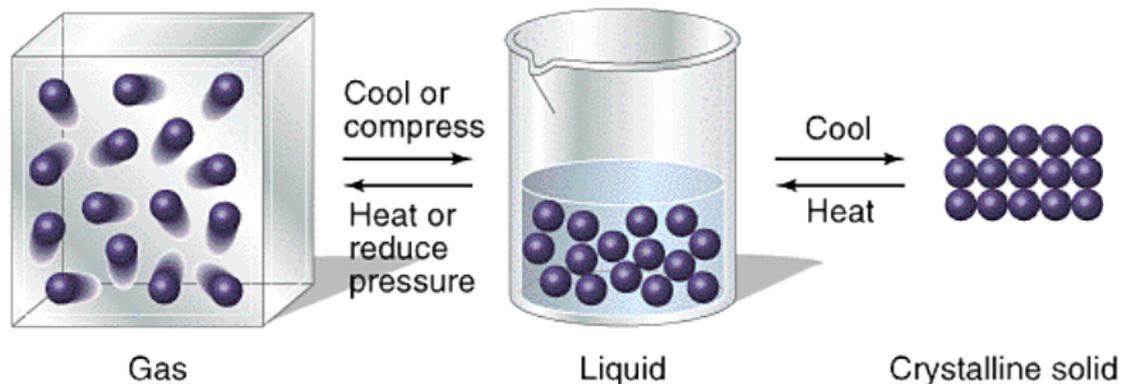


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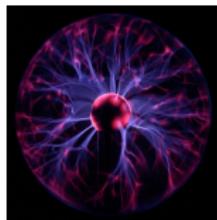


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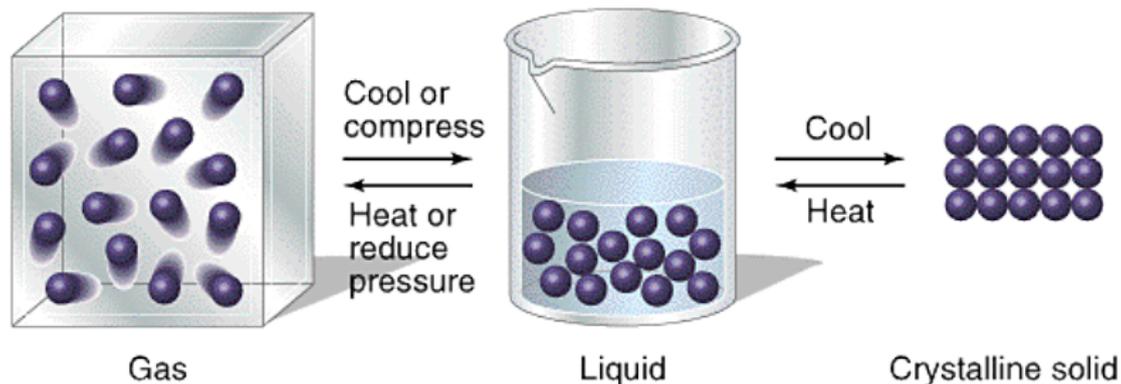
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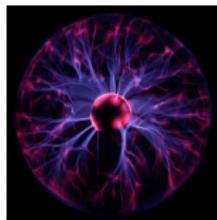
Plasma

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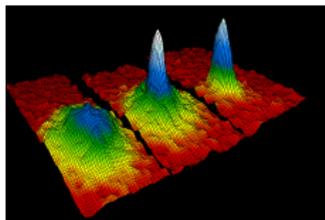
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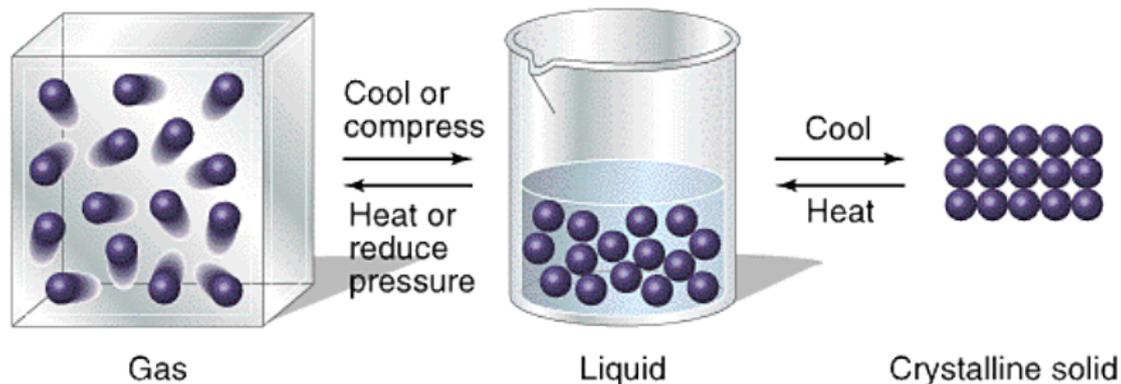
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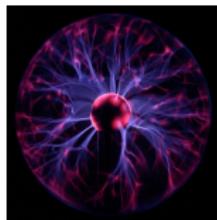
Bose-Einstein condensate

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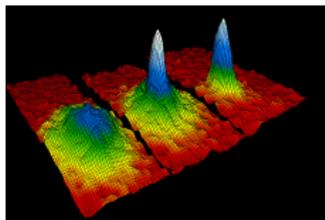
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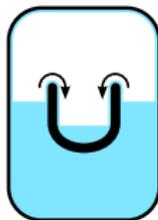
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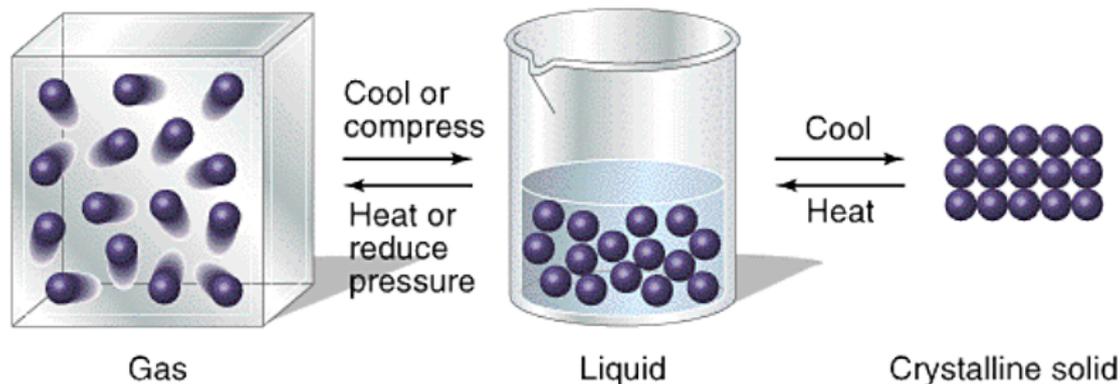
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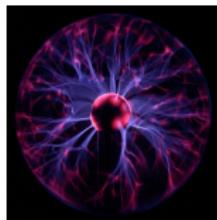
Superfluid

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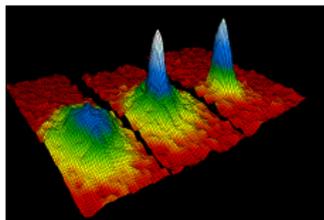
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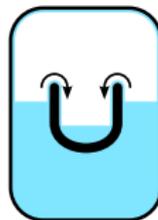
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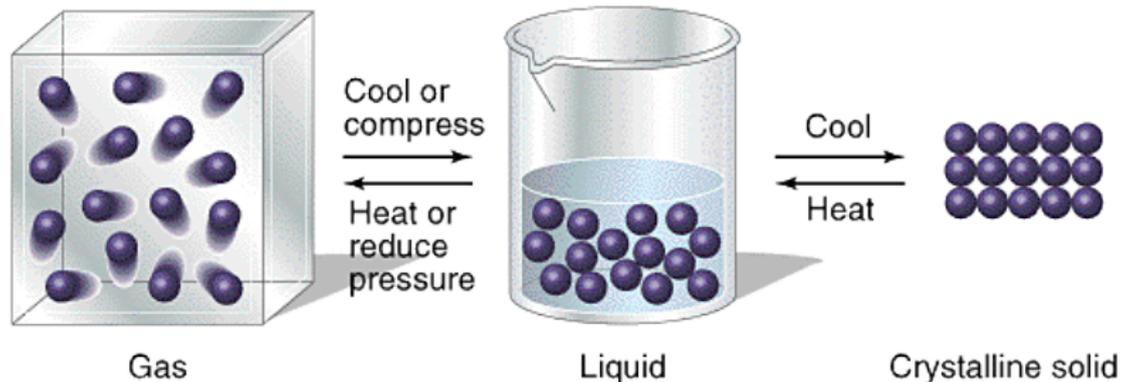
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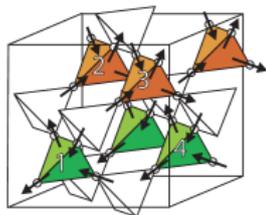
Glass

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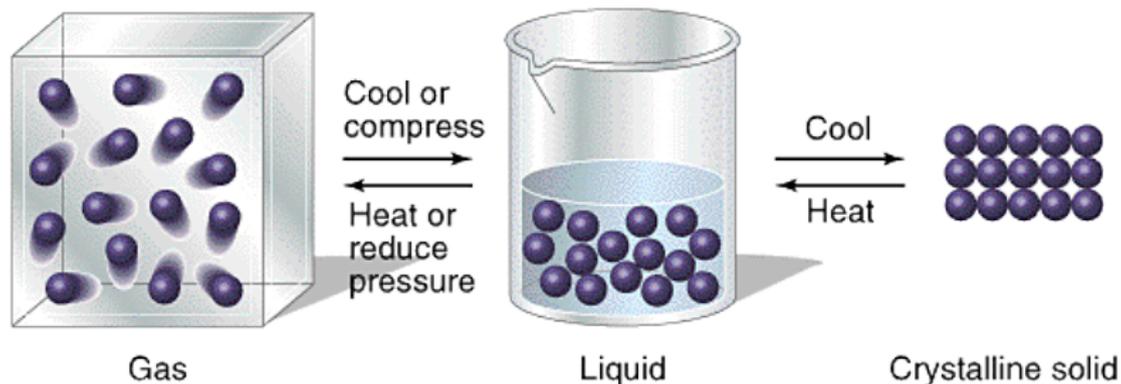
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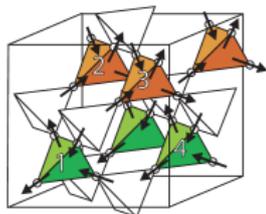
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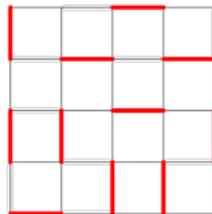
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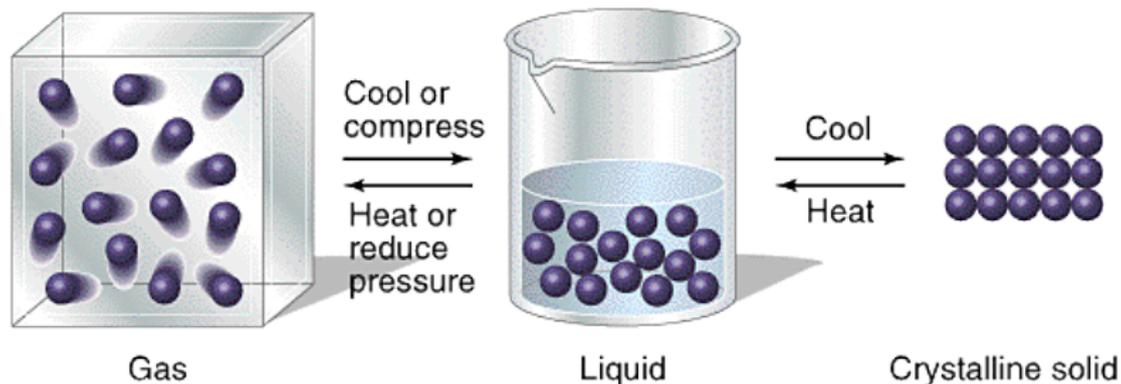
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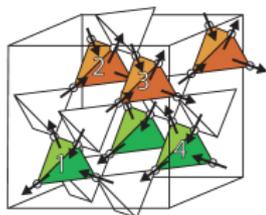
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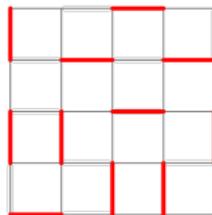
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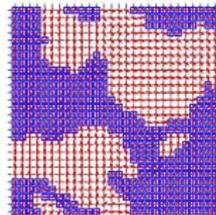
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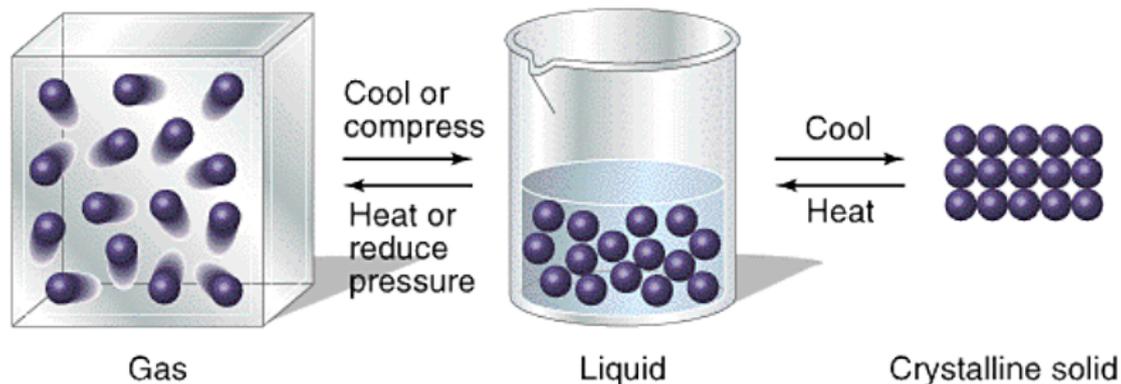
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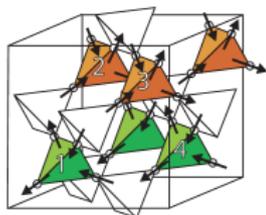
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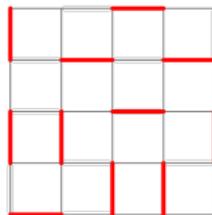
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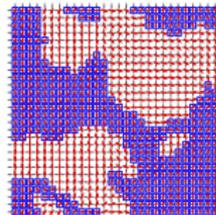
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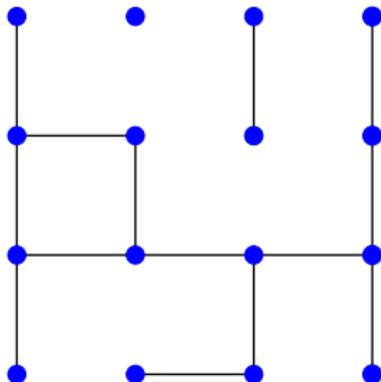
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- ▶ **Weak disorder:** long-range order is not destroyed and the nature of the ordered phase is unchanged

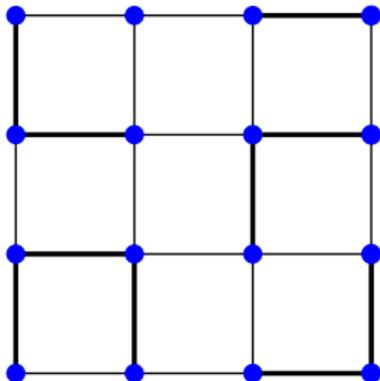


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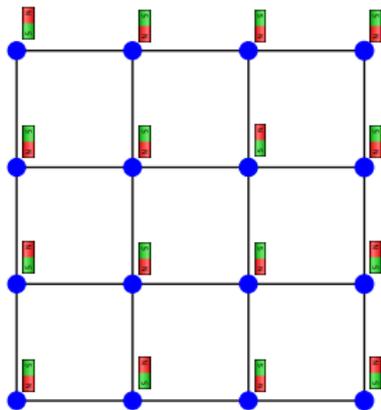


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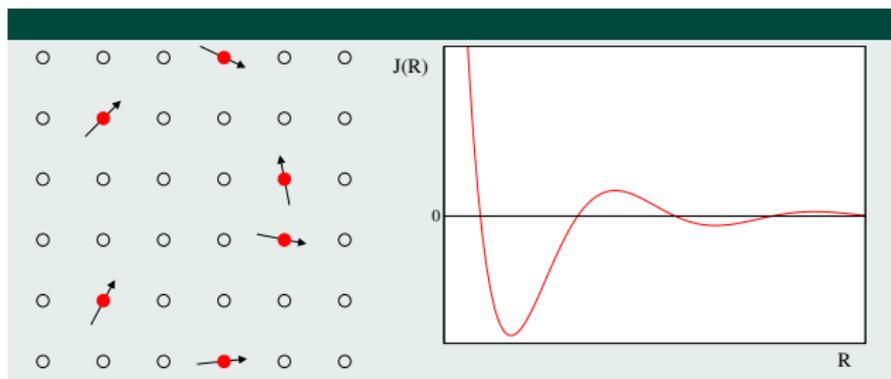
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- ▶ **Strong disorder**: no long-range order, new phases of matter; typically encompasses the presence of **frustration** – **spin glasses**.

What is a spin glass?

Classical example of spin glass: noble metals weakly diluted with transition metal ions, interacting via the RKKY interaction,

$$J(\mathbf{R}) = J_0 \frac{\cos(2k_F R + \phi_0)}{(k_F R)^3}$$

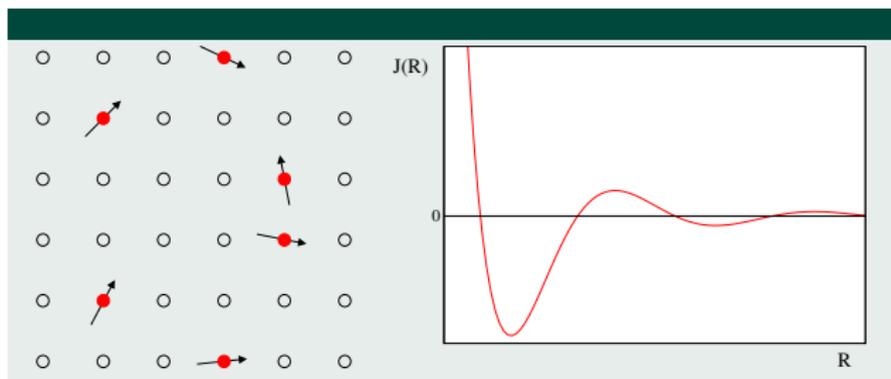


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- ▶ no long-range order down to $T = 0$
- ▶ phase transition to short-range ordered, "glassy" phase
- ▶ diverging relaxation times, memory, rejuvenation etc.

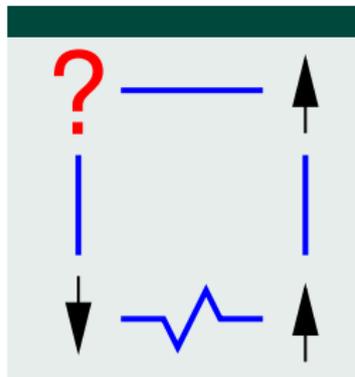


The Edwards-Anderson model

Simplify to the essential properties, **disorder** and **frustration** to yield the Edwards-Anderson (EA) model,

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j, \quad \mathbf{s}_i \in \text{O}(n)$$

where J_{ij} are *quenched*, random variables.

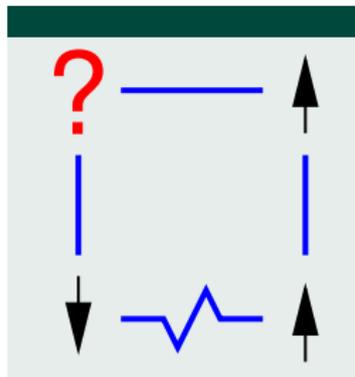


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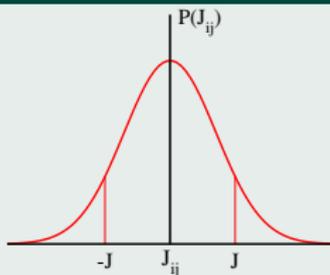
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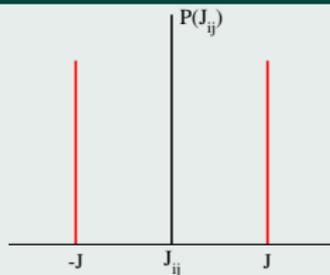


Coupling distributions

Gaussian



bimodal

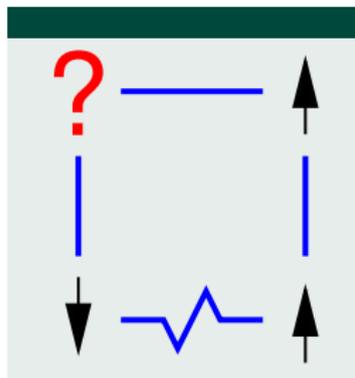


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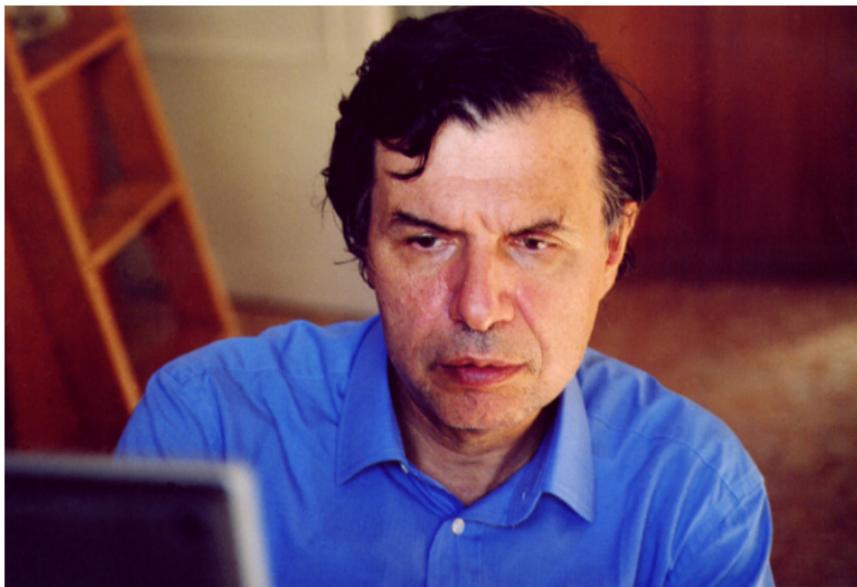


Has been investigated for ≈ 30 years, however no agreement on general case. Mean-field model with

$$J_{ij} = \frac{\pm 1}{\sqrt{N}},$$

known as Sherrington-Kirkpatrick (SK) model can be solved in the framework of “replica-symmetry breaking” (RSB) (Parisi et al., 1979/80).

Giorgio Parisi



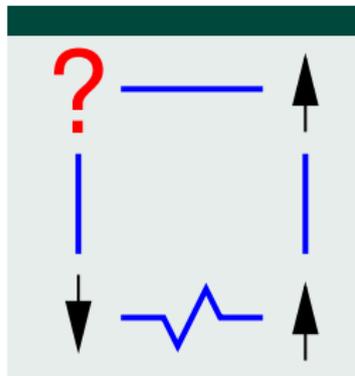
Nobel Prize 2021

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Applications

System has applications in a range of fields:

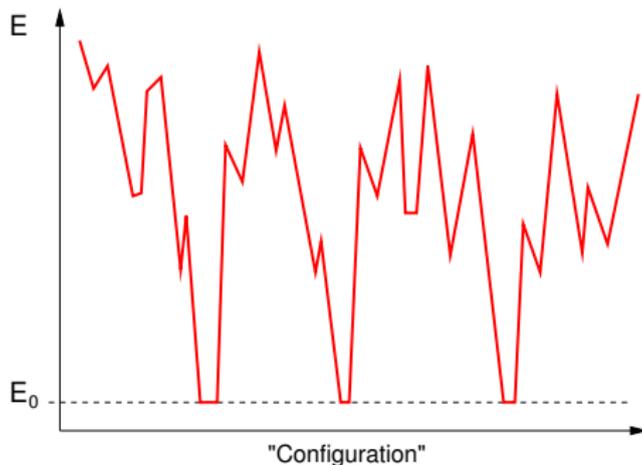
- ▶ possible role in high- T_c superconductors
- ▶ model of associative memory (Hopfield model), machine learning
- ▶ gene expression networks
- ▶ realized in D-Wave quantum computer

Ground-state calculations

At low temperatures, there are several (many) competing, **metastable** states, leading to very *slow dynamics*.

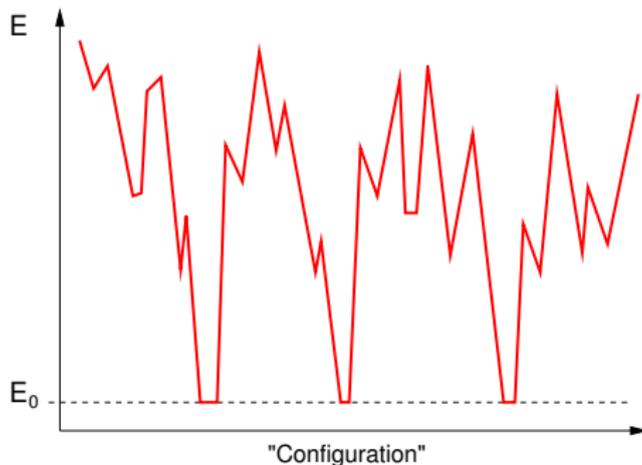
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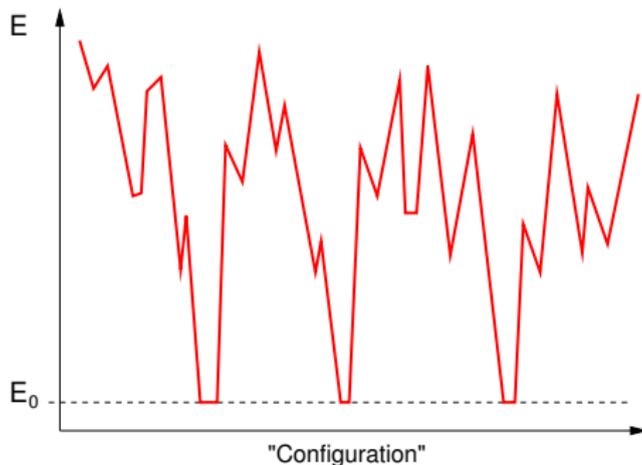
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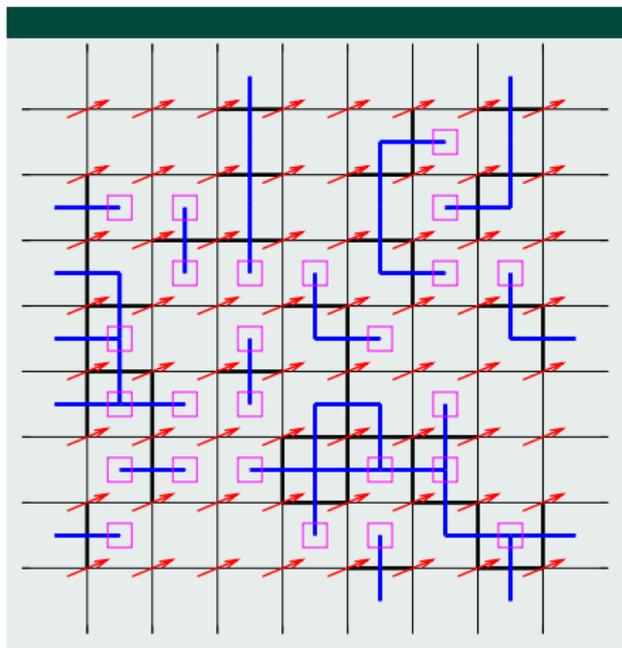
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Finding them, however, can be difficult. In some cases it is **NP hard**.

Ising ground states as perfect matchings

System energy equals total weight of **energy strings** pairing frustrated plaquettes (Toulouse, 1977),

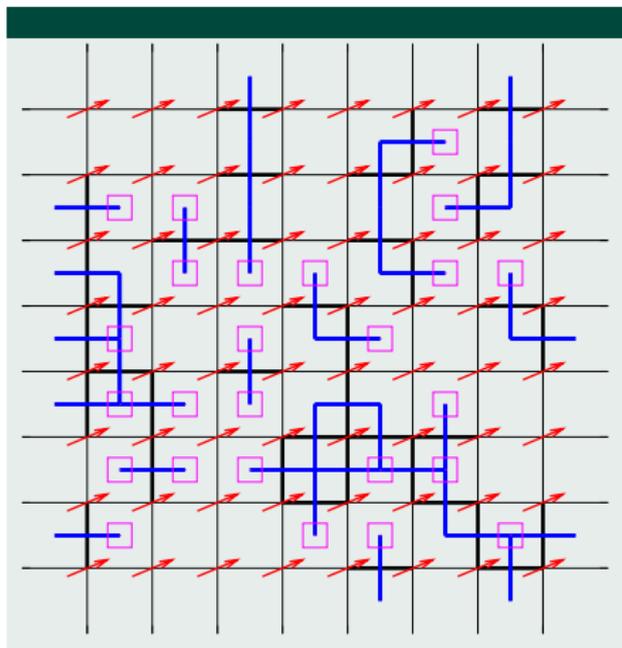
$$E = - \sum_{\text{strings}} |J_{ij}| + \text{const.}$$



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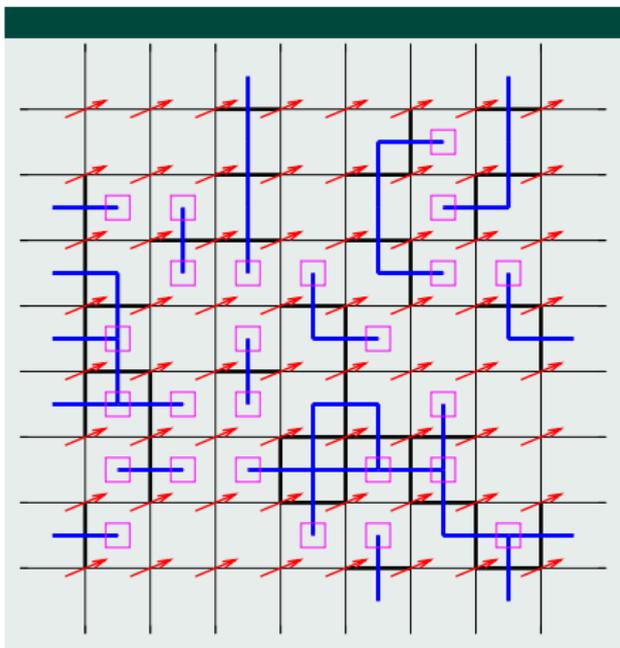


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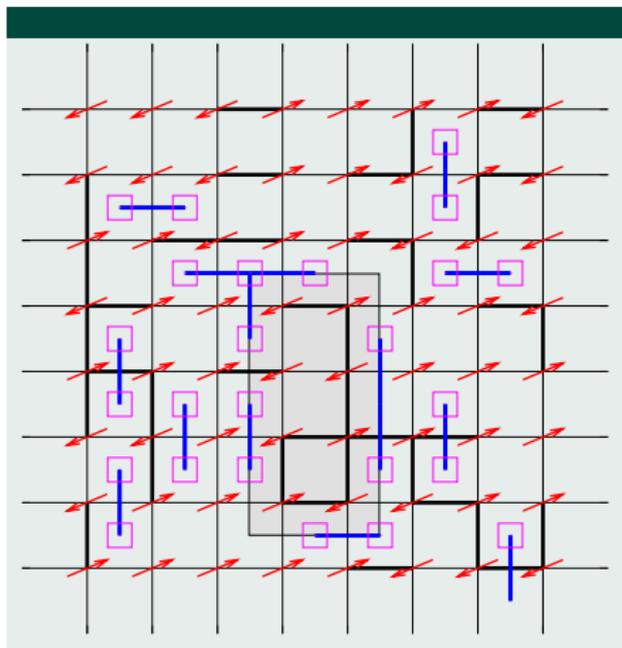


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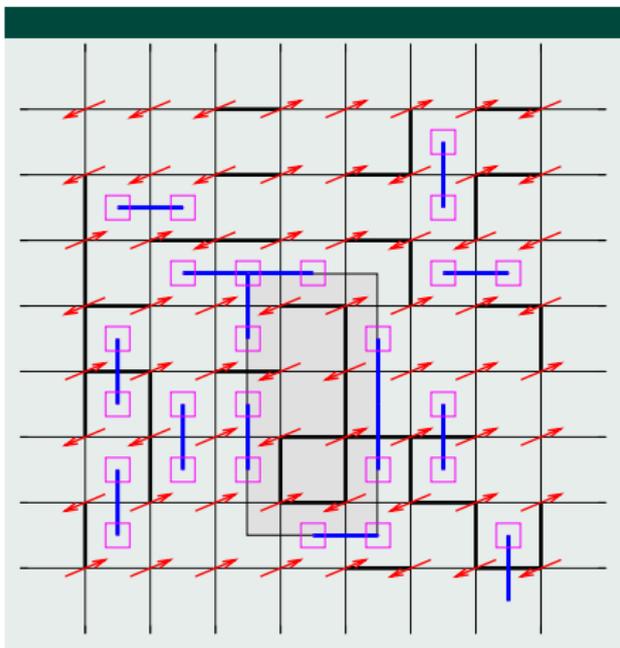


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- ▶ matching solution always corresponds to spin configuration for **planar** graphs
- ▶ can be solved in polynomial time using the “blossom” algorithm (Edmonds, 1965)
- ▶ **space complexity is $O(V^2)$**

Ising spin glass in 2D

Complex energy landscape leads to **slow relaxation**: sizes restricted to $L \approx 128$ (MC).

Ising spin glass in 2D

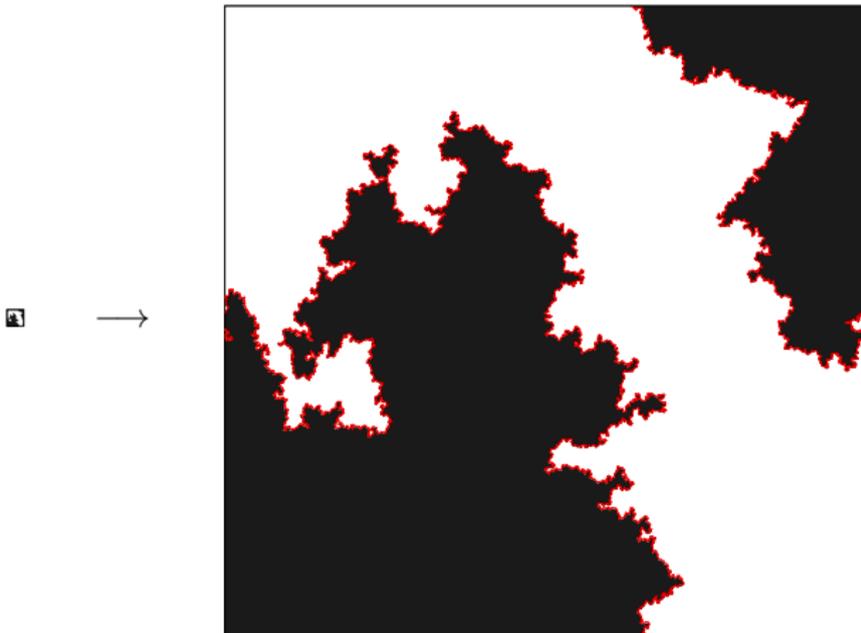
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With suitably constructed **combinatorial optimization** methods we can treat large system sizes up to $10\,000 \times 10\,000$ spins **exactly** (for $T = 0$).

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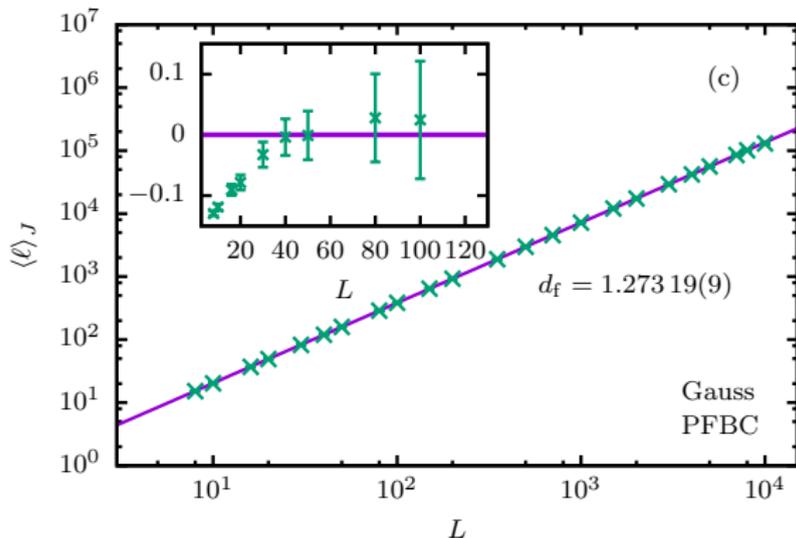
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Fractal dimension

Fractal dimension of domain wall.



$$\langle \ell \rangle_J(L) = A_\ell L^{d_f} (1 + B_\ell L^{-\omega}) + \frac{C_\ell}{L} + \frac{D_\ell}{L^2} + \dots$$

Results

Perform calculations for periodic-free and periodic-periodic boundary conditions.

	PFBC	PPBC
$-e_\infty$	1.3147876(7)	1.314788(3)
θ	-0.2793(3)	-0.2788(11)
d_f	1.27319(9)	1.2732(5)

Results are fully consistent with each other.

Based on SLE and further assumptions, Amoruso et al. (2006) proposed

$$d_f = 1 + \frac{3}{4(3 + \theta)}.$$

$d_f = 1.27319(9)$ would imply $\theta = -0.2546(9)$ which is **not compatible** with the direct estimate.

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$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - \sum_i h_i s_i$$

h_i quenched random variables drawn, e.g., from a Gaussian,

$$h_i \sim \mathcal{N}(0, h)$$

or a bimodal distribution,

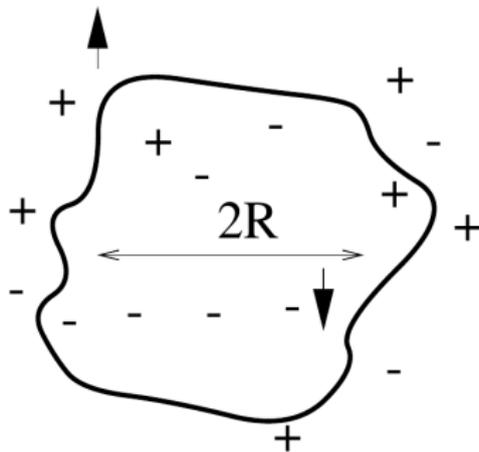
$$P(h_i) = \frac{1}{2} \delta_{h_i, -1} + \frac{1}{2} \delta_{h_i, +1}.$$

Imry and Ma argument

Is the FM phase stable?

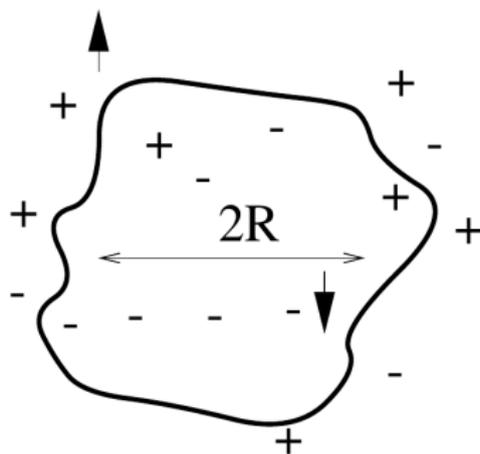
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Following Imry and Ma (1975), consider a cluster of spins of (linear) size R . Overturning it will cost a surface energy of

$$E_J \sim JR^{d-1}$$

but potentially yield a gain in random-field energy of

$$E_{\text{RF}} \sim hR^{d/2}$$

Imry and Ma argument (cont'd)

leading to a balance of

$$\Delta E(R) \sim JR^{d-1} - hR^{d/2}.$$

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For large R , $\Delta E > 0$ for $d > 2$ and $\Delta E < 0$ for $d < 2$. Hence,

- ▶ FM order is stable in $d \geq 3$.
- ▶ FM order is destroyed by random fields in $d = 1$.
- ▶ $d = 2$ is marginal.

Imry and Ma argument (cont'd)

leading to a balance of

$$\Delta E(R) \sim JR^{d-1} - hR^{d/2}.$$

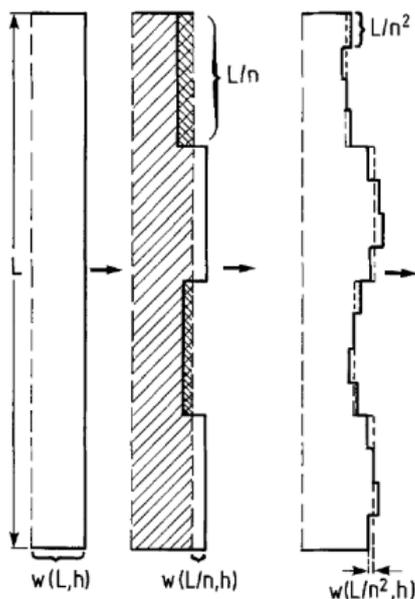
For large R , $\Delta E > 0$ for $d > 2$ and $\Delta E < 0$ for $d < 2$. Hence,

- ▶ FM order is stable in $d \geq 3$.
- ▶ FM order is destroyed by random fields in $d = 1$.
- ▶ $d = 2$ is marginal.

Aizenman and Wehr (1989) proved unique Gibbs state for $d \leq 2$, so no long-range order in 2D.

Domain-wall roughness

Binder (1983) considered the energy balance for a domain-wall, comparing the interface energy $2JL$ and the gain in field energy, ΔU .



Taking the interface roughness into account, he finds

$$\Delta U \sim -(h^2/J)L \ln L / \ln n,$$

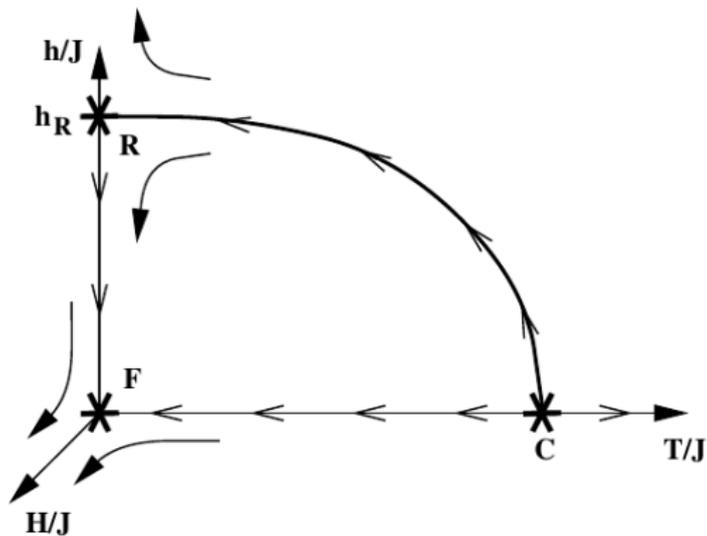
where n denotes the scale of resolution for the interface.

$U = 2JL - \Delta U$ changes sign at length scale

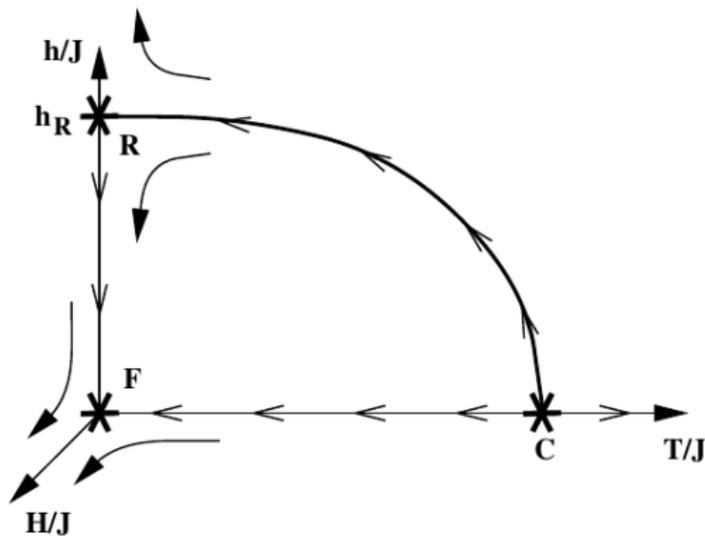
$$L_b \sim \exp[c(J/h)^2].$$

L_b is known as **breakup length**.

Renormalization group

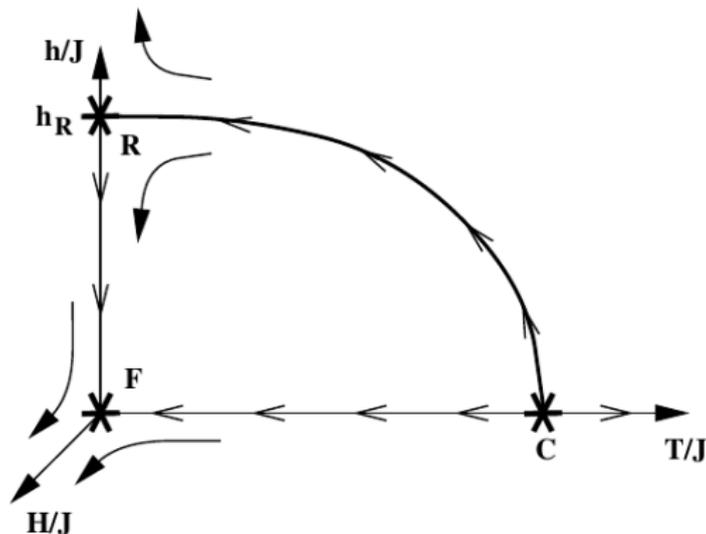


Renormalization group



The critical behavior of the RFIM can be studied at $T = 0$, i.e., from ground states!

Renormalization group



The critical behavior of the RFIM can be studied at $T = 0$, i.e., from ground states!

Renormalization group flow equation for $w = h/J$ (Bray and Moore, 1985),

$$dw/dl = -(\epsilon/2)w + Aw^3.$$

Break-up length

Sample ground-state configurations for $L = 512$.



$$h = 0.6$$

Break-up length

Sample ground-state configurations for $L = 512$.



$$h = 0.7$$

Break-up length

Sample ground-state configurations for $L = 512$.



$$h = 0.8$$

Break-up length

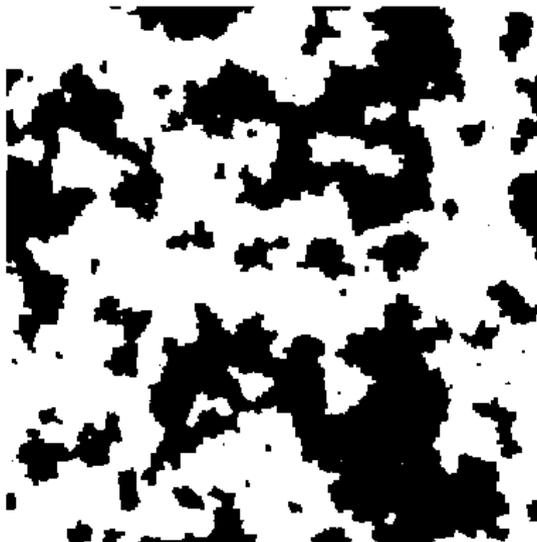
Sample ground-state configurations for $L = 512$.



$$h = 0.9$$

Break-up length

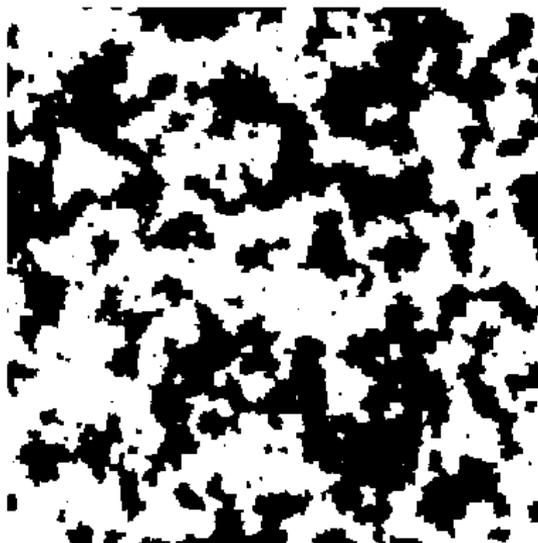
Sample ground-state configurations for $L = 512$.



$$h = 1.0$$

Break-up length

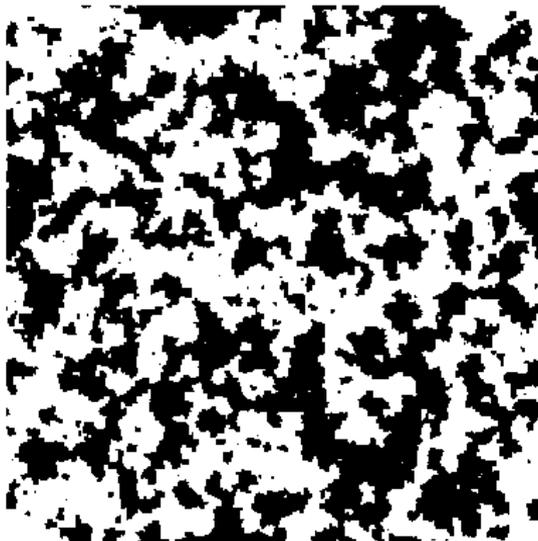
Sample ground-state configurations for $L = 512$.



$$h = 1.1$$

Break-up length

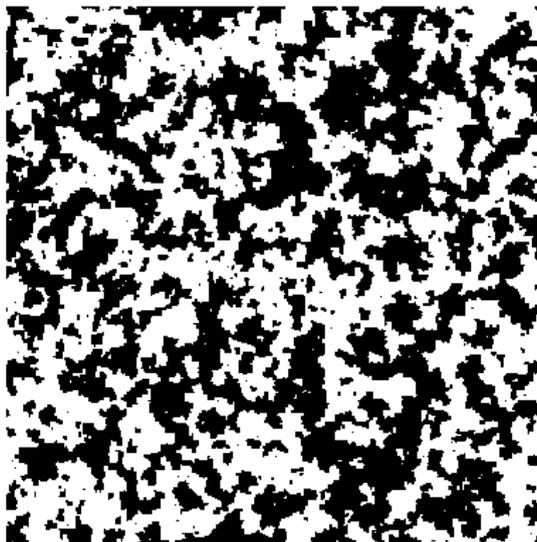
Sample ground-state configurations for $L = 512$.



$$h = 1.2$$

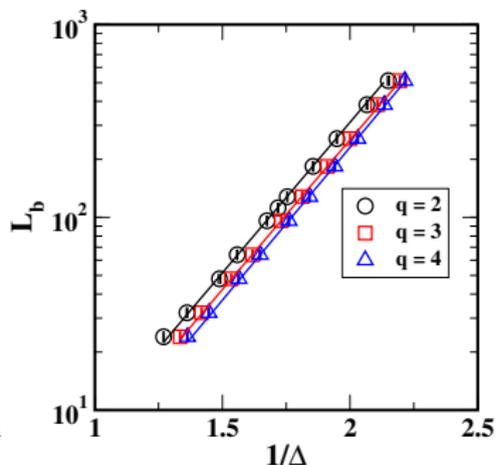
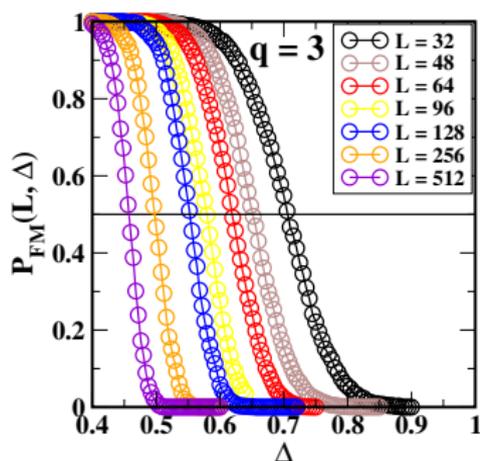
Break-up length

Sample ground-state configurations for $L = 512$.

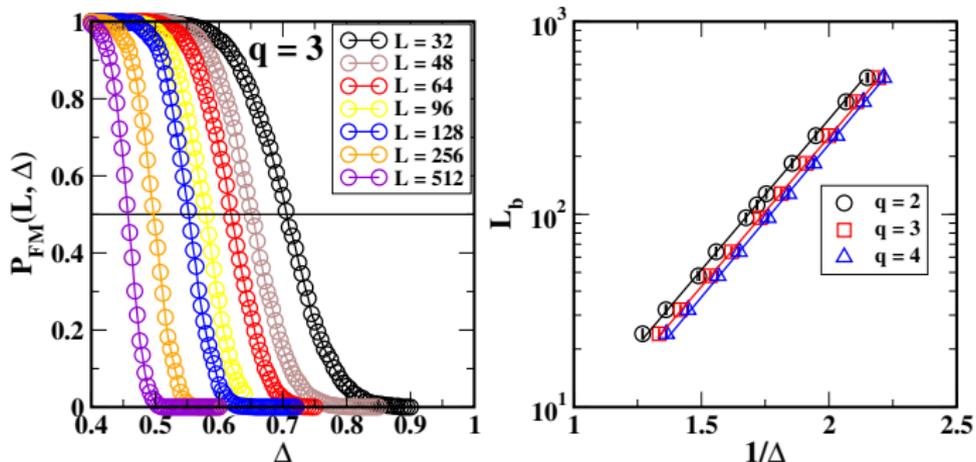


$$h = 1.3$$

Break-up length (cont'd)

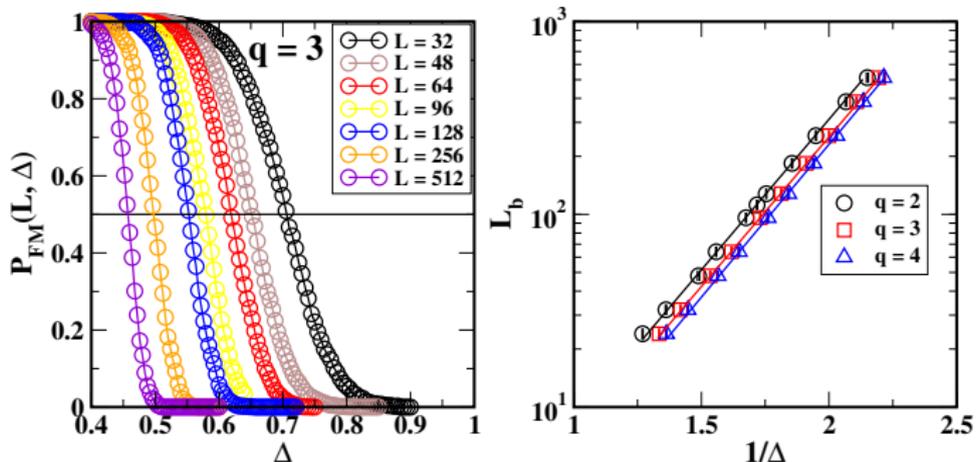


Break-up length (cont'd)



Define L_b as system size such that 50% of disorder samples at given h are FM (Seppälä et al., 1998).

Break-up length (cont'd)

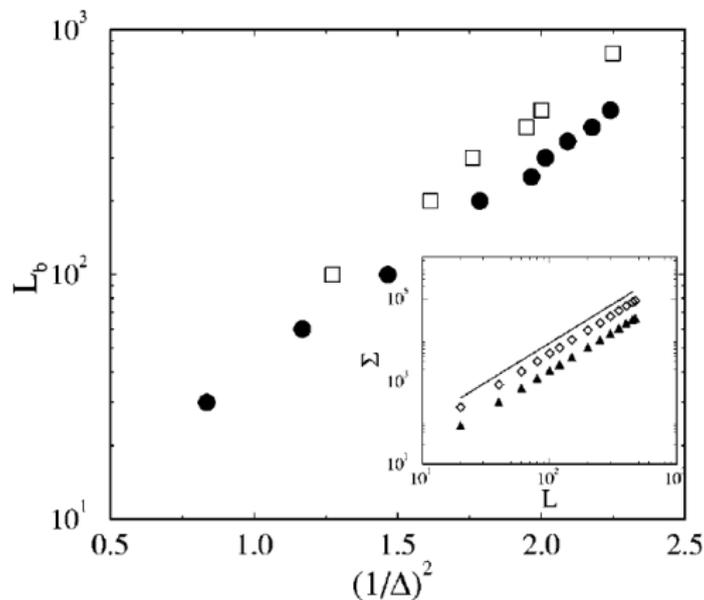


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What is the correct form?

$$L_b \sim \exp(A/h) \quad \text{or} \quad \exp(A/h^2)$$

Break-up length (cont'd)

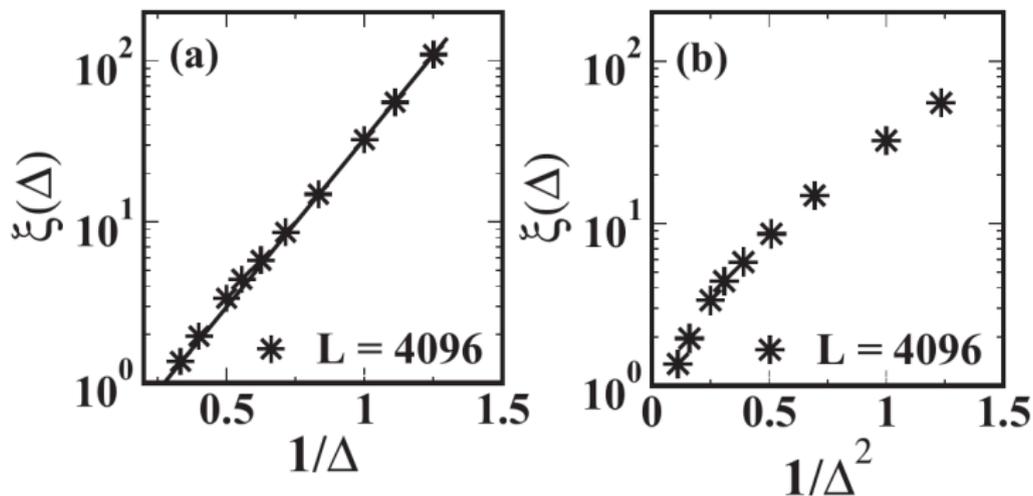


Seppälä et al., 1998

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Break-up length (cont'd)



Shrivastav et al. 2014

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Maximum flows and graph cuts

Split up Ising model Hamiltonian,

$$-\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} s_i s_j = W^+ + W^- - W^\pm = K - 2W^\pm, \quad (1)$$

where $K = \sum_{\langle ij \rangle} J_{ij}$, and

$$W^+ = \sum_{\substack{\langle ij \rangle \\ s_i = s_j = +1}} J_{ij}, \quad W^- = \sum_{\substack{\langle ij \rangle \\ s_i = s_j = -1}} J_{ij}, \quad W^\pm = \sum_{\substack{\langle ij \rangle \\ s_i \neq s_j}} J_{ij} \quad (2)$$

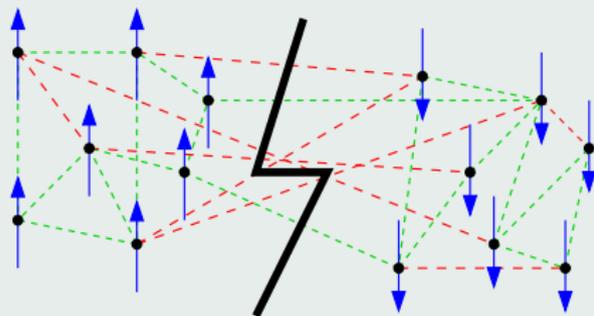
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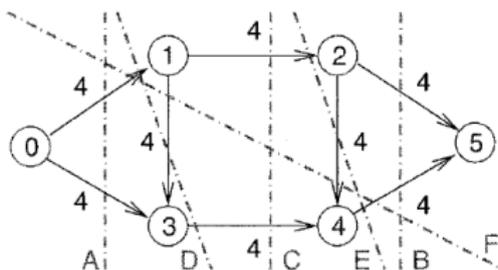
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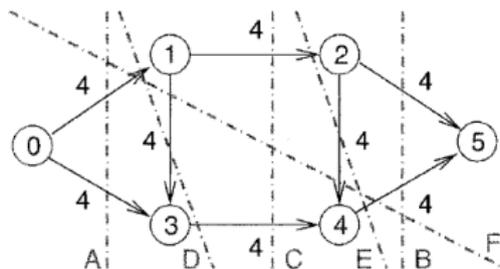


Then, a ground state is given by a configuration with **minimal cut** W^\pm , which divides the spins between the “up” and “down” states.

Maximum flows and graph cuts (2)

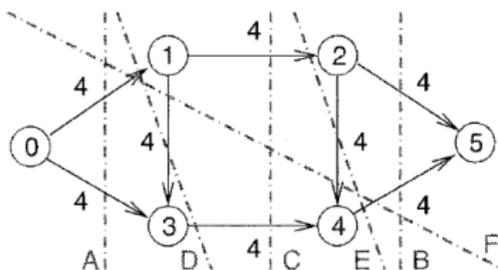


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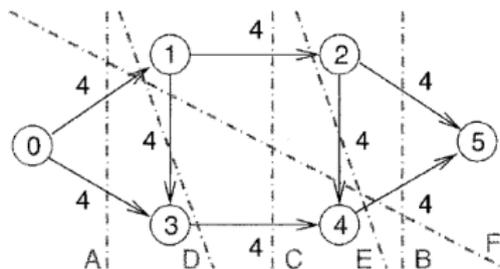
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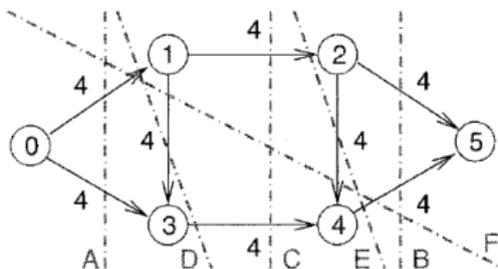
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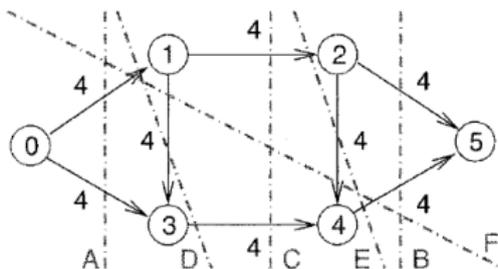
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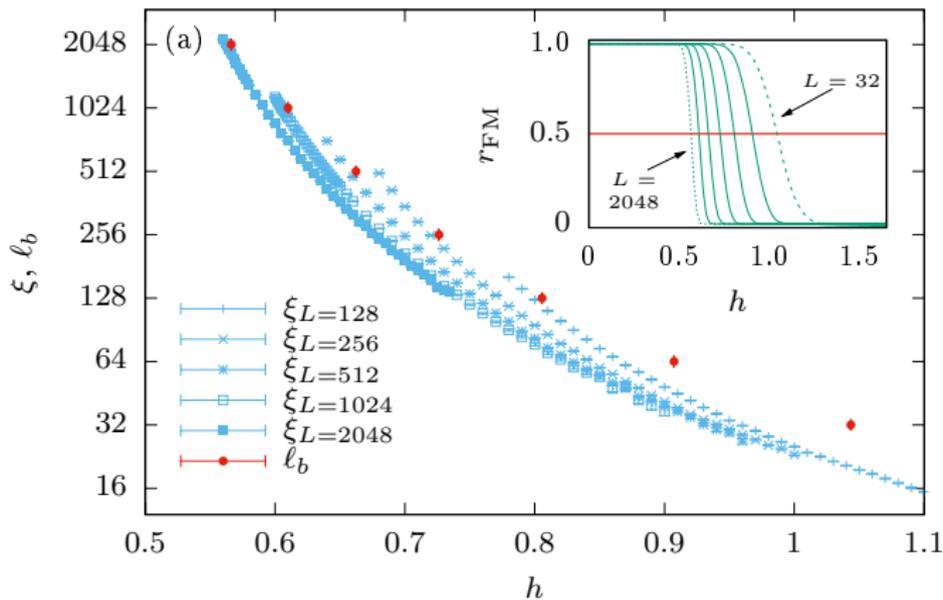
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Numerical study

We use **exact** ground-state algorithms to study the breakup length ℓ_b and the **correlation lengths** ξ and ξ^{dis} for 10^6 samples and lattice sizes $L = 128, 256, 512, 1024, \text{ and } 2048$.

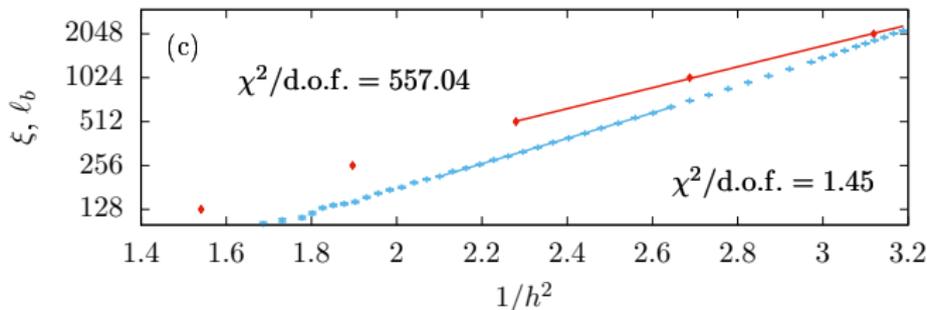
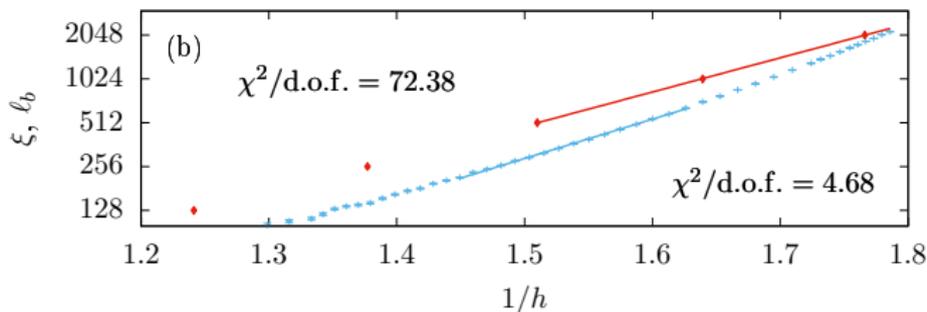
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Correlation length: triangular lattice

Strong evidence for $\xi \sim \exp(A/h^2)$ form on the square lattice.

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Hayden, Raju and Sethna, 2019: since $w \leftrightarrow -w$ on non-bipartite lattices, the RG equation should take the form

$$dw/dl = -(\epsilon/2)w + Bw^2 + Aw^3 + \dots,$$

implying a leading divergence $\xi \sim \exp(A/h)$ for the **triangular** lattice.

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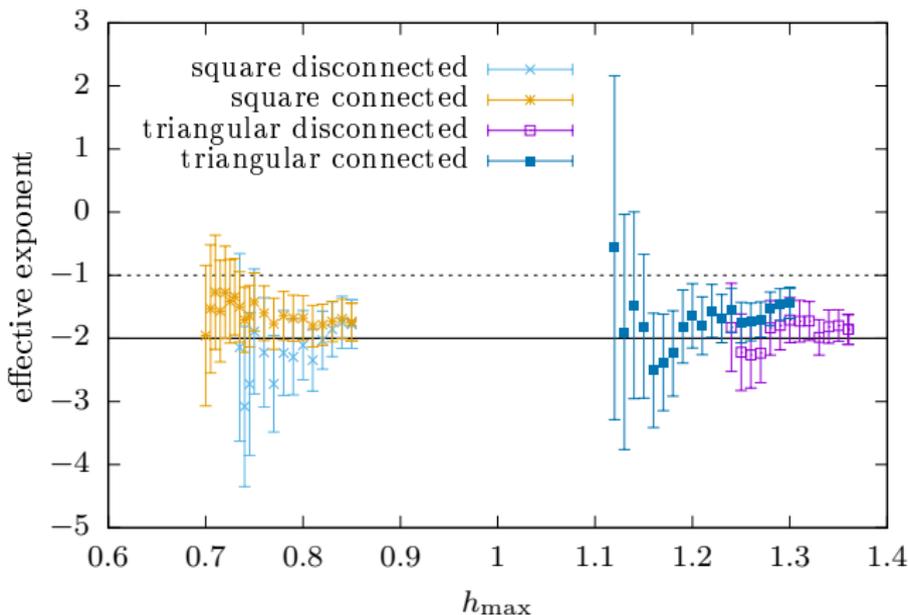
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Is this supported by the data?

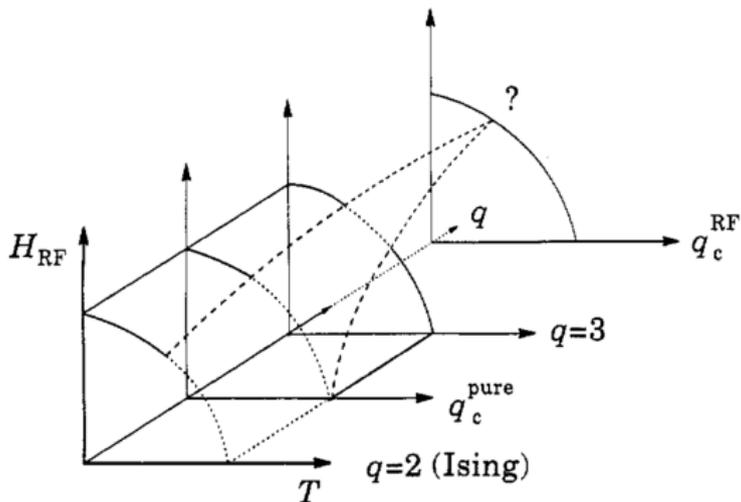
Correlation length: comparison

We find clear evidence for $\xi \sim \exp(A/h^2)$ for the connected and disconnected correlation lengths in the square and triangular lattices.



Random-field Potts model

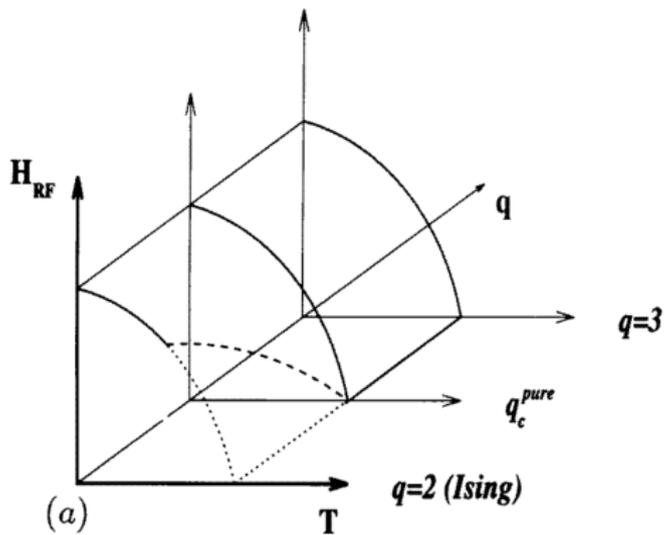
Very little work to date:



Blankschtein, Shapir, Aharony, 1984

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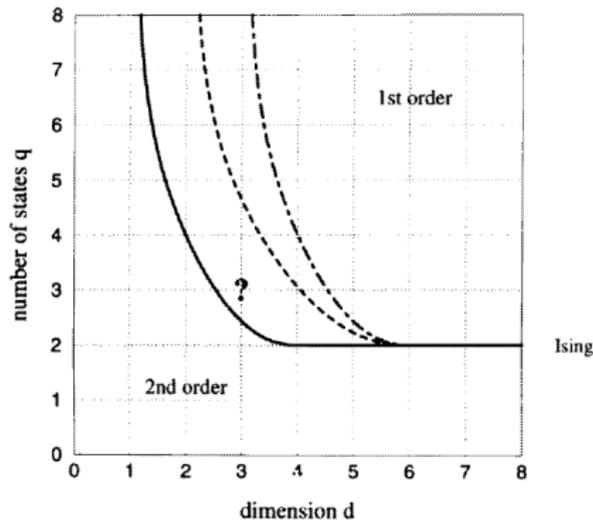
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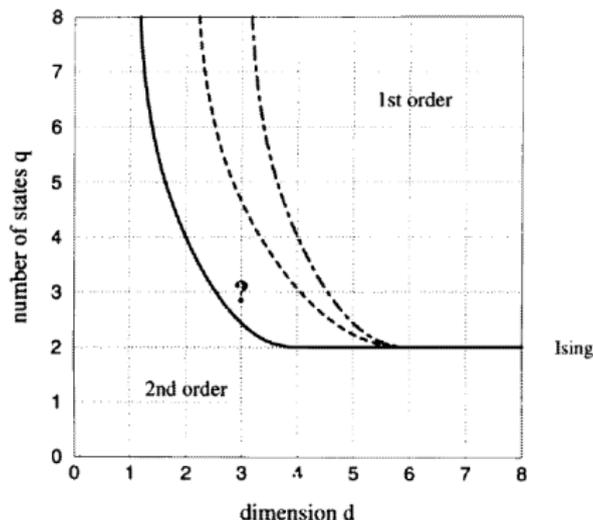
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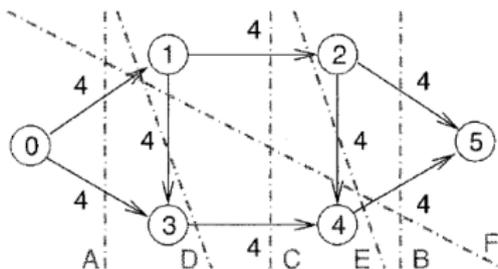
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Most recent study by Eichhorn and Binder (1995/96): possible 2nd order transition for 3D $q = 3$ model.

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Graph cuts and the Potts model

We consider the Hamiltonian

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We need to revert to **approximation methods**.

Approximate graph cuts

Boykov, Veksler and Zabih (2001) propose a method for problems in computer vision:

$$E(\{s_i\}) = \sum_{i,j} V_{ij}(s_i, s_j) + \sum_i D_i(s_i).$$

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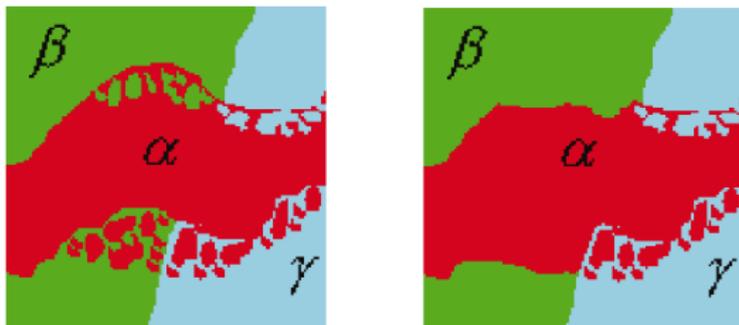
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► **α - β -swap move**

picks two labels $\alpha \neq \beta \in \{0, 1, \dots, q-1\}$ and freeze all labels apart from α and β



Approximate graph cuts

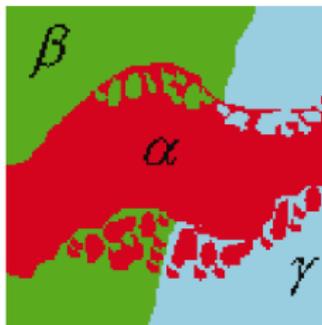
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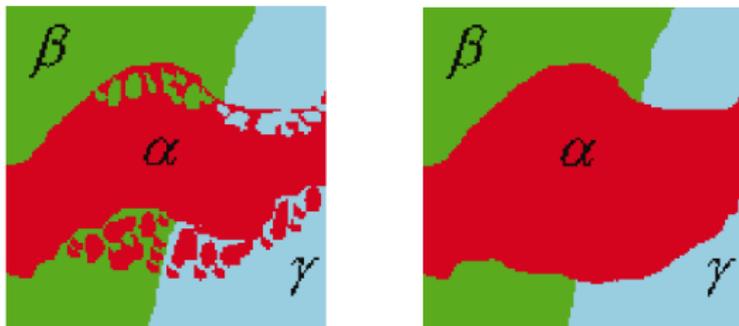
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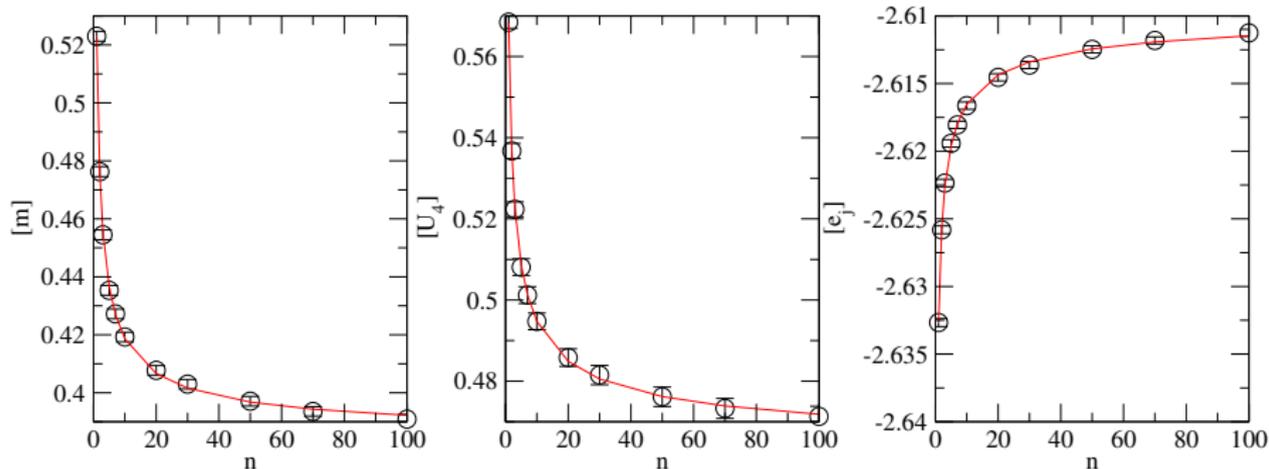


Works well in **computer vision** (paper has 10,000 citations!). How about the RFPM?

Results: 3D $q = 3$ RFPM – initial conditions

Use repeated runs to increase success probabilities.

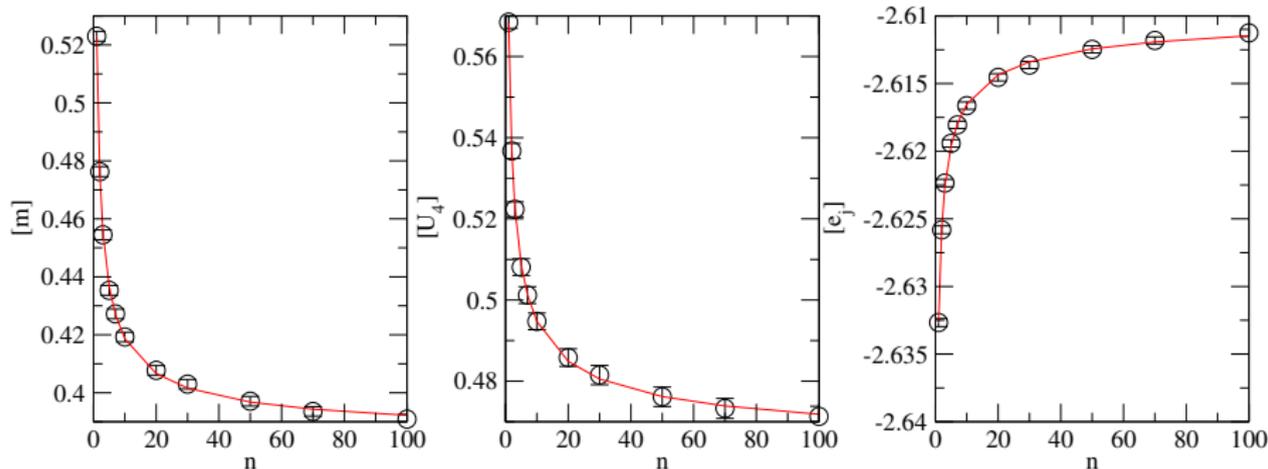
$L = 64, \Delta = 1.7$



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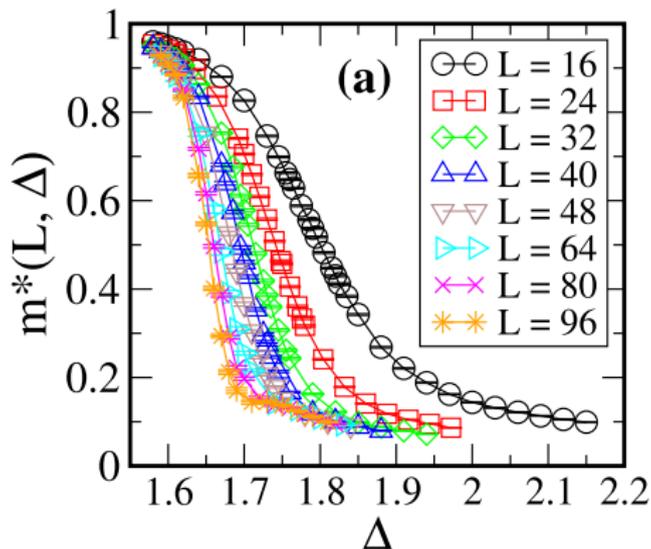


Quantities converge in power laws:

$$\mathcal{O}(n) = an^{-b}(1 + cn^{-e}) + \mathcal{O}^*.$$

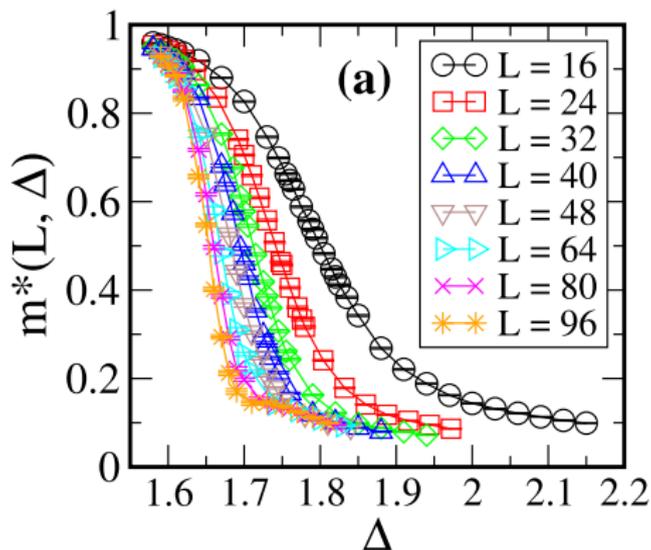
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Sample thermodynamic quantities either for $n = 100$ or extrapolate.



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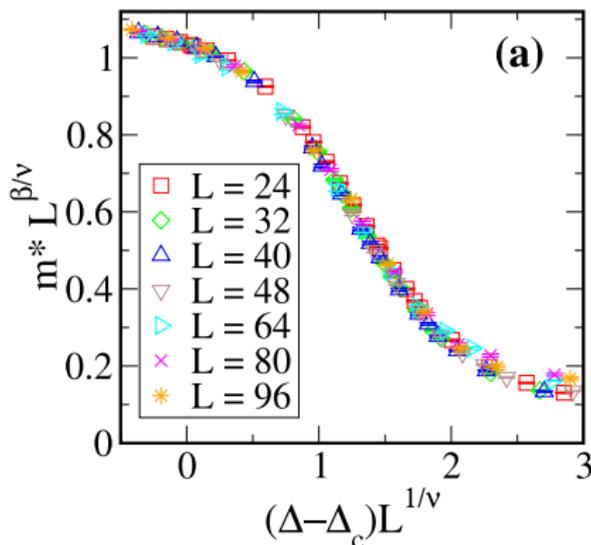


Scaling form of the magnetization:

$$m^*(\Delta, L) = L^{-\beta/\nu} \widetilde{\mathcal{M}} \left[(\Delta - \Delta_c) L^{1/\nu} \right],$$

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n	Δ_c	$1/\nu$	β/ν	$\bar{\gamma}/\nu$	S_1	S_2
1	1.636(2)	0.837(9)	0.0460(9)	2.9084(14)	2.30	2.38
5	1.626(3)	0.812(6)	0.0403(8)	2.9220(15)	1.82	1.69
10	1.623(5)	0.828(15)	0.0387(7)	2.9230(15)	1.28	1.58
50	1.617(4)	0.797(4)	0.0340(8)	2.9323(16)	1.25	1.38
100	1.616(1)	0.774(6)	0.0330(10)	2.9337(15)	1.20	1.36
∞	1.606(3)	0.723(4)	0.0306(23)	2.9402(30)	0.82	0.87

Table: A summary of exponents from the FSS of the $m(L, \Delta, n)$ for finite as well as infinite n . The numbers in the parenthesis denote the error bars in the last significant digit.

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$$m^*(\Delta, L) = L^{-\beta/\nu} \widetilde{\mathcal{M}} \left[(\Delta - \Delta_c) L^{1/\nu} \right],$$

Results: 3D $q = 3$ RFPM – specific heat

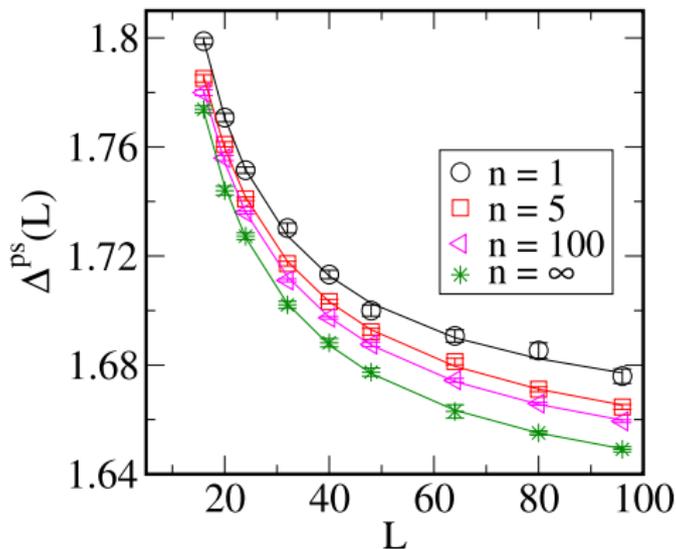
No direct access to fluctuations in ground states. Hence consider

$$C(\Delta) = \frac{\partial[e_J(\Delta)]}{\partial\Delta}.$$

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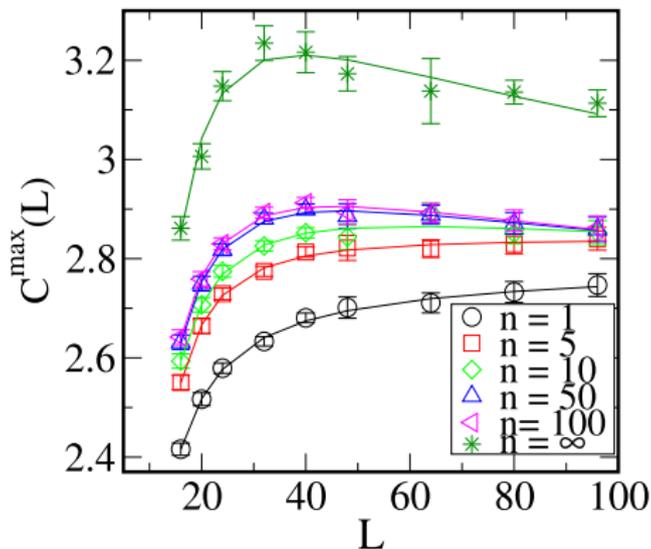
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n	Δ_c	$1/\nu$	α/ν	ω	Q_1	Q_2
1	1.644(6)	0.850(70)	0.023(12)	2.67(87)	0.74	0.71
5	1.626(3)	0.774(32)	-0.002(11)	2.62(68)	0.32	0.70
10	1.621(3)	0.767(25)	-0.019(13)	2.39(61)	0.14	0.52
50	1.620(2)	0.776(21)	-0.046(20)	1.87(53)	0.12	0.50
100	1.620(2)	0.780(21)	-0.049(20)	1.86(52)	0.15	0.49
∞	1.611(4)	0.733(28)	-0.059(20)	2.52(73)	0.14	0.93

Table: A summary of exponents from the fits of the peak positions $\Delta^{\text{ps}}(L, n)$ and the heights of the specific heat $C^{\text{max}}(L, n)$. Q_1 is the quality of the fit for the data of $\Delta^{\text{ps}}(L, n)$, and Q_2 is the quality of the fit for the data of $C^{\text{max}}(L, n)$. The numbers in the parenthesis denote the error bars in the last significant digits.

$$C^{\text{max}}(L) = C_0 + aL^{\alpha/\nu}(1 + bL^{-\omega}).$$

Results: 3D $q = 3$ RFPM – susceptibility

We cannot make use of a fluctuation-dissipation relation as the ground state is unique (for continuous fields). Hence we could rely on

$$\chi^\mu(\Delta) = \left[\frac{\partial M^\mu(\{h_i^\alpha\}, H)}{\partial H} \right]_{H=0}.$$

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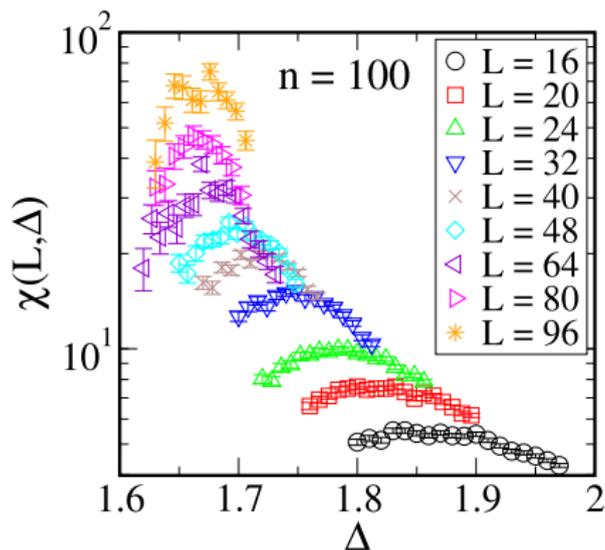
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Without explicitly breaking the symmetry, however, there is no peak in this χ . Scaling arguments imply that one should use a field $H \sim L^{3/2}$.

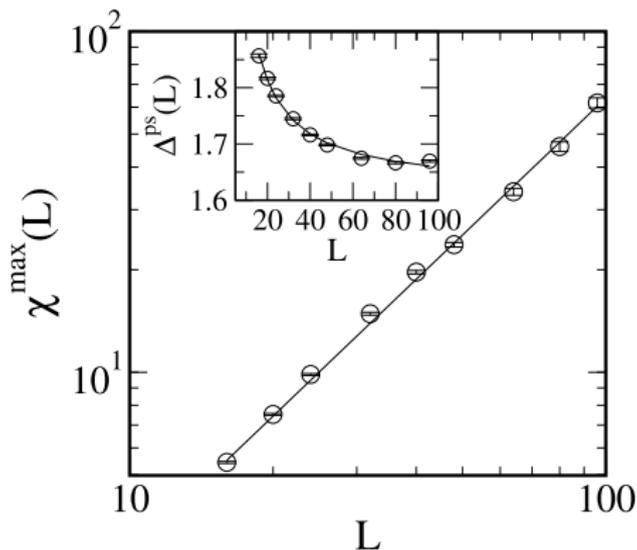
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Consider the scaling form

$$\chi(L, \Delta) = L^{\gamma/\nu} \tilde{\chi} \left[(\Delta - \Delta_c) L^{1/\nu} \right].$$

Results: 3D $q = 3$ RFPM – exponents

In summary, we have the following estimates:

	RFIM	$q = 3$ RFPM
ν	1.38(10)	1.383(8)
α	-0.16(35)	-0.082(28)
β	0.019(4)	0.0423(32)
γ	2.05(15)	2.089(84)
η	0.5139(9)	0.49(6)
$\bar{\eta}$	1.028(2)	1.060(3)
θ	1.487(1)	1.43(6)
$\alpha + 2\beta + \gamma$	2.00(31)	2.08(9)

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2D spin glass:

- ▶ new mapping allows to treat huge systems up to $10\,000 \times 10\,000$ spins
- ▶ strong scaling corrections in frustrated systems
- ▶ connection to stochastic Loewner evolution

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2D RFIM:

- ▶ clear evidence for $\sim \exp(A/h^2)$ scaling predicted by Binder
- ▶ no violation of universality for different lattice structures
- ▶ complete lack of self-averaging of the correlation length

Conclusions

- ▶ hard optimization problems are ubiquitous in statistical mechanics problems
- ▶ for the hardest problems, general-purpose techniques are not sufficient
- ▶ use results from combinatorial problems for non-combinatorial ones

3D $q = 3$ RFPM:

- ▶ approximate ground states from graph cuts and α expansion
- ▶ systematic extrapolation to $n \rightarrow \infty$
- ▶ critical exponents close to, but potentially different from 3D RFIM
- ▶ two-exponent scaling, $\bar{\gamma}/\nu = 2.904(30) \approx 2\gamma/\nu = 3.02(12)$
- ▶ hyperscaling violation, $(d - \theta)\nu = 2.17(8) \approx 2 - \alpha = 2.08(10)$ with $\theta = 1.43(6)$

Acknowledgements

References

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Thank you for your attention!