Universal fragility of spin-glass ground-states under single bond changes

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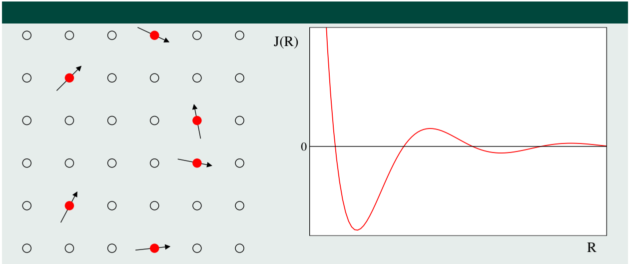
Spin glass history

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

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



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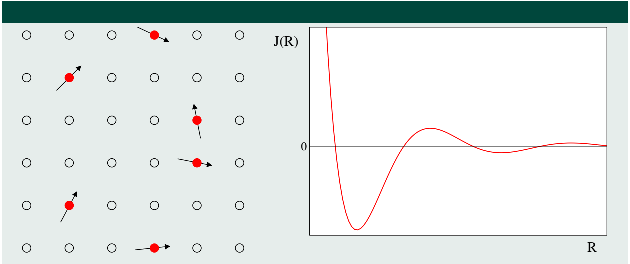
Emergent properties:

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

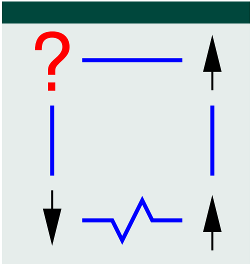


The EA model

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

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{ij}\, s_i s_j, \quad s_i = \pm 1$$

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



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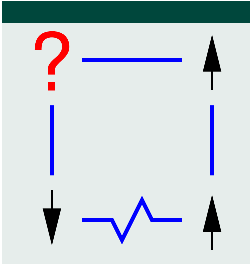
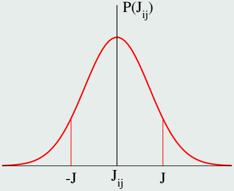
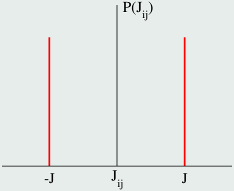


Coupling distributions

Gaussian



bimodal



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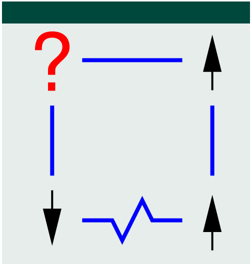


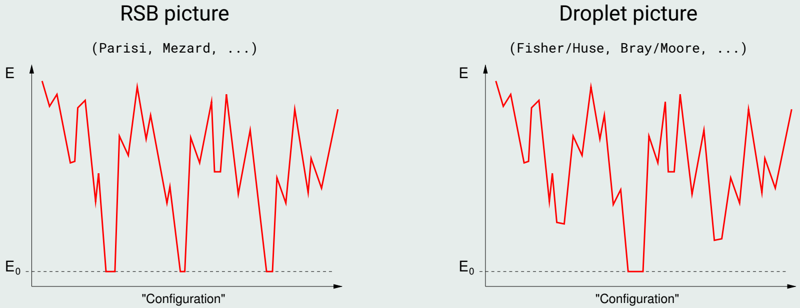
Has been investigated for $\approx$ 30 years, however no agreement on general case. Mean-field model with

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

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

The “pictures”

Behavior of systems in $d = 2$, $d = 3$ incompletely understood, even after 40 years of research.



- **many pure states**
- global (gapless) excitations
- non-self-averaging and continuous distribution of $P(q)$

- **only two pure states**
- global excitations cost an infinite energy
- $P(q)$ is self-averaging

The overlap distribution

The spin-glass order parameter is the overlap between two real replicas,

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

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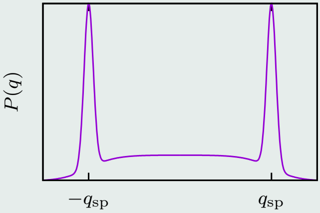
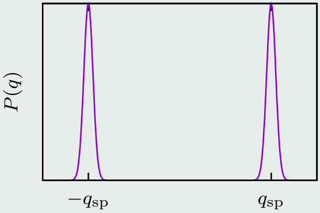
RSB picture

`(Parisi, Mezard, ...)`



Droplet picture

`(Fisher/Huse, Bray/Moore, ...)`



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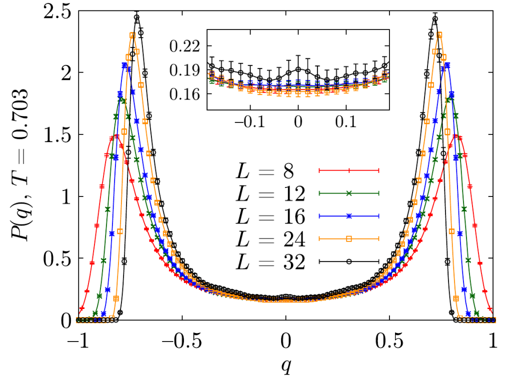

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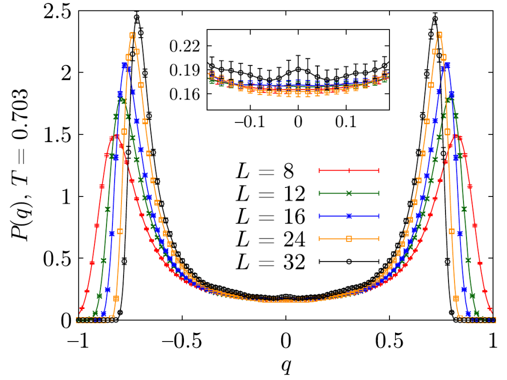

⇒ for $d = 3$, they look more in favor of RSB, but this remains disputed

Spin-glass excitations

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$$\Delta E \sim L^\theta$$

with $\theta > 0$ in 3D.

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RSB theory: excitations with **space-filling** interfaces and

$$\Delta E \sim \mathrm{O}(1)$$

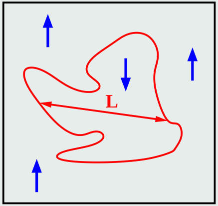
irrespective of L.

Spin stiffness and zero-temperature scaling

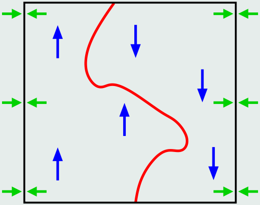
Edwards-Anderson model: $\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij}\, s_i s_j, \quad s_i = \pm 1$

Ferromagnet

(Peierls)



$$\Delta E \sim L^{d-1}$$



Spin glass

(Bray/Moore, 1987)

Distribution of couplings evolving under RG transformations, asymptotic width scales as

$$J(L) \sim J L^{\theta(d)}.$$

Spin-stiffness exponent θ determines lower critical dimension. For $\theta < 0$,

$$\xi \sim T^{-\nu}, \quad \nu = -1/\theta.$$

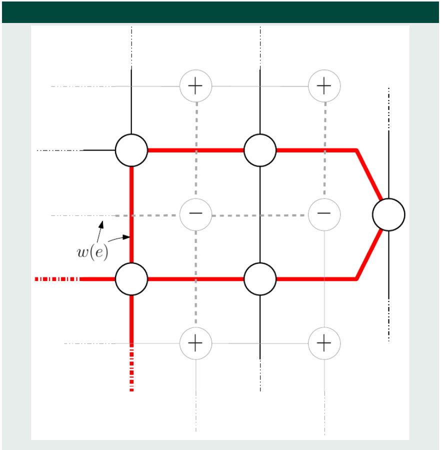
Numerically, θ can be determined from inducing droplets or domain walls with a change of *boundary conditions*,

$$\Delta E = |E_{\mathrm{AP}} - E_{\mathrm{P}}| \sim L^{\theta}.$$

Matching on auxiliary graph

Use mapping of the Ising problem to minimum-cut:

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

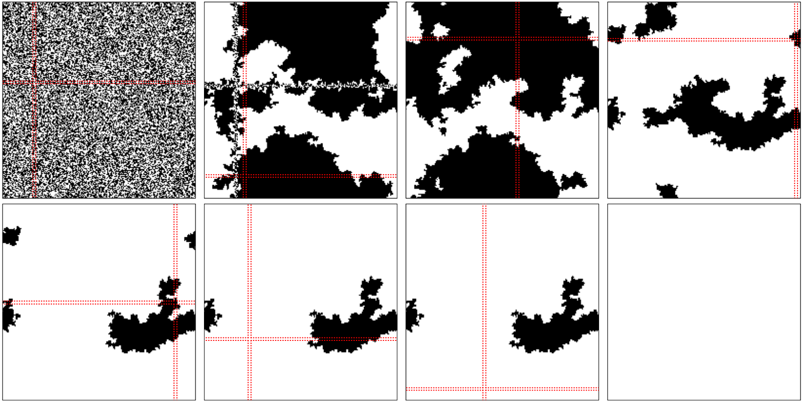


- GS search again corresponds to **minimum-weight perfect matching problem**

  `(Thomas & Middleton, 2007; Pardella & Liers, 2008)`
- matching solution always corresponds to spin configuration for **planar** graphs
- we use a windowing technique to also treat **fully periodic boundaries**
- **space complexity is O(V)**

Windowing technique

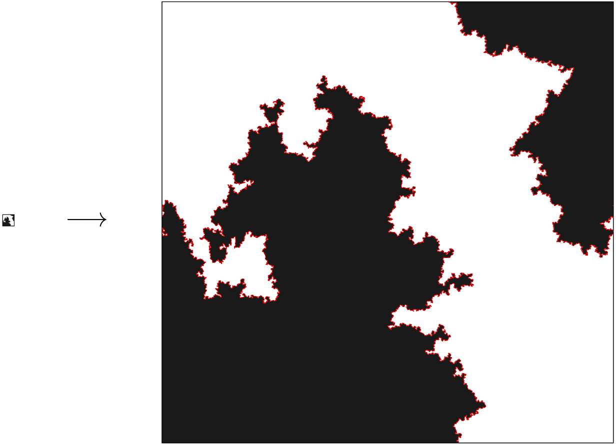
Determine exact ground-states for fully periodic systems in polynomial time.



Ising spin glass in 2D

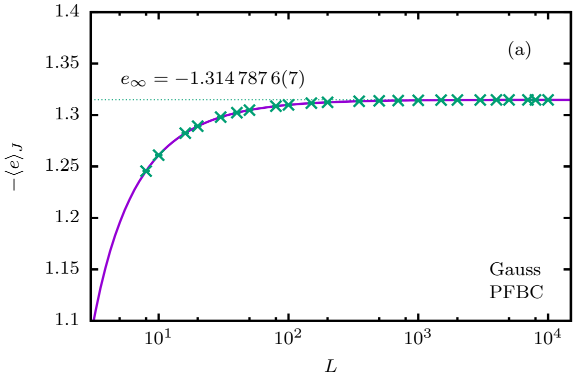
Complex energy landscape leads to slow relaxation: sizes restricted to $L \approx 128$ (MC) or maybe $L = 256$ (GS techniques).

A newly developed **combinatorial optimization** method allows us to treat large system sizes up to $10\,000 \times 10\,000$ spins **exactly** (for $T = 0$).



Ground-state energy

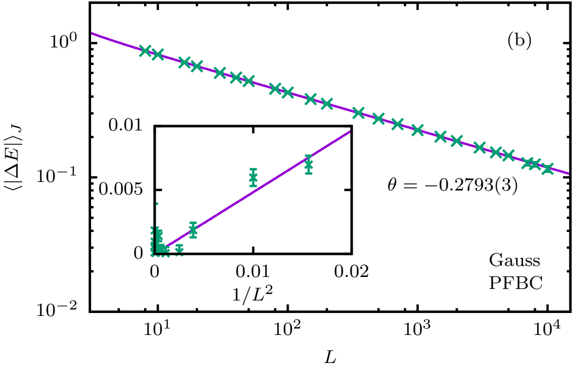
Average ground-state energy per spin.



$$\langle e(L)\rangle_J = e_\infty + \hat{A}_E L^{-(d-\theta)} + (\hat{C}_E - e_\infty/2)L^{-1} - (\hat{C}_E/2)L^{-2}$$

Defect energies

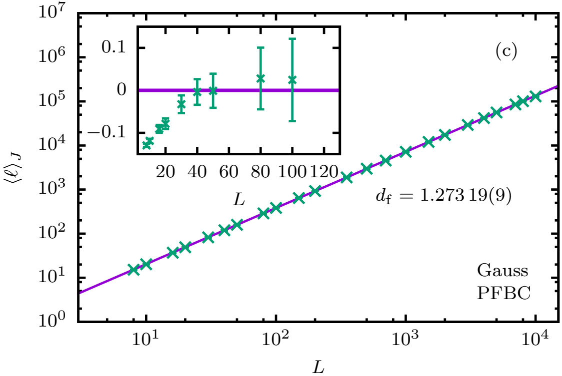
Defect energy.



$$\langle|\Delta E(L)|\rangle_J(L) = A_\theta L^\theta (1 + B_\theta L^{-\omega}) + \frac{C_\theta}{L} + \frac{D_\theta}{L^2} + \cdots ,$$

Fractal dimension

Fractal dimension of domain wall.



$$\langle \ell \rangle_J(L) = A_\ell L^{d_\mathrm{f}}(1 + B_\ell L^{-\omega}) + \frac{C_\ell}{L} + \frac{D_\ell}{L^2} + \cdots .$$

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

$$d_\mathrm{f} = 1 + \frac{3}{4(3+\theta)}.$$

$d_\mathrm{f} = 1.27319(9)$ would imply $\theta = -0.2546(9)$ which is **not compatible** with the direct estimate.

General spin stiffness

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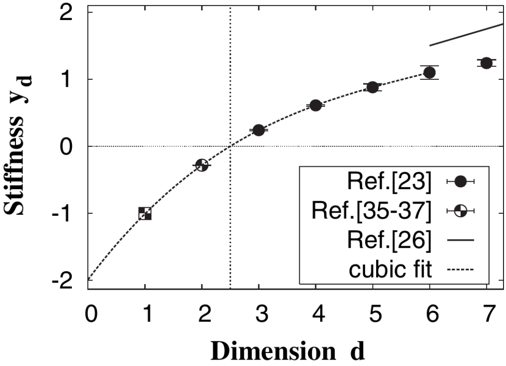

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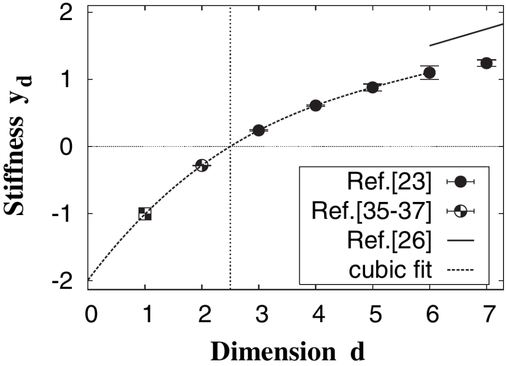

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⇒ not consistent with RSB in $d = 3$ (?)

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$\Rightarrow$ maybe droplets are not the **dominant** excitations?

Zero-energy droplets

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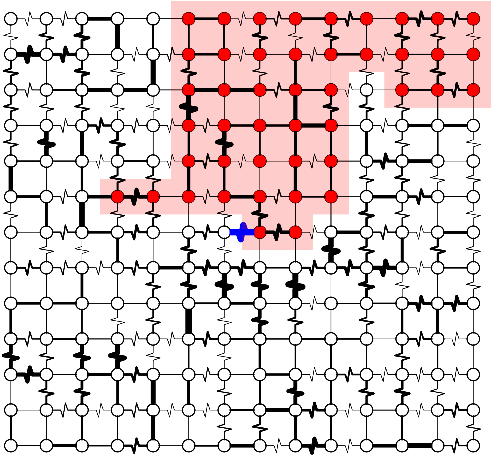
$\Rightarrow$ similar to question of bond chaos, but for a single-bond change

Zero-energy droplets (2)

Illustration of the cluster definition.



ZED energies

Droplet energy distributions depend on dimension and lattice structure.

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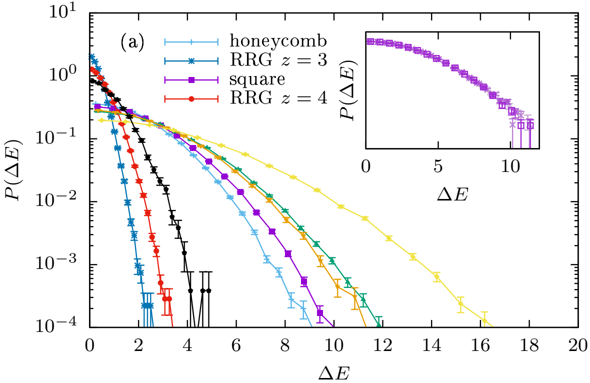

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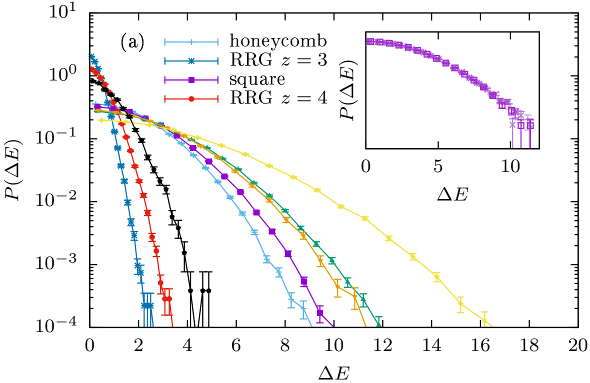

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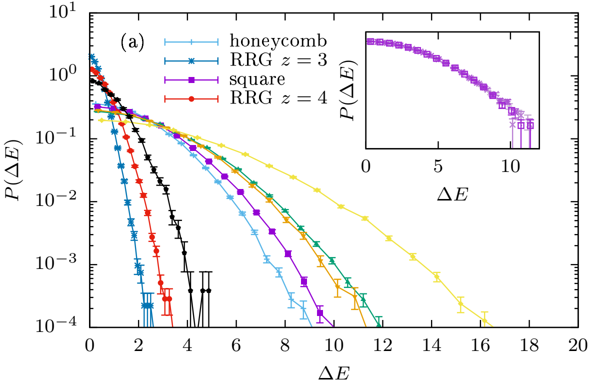

$\Rightarrow$ ZED energies do *not* scale with system size

$\Rightarrow$ in fact ΔE has a rigorous upper bound

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Critical coupling strengths mostly depend on the coordination number.

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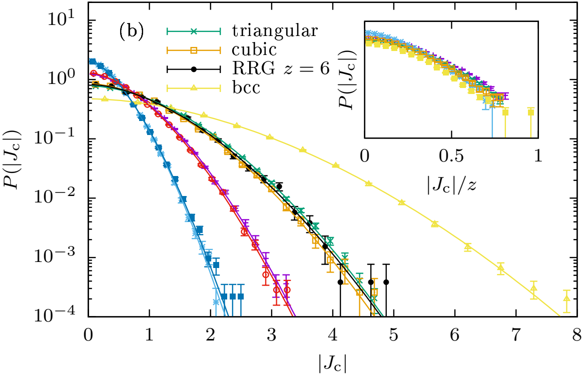

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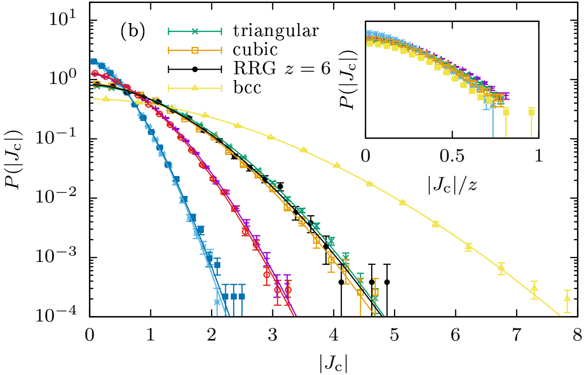

Probability densities of critical couplings follow stretched exponential distributions:

$$P(|J_c|) = k_c \exp(-a_c |J_c|^{\beta_c}),$$

ZED geometry

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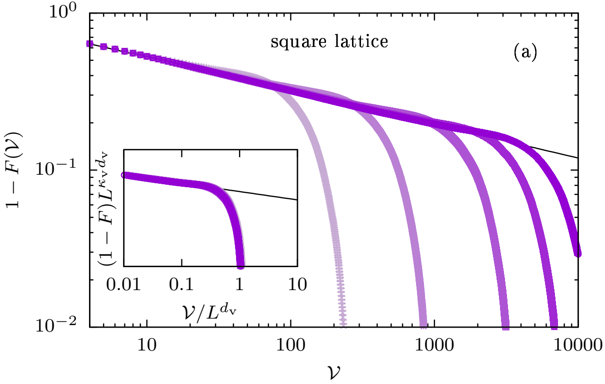

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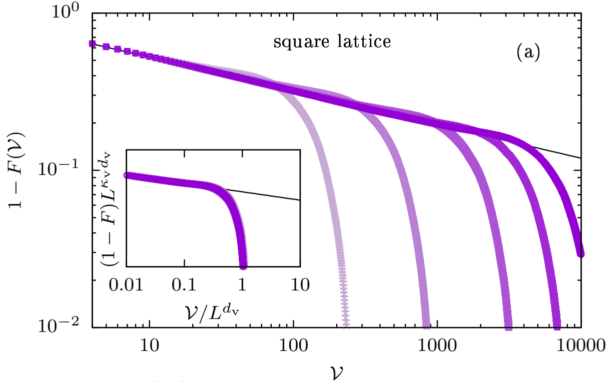

The tails show power-law behavior,

$$P(|D| \geq \mathcal{V}) = 1 - F(\mathcal{V}) = \frac{1}{\mathcal{V}_0^{\kappa_v}} \Omega\left(\frac{\mathcal{V}}{\mathcal{V}_0}\right) \sim k_v \mathcal{V}^{-\kappa_v},$$

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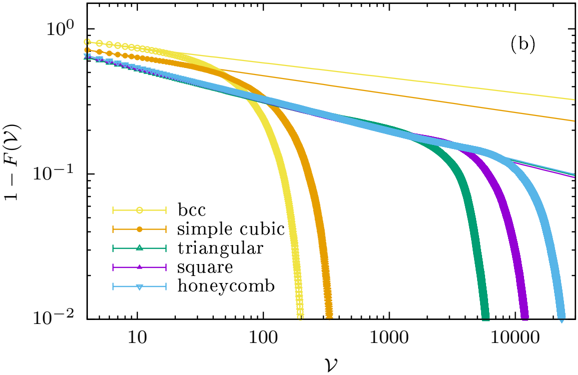

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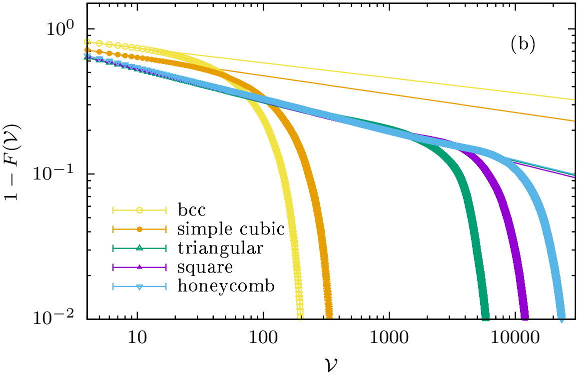

$\Rightarrow$ decay exponent $\kappa_{\rm v}$ only depends on lattice dimension

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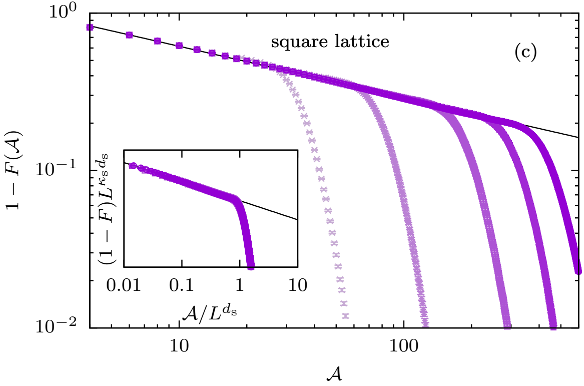

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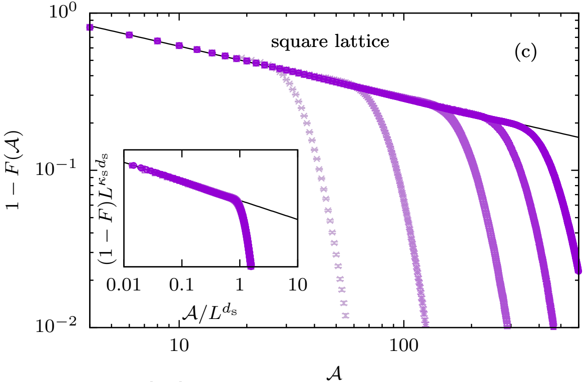

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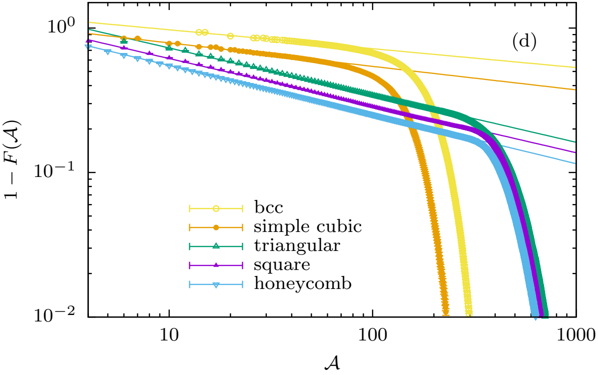

ZED geometry (2)

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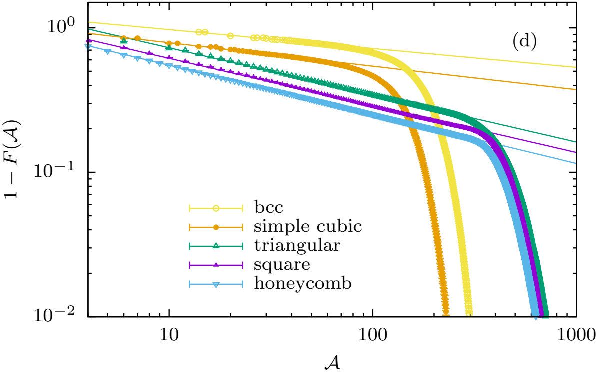

⇒ decay exponent κ_s only depends on lattice dimension

ZED fractality

$P(|D|)$ and $P(|\partial D|)$ follow power laws with exponent $-(\kappa+1)$, such that $\langle\mathcal{V}\rangle$ and $\langle\mathcal{A}\rangle$ **diverge** as long as $\kappa < 1$.

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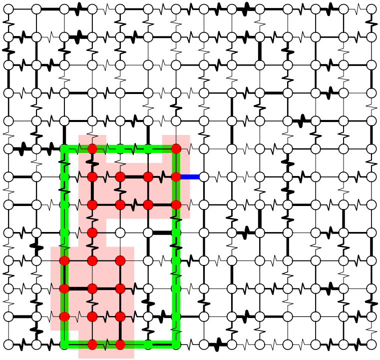

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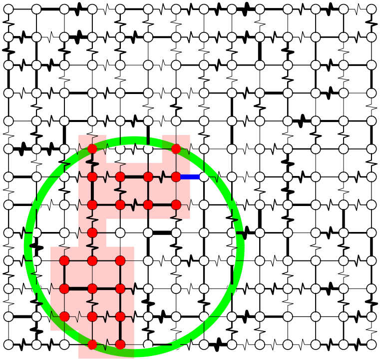

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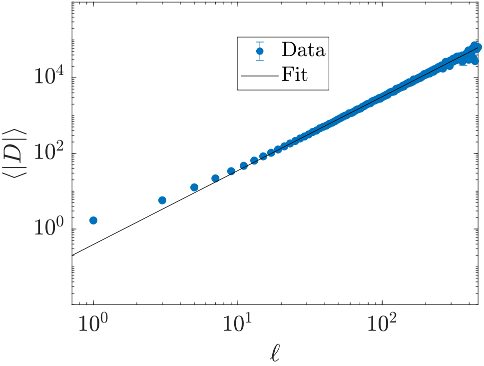

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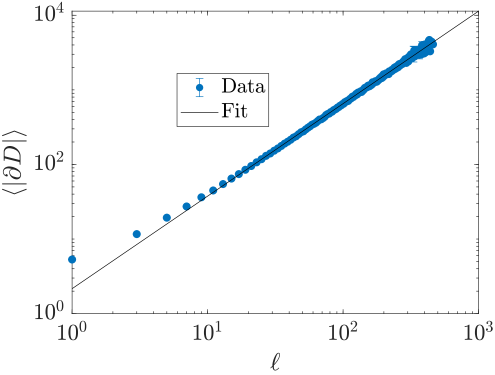

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In two dimensions:

volume fractal dimension: $d_\mathrm{v} = 1.954(8)$

surface fractal dimension: $d_\mathrm{s} = 1.24(2)$

We have that

$$\langle\mathcal{V}\rangle \propto \mathcal{V}_0 \propto L^{d_\mathrm{v}}$$

and

$$\langle\mathcal{A}\rangle \propto \mathcal{A}_0 \propto L^{d_\mathrm{s}}.$$

ZED properties

ZED exponents show universality in 2D, and maybe also in 3D.

Table: Parameters of the stretched exponential form, as well as values of the scaling exponents κ_v for the droplet volume and κ_s for the droplet boundary, for the different lattices considered.

Lattice	a_c	β_c	κ_v	κ_s
honeycomb	$2.76(1)$	$1.59(1)$	$0.212(1)$	$0.34(2)$
square	$1.204(9)$	$1.68(1)$	$0.214(1)$	$0.334(1)$
triangular	$0.532(9)$	$1.78(1)$	$0.21(1)$	$0.327(2)$
simple cubic	$0.61(1)$	$1.74(2)$	$0.127(1)$	$0.163(2)$
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ZEDs are excitations with

- $\mathrm{O}(1)$ energy
- fractal dimension $d_{\mathrm{v}} \lesssim d$ and $d-1 < d_{\mathrm{s}} < d$ (in $d=2$), i.e., not space-filling domain walls

TNT and chaotic pairs

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Conclusions

Domain walls:

- new techniques allow to study systems up to $10\,000 \times 10\,000$ spins
- windowing method enables ground-state calculations for toroidal graphs
- careful FSS analysis yields $e_\infty = -1.3147876(7)$, $\theta = -0.2793(3)$ and $d_\mathrm{f} = 1.27319(9)$ for the Gaussian model

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Zero-energy droplets:

- SG ground states are highly fragile with respect to single-bond perturbations
- ZEDs are extended excitations with volumes and surface areas diverging with system size
- ZED energies are strictly bounded, i.e., O(1), also in 3D
- fractal dimensions $d_\mathrm{v} \approx 2$ and $d_\mathrm{s} = 1.24(2)$ in 2D
- conventional droplets are *not* the lowest-energy extensive excitations in 3D
- these results point towards an intermediate picture between RSB and droplet theory

`H. Khoshbakht and MW, Phys. Rev. B 97, 064410 (2018)`
`M. Shen, G. Ortiz, Y.-Y. Liu, MW, and Z. Nussinov, arXiv:2305.10376 (2023)`