Critical behaviour of disordered Potts models

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- Introduction of the model
- Perturbative results
- Observables
- Analysis techniques
- Numerical results for the first order regime in 2D
- ... and in 3D ?
- Conclusions

section zero

Definition of the critical exponents:

	critical exponents
physical quantity	singularity
specific heat	$C_v(T) \sim \|T - T_c\|^{-\alpha}$
order parameter	$m(T) \sim \|T - T_c\|^{\beta}, \quad T < T_c$
susceptibility	$\chi(T) \sim \|T - T_c\|^{-\gamma}$
critical isotherm	$m_{T_c}(h) \sim \|h\|^{1/\delta}$
correlation length	$\xi(T) \sim \|T - T_c\|^{-\nu}$
correlation function	$\langle \mathbf{s}(\mathbf{r}_1) \cdot \mathbf{s}(\mathbf{r}_2) \rangle \sim \|\mathbf{r}_1 - \mathbf{r}_2\|^{-(d-2+\eta)}, \quad T = T_c$
	$\langle \mathbf{s}(\mathbf{r}_1) \cdot \mathbf{s}(\mathbf{r}_2) \rangle \sim \mathrm{e}^{\|\mathbf{r}_1 - \mathbf{r}_2\|/\xi(T)}, \quad T > T_c$
	$\langle \mathbf{s}(\mathbf{r}_1) \cdot \mathbf{s}(\mathbf{r}_2) \rangle \sim m^2(T) + \mathrm{e}^{\|\mathbf{r}_1 - \mathbf{r}_2\|/\xi(T)}, \quad T < T_c$

Here we usually deal with $x_\sigma = \beta/\nu$ and $x_\varepsilon = (1 - \alpha)/\nu$.

Experimental results

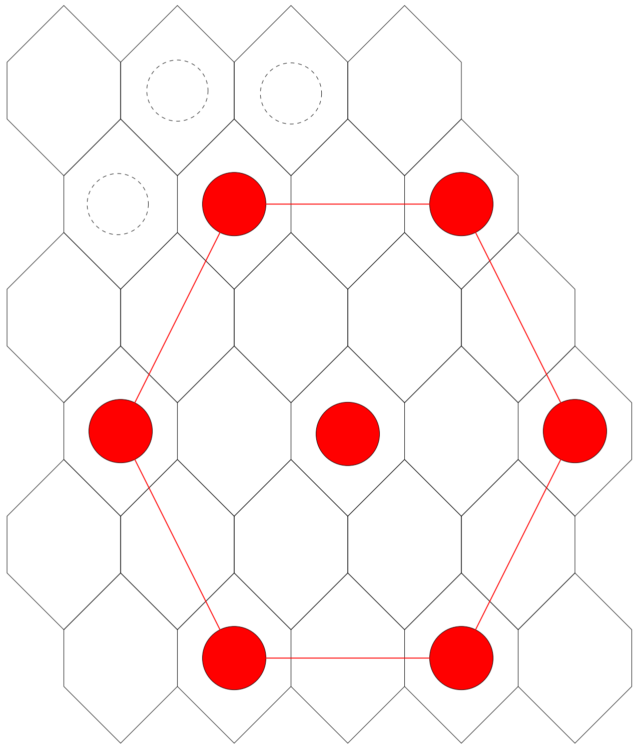
- Potts universality class
- Role of disorder

Experimental results

Order-disorder transitions of adsorbed atomic layers belong to different $2D$ universality classes.

Ex. The $(2 \times 2)-$2H/Ni(111) transition of hydrogen adsorbed on the (111) surface of Ni belongs to the $2D$ four-state Potts model universality class, (the ground state stable at low temperatures has a four-fold degenaracy due to the four possible coverings of the ad-atoms at the (111) surface).

Experimental results



Experimental results

Expected exponents are theoretical values of $q = 4$ PM

$$\beta = 1/12 \simeq 0.083,$$

$$\gamma = 7/6 \simeq 1.167,$$

$$\nu = 2/3 \simeq 0.667.$$

Experimental results

LEED experiments: measure exponents through the diffracted intensity $I(\mathbf{q})$.

$=$ two-dimensional Fourier transform of the pair correlation function of ad-atom density.

Long range fluctuations produce an isotropic Lorentzian with peak intensity given by the susceptibility and width given by inverse correlation length.

Long range order gives a background proportional to order parameter squared:

$$I(\mathbf{q}) = \langle m^2 \rangle \delta(\mathbf{q} - \mathbf{q}_0) + \frac{\chi}{1 + \xi^2(\mathbf{q} - \mathbf{q}_0)^2}.$$

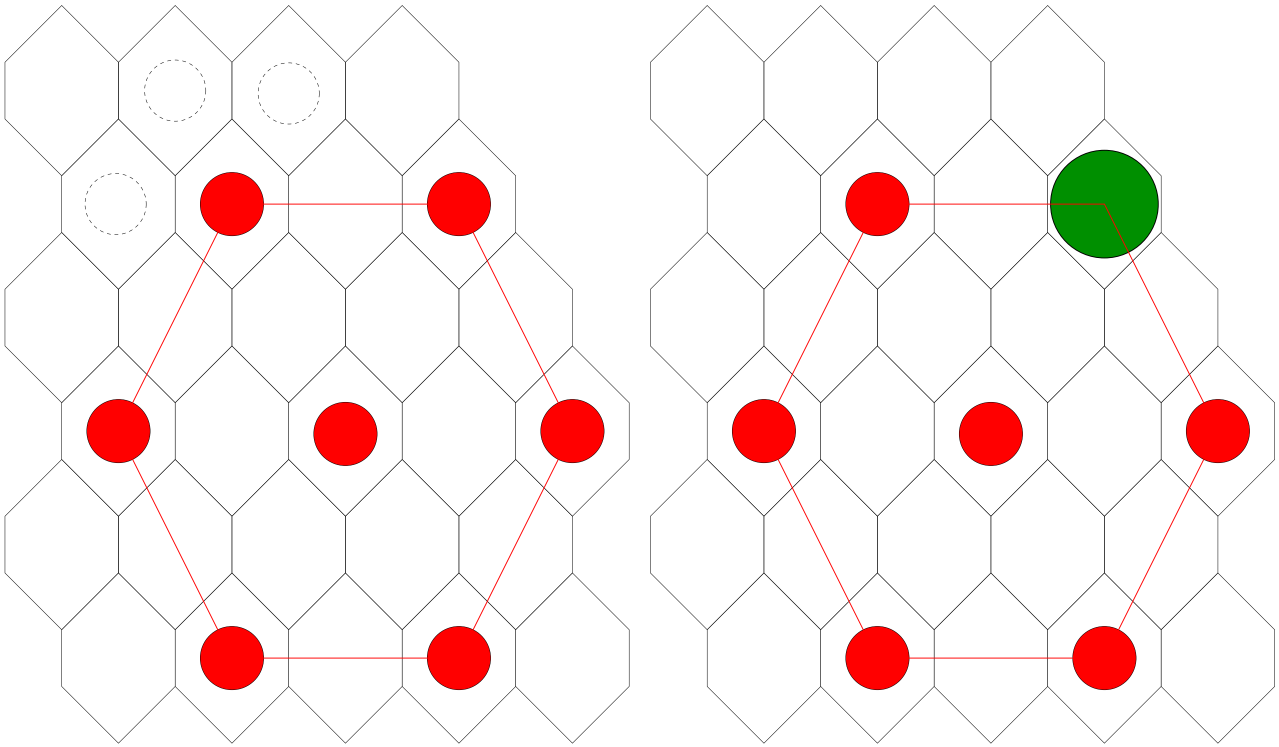
Experimental results

The following exponents were thus measured

$$\beta = 0.11 \pm 0.01, \ \gamma = 1.2 \pm 0.1, \ \nu = 0.68 \pm 0.05$$

in correct agreement with 4-state Potts values (the small deviation, especially for the exponent β, is attributed to the logarithmic corrections to scaling of the pure 4-state Potts model.

Experimental results



Experimental results

Presence of intentionally added oxygen impurities. Mobility of oxygen atoms is low enough at hydrogen order-disorder transition critical temperature that they essentially represent quenched impurities randomly distributed in the hydrogen layer. The exponents become

$$\beta = 0.135 \pm 0.010, \ \gamma = 1.68 \pm 0.15, \ \nu = 1.03 \pm 0.08,$$

$$(\beta = 0.11 \pm 0.01, \ \gamma = 1.2 \pm 0.1, \ \nu = 0.68 \pm 0.05)$$

$\rightarrow$ modification of universality class.

The model

- Different types of disorder
- The Potts model

The model

Since universality is expected to hold, the detailed structure of the Hamiltonian should not play any important role in universal quantities like critical exponents.

Randomness:

$$-\beta\mathcal{H} = \sum_{(ij)} K_{ij}\mathbf{s}_i\mathbf{s}_j + \sum_i \mathbf{H}_i\mathbf{s}_i + \sum_i D(\mathbf{s}_i\mathbf{n}_i)^2 + \ldots$$

where K_{ij}, $\mathbf{H}_i$, or $\mathbf{n}_i$ are independent random quenched variables drawn from some probability distributions $P[K_{ij}]$, $P[\mathbf{H}_i]$, or $P[\mathbf{n}_i]$.

Usually, uncorrelated quenched random variables,
$\overline{K_{ij}} \equiv \int K\mathcal{P}[K]\mathrm{d}K = K_0$, and $\overline{K_{ij}K_{kl}} = \Delta\delta_{ik}\delta_{jl}$.

The model

Special cases of probability distributions e.g.:

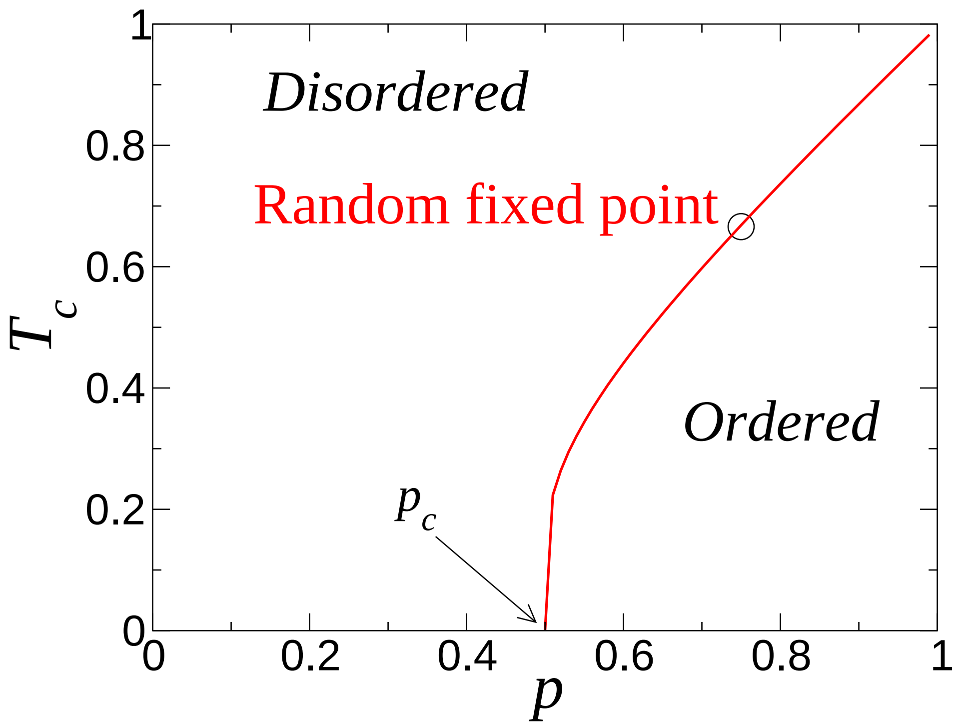
i) *dilution problems*, non magnetic impurities are randomly distributed on the bonds or sites of the lattice,

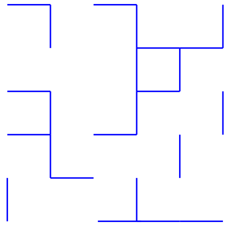
$$\mathcal{P}[K_{ij}] = \prod_{(ij)} [p\delta(K_{ij} - K) + (1 - p)\delta(K_{ij})],$$

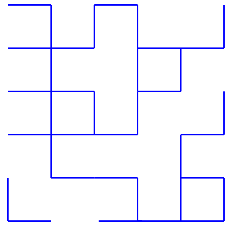
ii) *binary distributions*, e.g. disordered alloy of two magnetic species

$$\mathcal{P}[K_{ij}] = \prod_{(ij)} [p\delta(K_{ij} - K) + (1 - p)\delta(K_{ij} - Kr)],$$

The model







The model

The Potts model:

The 2-dimensional q-state Potts model is defined by:

$$-\beta\mathcal{H} = \sum_{(i,j)} K_{ij}\delta_{\sigma_i,\sigma_j}$$

$\{\sigma_i\}$ can take q values $0, 1, \ldots q-1$ and the “exchange couplings” $K_{ij} = J_{ij}/k_B T$ are quenched independent random variables.

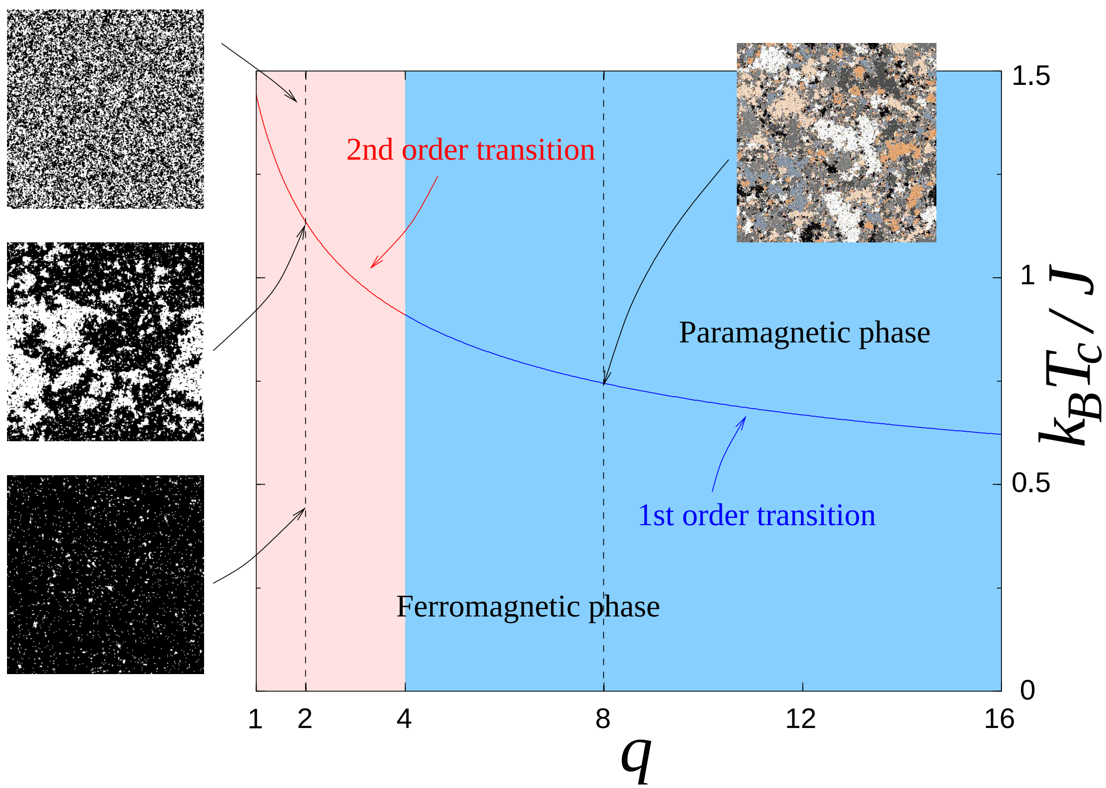
The model

The $q-$state Potts model is the natural candidate for the investigations of influence of disorder - the pure model exhibits two different regimes:

- a second order phase transition when $q \leq 4$ ($2D$)
- a first order one for $q > 4$ ($2D$).

In $3D$, ordering is easier and the transition becomes weakly first-order at $q = 3$ already.

The model



2nd order transition
1st order transition
Paramagnetic phase
Ferromagnetic phase
1.5
1
0.5
0
1
2
4
8
12
16
q
$k_B T_c / J$

Perturbative results

- Replica limit and Harris criterion
- First-order transitions
- Perturbative expansions
- Replica symmetry and replica symmetry breaking

Perturbative results

For a specific disorder realization $[K_{ij}]$, the Hamiltonian, P.F. and free energy are

$$
\begin{aligned}
-\beta\mathcal{H}[K_{ij},\sigma_i] &= \sum_{(ij)}(K_0+\delta K_{ij})\delta_{\sigma_i,\sigma_j}, \\
Z[K_{ij}] &= \int \mathcal{D}[\sigma_i]\mathrm{e}^{-\beta\mathcal{H}[K_{ij},\sigma_i]}, \\
F[K_{ij}] &= -k_BT\ln Z[K_{ij}].
\end{aligned}
$$

quantities of interest $\rightarrow$ average over the distribution $\mathcal{P}[K_{ij}]$,

$$
F = \overline{F[K_{ij}]} = -k_BT\int \mathcal{D}[K_{ij}]\mathcal{P}[K_{ij}]\ln Z[K_{ij}].
$$

Perturbative results

Averaging the log of P.F. is possible through the identity

$$\ln Z = \lim_{n \to 0} \frac{1}{n}(Z^n - 1),$$

which requires n copies (with labels α) with the same $[K_{ij}]$,

$$(Z[K_{ij}])^n = \int \left(\prod_{\alpha=1}^{n} \mathcal{D}[\sigma_i^{(\alpha)}] \right) \mathrm{e}^{-\beta \sum_\alpha \mathcal{H}[K_{ij}, \sigma_i^{(\alpha)}]},$$

and then to perform integrations,

$$\overline{\mathrm{e}^{-X}} = \mathrm{e}^{-\bar{X} + \frac{1}{2}(\overline{X^2} - \bar{X}^2) + \dots},$$

Perturbative results

leading to

$$\overline{(Z[K_{ij}])^n} = \int \left(\prod_{\alpha=1}^{n} \mathcal{D}[\sigma_i^{(\alpha)}] \right)$$

$$\times e^{-\sum_\alpha (K_0 + \overline{\delta K}) \sum_{(ij)} \delta_{\sigma_i^{(\alpha)}, \sigma_j^{(\alpha)}}}$$

$$\times e^{\sum_{\alpha \neq \beta} (\overline{\delta K^2} - \overline{\delta K}^2) \sum_{(ij)} \delta_{\sigma_i^{(\alpha)}, \sigma_j^{(\alpha)}} \delta_{\sigma_i^{(\beta)}, \sigma_j^{(\beta)}} + \ldots}$$

Perturbative results

Leading term: $\overline{\delta K_{ij}}$ has RG eigenvalue $y_t = d - x_\varepsilon$ and corresponds to a shift of the transition temperature (relevant effect).

Next term: $\overline{\delta K^2} - \overline{\delta K}^2$ has RG eigenvalue $y_H = d - 2x_\varepsilon$ and all following terms are irrelevant[a].

[a] The leading (unperturbed) term is written in the continuum limit as $-\beta\mathcal{H}_c = m_0 \int \sum_\alpha \varepsilon_\alpha(\mathbf{r})\mathrm{d}^2 r$ where m_0 stands for $K_0 + \overline{\delta K}$ while the perturbation is written $g_0 \int \sum_{\alpha \neq \beta} \varepsilon_\alpha(\mathbf{r})\varepsilon_\beta(\mathbf{r})\mathrm{d}^2 r$ with g_0 corresponding to $\overline{\delta K^2} - \overline{\delta K}^2$.

Perturbative results

Using hyperscaling relation, the Harris scaling dimension of disorder is rewritten

$$y_H = \alpha/\nu.$$

- disorder is a relevant perturbation when the specific heat exponent α of the pure system is positive
- it is irrelevant (and universal properties are thus unaffected by randomness) when α is negative.
- In borderline case $\alpha = 0$, randomness is marginal to leading order, e.g. RBIM in 2D.

Perturbative results

First-order transitions were considered later (Imry and Wortis, Aizenman and Wehr, Hui and Berker).

Intuitively, the existence of a latent heat corresponds to a discontinuity of the energy density $\rightarrow$ vanishing energy density scaling dimension.

Disorder is always relevant in this sense.

Perturbative results

$\overline{Z^n}$ couples the replicas via energy-energy interactions

$$\sum_{\alpha \neq \beta} (\overline{\delta K^2} - \overline{\delta K}^2) \sum_{\mathbf{r}} \varepsilon_{\alpha}(\mathbf{r}) \varepsilon_{\beta}(\mathbf{r})$$

which are treated as a perturbation around the pure fixed point ($q \leq 4$)[a].

[a] $\varepsilon_\alpha(\mathbf{r})$ is a short notation for $\delta_{\sigma_i^{(\alpha)} \sigma_j^{(\alpha)}}$. Second cumulant of the coupling distribution will be denoted g_0

Perturbative results

Two different schemes:

i) *replica symmetric scenario*, where all the replicas are coupled through the same interaction strength,

$$\sum_{\alpha\neq\beta} g_0 \sum_{\mathbf{r}} \varepsilon_\alpha(\mathbf{r})\varepsilon_\beta(\mathbf{r}),$$

ii) *replica symmetry breaking scenario*, where the coupling between replicas are replica-dependent,

$$\sum_{\alpha\neq\beta} g_{\alpha\beta} \sum_{\mathbf{r}} \varepsilon_\alpha(\mathbf{r})\varepsilon_\beta(\mathbf{r}).$$

Perturbative results

- consider $2D$ Potts model with weak bond randomness,
- compute the scaling dimensions $x'_\sigma(n)$ and $x'_\varepsilon(n)$ around Ising model conformal field theory,
- take the replica limit $n \to 0$.

Expansions performed in terms of the disorder strength

$$\overline{\delta K_{ij}^2} - \overline{\delta K_{ij}}^2,$$

and exponents are given in powers of $y_H = \alpha/\nu$.

Perturbative results

For scaling operator ϕ, the perturbed correlation function $\langle\phi(0)\phi(\mathbf{R})\rangle_g$ corresponds, in the limit $n \to 0$, to the average correlator $\overline{\langle\phi(0)\phi(\mathbf{R})\rangle}$.

$$\langle\phi(0)\phi(\mathbf{R})\rangle_g = \frac{\mathrm{Tr}\,\phi(0)\phi(\mathbf{R})\mathrm{e}^{-\beta(\mathcal{H}_c+\mathcal{H}_g)}}{\mathrm{Tr}\,\mathrm{e}^{-\beta(\mathcal{H}_c+\mathcal{H}_g)}}$$

where perturbation term $-\beta\mathcal{H}_g = g_0 \int \sum_{\alpha\neq\beta} \varepsilon_\alpha(\mathbf{r})\varepsilon_\beta(\mathbf{r})\mathrm{d}^2 r$ acts on 'critical' Hamiltonian

$-\beta\mathcal{H}_c = m_0 \int \sum_\alpha \varepsilon_\alpha(\mathbf{r})\mathrm{d}^2 r + h_0 \int \sum_\alpha \sigma_\alpha(\mathbf{r})\mathrm{d}^2 r$.

Perturbative results

Using

$$e^{-\beta(\mathcal{H}_c+\mathcal{H}_g)} \simeq (1 - \beta\mathcal{H}_g + \ldots)e^{-\beta\mathcal{H}_c}$$

expansion in terms of unperturbed correlators:

$$\begin{aligned}\langle\phi(0)\phi(\mathbf{R})\rangle_g &= \langle\phi(0)\phi(\mathbf{R})\rangle_0 - \beta\langle\mathcal{H}_g\phi(0)\phi(\mathbf{R})\rangle_0 \\ &+ \frac{1}{2}\beta^2\langle{\mathcal{H}_g}^2\phi(0)\phi(\mathbf{R})\rangle_0 + \ldots\end{aligned}$$

and renormalization of coupling constant follows.

Perturbative results

RS: Collecting results of Dotsenko and co-workers, new thermal and magnetic scaling dimensions (with primes) in terms of the original ones (unprimed) are:

$$x'_\varepsilon = x_\varepsilon + \frac{1}{2} y_H + \frac{1}{8} y_H^2 + O(y_H^3)$$

$$x'_\sigma = x_\sigma + \frac{1}{32} \frac{\Gamma^2(-\frac{2}{3})\Gamma^2(\frac{1}{6})}{\Gamma^2(-\frac{1}{3})\Gamma^2(-\frac{1}{6})} y_H^3 + O(y_H^4)$$

$$y_H = d - 2x_\epsilon(\text{pure}) \propto q - 2.$$

Perturbative results

RSB: leads to different fixed point structure.

$g_{\alpha\beta}$ now depends on the pair indices, leading to a modified thermal exponent

$$x''_{\varepsilon} = x_{\varepsilon} + \frac{1}{2} y_H + O(y_H^3),$$

while to y_H^3 order, the magnetic scaling index remains the same as in the replica symmetric scenario.

Perturbative results

Are these effects measurable?

At $q = 3$ we have $x_\varepsilon = 4/5$ and $y_H = 2/5$.

Scheme	Scaling dimensions				
	x_σ	x_ε	x_{σ^2}	x_{σ^0}	x_{ε^0}
Pure system	0.13333	0.800	0.13333	0.13333	0.800
RS	0.13465	1.000	0.11761	0.18303	1.090
RSB	0.13465	1.020	0.12011	–	–
	!!!	2.5 %	1.9 %		

Observables

- Monte Carlo versus transfer matrices
- Physical quantities

Observables

Monte Carlo simulations

Main recipe of cluster algorithms is identification of clusters of sites using a bond percolation process connected to the spin configuration. Spins of clusters are independently flipped. A cluster algorithm is efficient if percolation threshold coincides with the transition point of the spin model, which guarantees that clusters of all sizes will be updated in a single MC sweep.

For Potts model, percolation process involved is through the mapping onto the *random graph model* (Fortuin-Kasteleyn representation).

Observables

Monte Carlo simulations

- *Order parameter density:*

$$M = \langle \sigma \rangle, \quad \sigma = \frac{q\rho_{\mathrm{max}} - 1}{q-1},$$

where ρ_{max} is fraction of spins in majority orientation. To obtain the *local order parameter* $\langle \sigma(i) \rangle$ at site i, it is counted 1 when the spin at site i is in the majority state and 0 otherwise.

Observables

- *Susceptibility:*

$$k_B T \chi = L^d (\langle \sigma^2 \rangle - \langle \sigma \rangle^2).$$

- *Energy density:*

$$E = \langle \varepsilon \rangle, \quad \varepsilon = \frac{1}{2L^2} \sum_{(i,j)} K_{ij} \delta_{\sigma_i,\sigma_j}.$$

- *Specific heat:*

$$C/k_B = L^d (\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2).$$

Observables

- *Correlation functions:* connected spin spin correlation function $G_\sigma(i,j) = \langle\sigma(i)\sigma(j)\rangle - \langle\sigma^2\rangle$ at criticality obtained by the estimator of the paramagnetic phase,

$$\frac{q\langle\delta_{\sigma_i,\sigma_j}\rangle - 1}{q-1},$$

i.e. probability that spins at sites i and j belong to the same finite cluster.

Observables

All these quantities are then averaged over the disorder realisations

$$\overline{\langle \ldots \rangle} = \int \langle \ldots \rangle \mathcal{P}[\langle \ldots \rangle] \mathrm{d} \langle \ldots \rangle .$$

Observables

Transfer matrix technique

A unique connectivity label $\eta_i = \eta$ attributed to all sites i interconnected through a part of the lattice previously built on a strip of length m. In connectivity space, $|Z(m)\rangle$ is a vector whose components are the partial partition function $Z(m, \{\eta_i\}_m)$ whose connectivity on last row is $\{\eta_i\}_m$.

The connectivity transfer matrix: $|Z(m+1)\rangle = \mathbf{T}_m |Z(m)\rangle$ and partition function of strip of length m:

$$|Z(m)\rangle = \prod_{k=1}^{m-1} \mathbf{T}_k |Z(1)\rangle.$$

Observables

For a pure system, $Z = \mathrm{Tr}\,\mathbf{T}^m$,

$\mathbf{T}^m = \sum_n |t_n\rangle t_n^m \langle t_n| \rightarrow |t_0\rangle t_0^m \langle t_0|$,

$$f_0 = -\frac{1}{m} k_B T \ln Z = -k_B T \ln t_0,$$

Quenched free energy density: Lyapunov exponent of product of infinite number of transfer matrices $\mathbf{T}_k$

$$\overline{f_L} = -k_B T \Lambda_0(L),$$

$$\Lambda_0(L) = \lim_{m\to\infty} \frac{1}{m} \ln \left\| \left(\prod_{k=1}^{m} \mathbf{T}_k \right) |v_0\rangle \right\|,$$

$|v_0\rangle$ is unit initial vector.

Analysis of data

- Temperature dependence
- FSS
- Short-time dynamics
- Conformal mappings

Analysis of data

Temperature dependence

According to their definition, critical exponents can be obtained from temperature-dependence study, e.g.

$$M(t) = B|t|^{\beta}(1 + \ldots), \quad t = K_c - K < 0.$$

Technically, one uses an effective temperature-dependent exponent,

$$\beta_{\text{eff}}(t) = \frac{\mathrm{d}\ln M(t)}{\mathrm{d}\ln|t|}, \quad \beta = \lim_{t \to 0} \beta_{\text{eff}}(t).$$

Analysis of data

Finite-size scaling

Standard Finite-Size Scaling: on a finite system, physical quantities cannot exhibit any singularity. They can be written as singular term corrected by some scaling function, e.g. $M_L(T) = |K - K_c|^\beta f(L/\xi)$. Function $f(x)$ depends on geometry, but at K_c, the following behaviour is obtained:

$$M_L(K_c) \underset{L\to\infty}{\sim} L^{-\beta/\nu}.$$

Analysis of data

Short-time dynamics scaling

For a system in the high temperature phase, suddenly quenched to critical temperature, a universal dynamic scaling behaviour emerges:

$$M(t, \tau, L, M_0) = b^{-\beta/\nu} M(b^{1/\nu} t, b^{-z}\tau, b^{-1}L, b^{x_0} M_0),$$

z is dynamic exponent (dependent on algorithm), $t = |K - K_c|$, M_0 is initial magnetisation, τ is the time (measured in MC sweeps).

In thermodynamic limit, and at criticality, expected evolution is given by $M(\tau, M_0) = \tau^{-\beta/\nu z} f(M_0 \tau^{-x_0/z})$.

Analysis of data

Conformal mappings: principle

Scale invariance coupled with rotation and translation invariance implies covariance under local scale transformations, i.e. conformal transformations. For any local field (energy density or magnetisation) the usual homogeneity assumption under a homogeneous rescaling $\mathbf{R} \to b\mathbf{R}$

$$\langle \phi(0)\phi(b\mathbf{R})\rangle = b^{-2x_\phi}\langle \phi(0)\phi(\mathbf{R})\rangle$$

is extended to local transformations with position dependent rescaling factor.

Analysis of data

In 2D conformal transformations are realized by analytic functions in complex plane $z \longrightarrow w(z)$ and covariance law of correlators becomes:

$$\langle \phi(w_1)\phi(w_2)\rangle = |w'(z_1)|^{-x_\phi}|w'(z_2)|^{-x_\phi}\langle \phi(z_1)\phi(z_2)\rangle .$$

Helpful in numerical analysis, since simulations are performed on finite systems of particular shape. Critical properties of infinite system $\langle \phi(z_1)\phi(z_2)\rangle \sim |z_1 - z_2|^{-2x_\phi}$ can be obtained by fitting data to transformed conformal expression.

Analysis of data

Conformal mappings: strip

- *Mapping onto a cylinder:* the logarithmic transformation

$$w(z) = \frac{L}{2\pi} \ln z = u + iv$$

maps the infinite plane onto a strip of finite width L with PBC and infinite length (cylinder). One gets on the strip

$$\langle \phi(0,0)\phi(u,v)\rangle = \left(\frac{2\pi}{L}\right)^{2x_\phi} \left[2\cosh\left(\frac{2\pi u}{L}\right) - 2\cos\left(\frac{2\pi v}{L}\right)\right]^{-x_\phi} .$$

Analysis of data

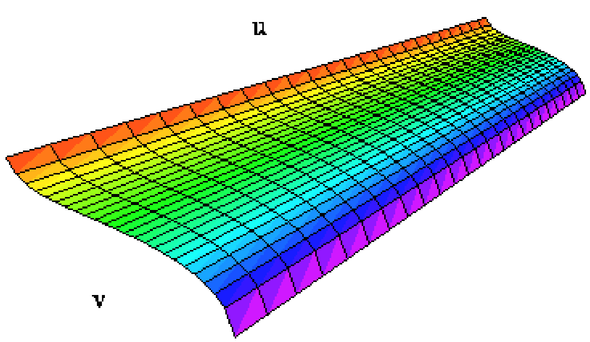
At large distances it becomes an exponential decay

$$\langle \phi(0,0)\phi(u,0)\rangle_{\rm pbc} = \left(\frac{2\pi}{L}\right)^{2x_\phi} \exp\left(-\frac{2\pi u x_\phi}{L}\right).$$

Analysis of data

With mapping $w(z) = \frac{L}{\pi} \ln z$, the half-infinite plane $\rightarrow$ strip with open boundaries in transverse direction. Transverse profile of order parameter density with fixed-free spins is given by

$$\langle \sigma(v) \rangle_{+f} = \text{const} \times \left[\frac{L}{\pi} \sin\left(\frac{\pi v}{L} \right) \right]^{-x_\sigma} F\left[\cos\left(\frac{\pi v}{2L} \right) \right].$$



Analysis of data

Conformal mappings: square

- *Mapping onto a square:* Schwarz-Christoffel

$$w(z) = \frac{N}{2\mathrm{K}}\mathrm{F}(z,k), \quad z = \mathrm{sn}\left(\frac{2\mathrm{K}w}{N}\right)$$

maps half-infinite plane $z = x + iy$ ($0 \leq y < \infty$) inside a square $w = u + iv$ of size $N \times N$.

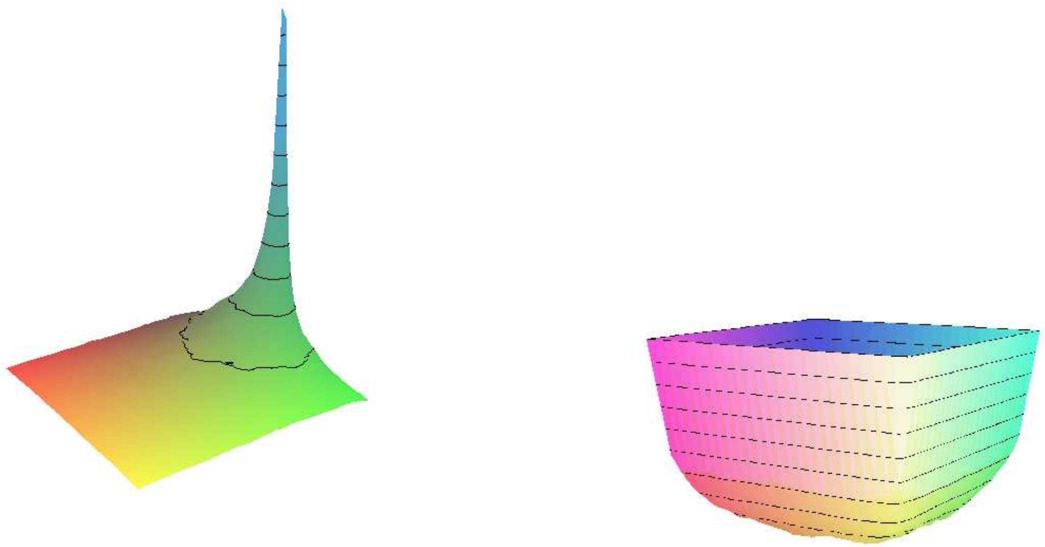
$F(z,k)$: elliptic integral of first kind,

$\mathrm{sn}\,(2\mathrm{K}w/N)$: Jacobian elliptic sine,

$\mathrm{K} = K(k)$: complete elliptic integral of first kind,

modulus k is solution of $K(k)/K(\sqrt{1-k^2}) = \frac{1}{2}$.

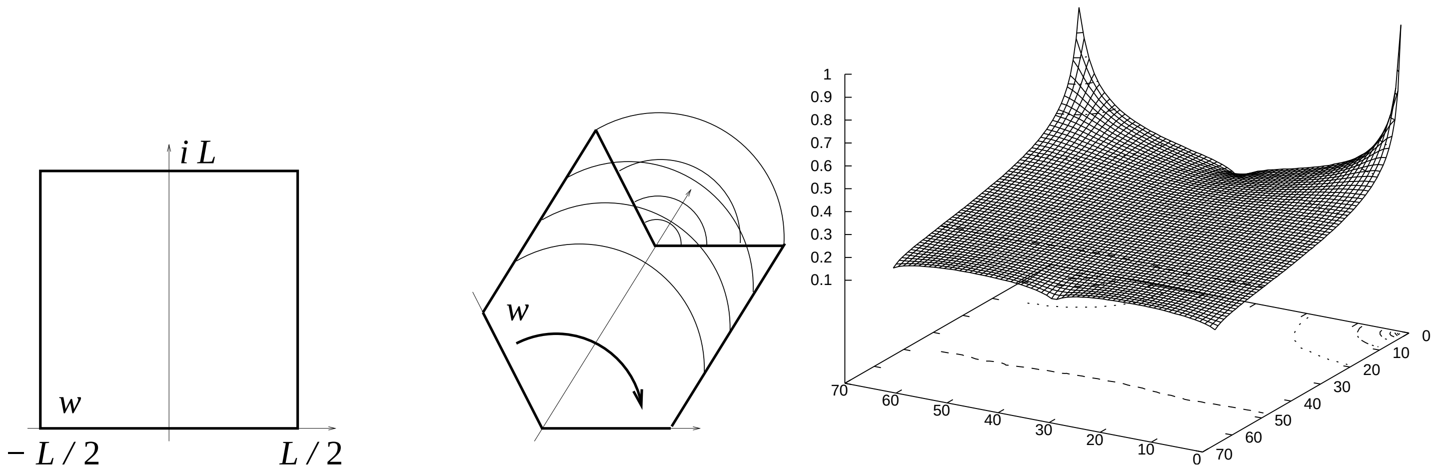
Analysis of data



Two-point correlation function or density profile in presence of ordering surface fields: $\langle \sigma(w) \rangle_{\text{sq.}} = \text{const} \times [\kappa(w)]^{-x_\sigma}$ where $\kappa(w) = \left(\Im\text{m}[z] \left(|1 - z^2||1 - k^2 z^2| \right)^{-1/2} \right)$ comes from SC mapping.

Analysis of data

Conformal mappings: square with “pillow” BC



Analysis of data

Summary	
infinite plane $\rightarrow$ PBC strip	$w = \frac{L}{2\pi} \ln z$
half-plane $\rightarrow$ open strip	$w = \frac{L}{\pi} \ln z$
infinite plane $\rightarrow$ "pillow" square	$z = \mathrm{sn}^2 \frac{2\mathrm{K}w}{L}$
half-plane $\rightarrow$ open square	$z = \mathrm{sn} \frac{2\mathrm{K}w}{L}$

Numerical results in $2D$: Regime $q > 4$

- Nature of the transition
- Location of the fixed point
- Critical exponents

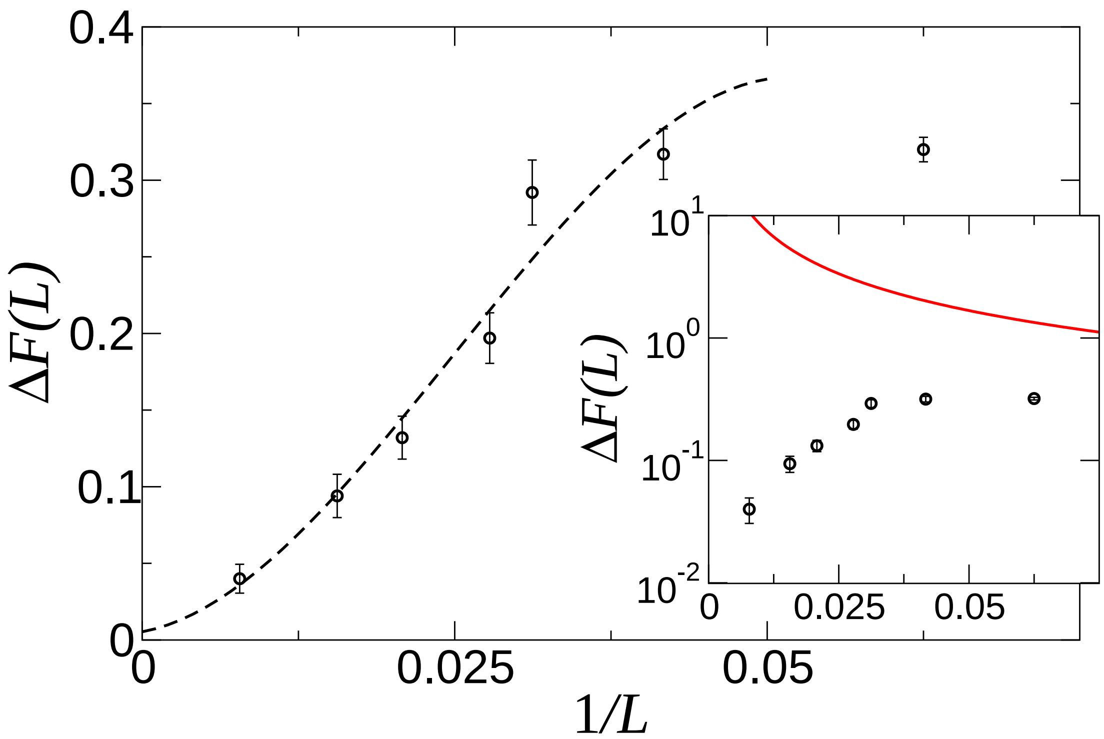
Numerical results in $2D$: Regime $q > 4$

Nature of the transition

When $q > 4$, what about the nature of the transition in the presence of disorder?

Free energy barrier $\Delta F(L)$, defined from energy histogram $\mathcal{P}(E)$ in MC simulations is according to $\mathrm{e}^{-\beta \Delta F(L)} = P_{\max}/P_{\mathrm{well}}$. Energy barrier $\Delta F(L) = -2\sigma_{\mathrm{o.d.}} L^{d-1}$ is found to vanish in the thermodynamic limit ($\sigma_{\mathrm{o.d.}}$ is order-disorder interface tension between two possibly coexisting phases).

Numerical results in $2D$: Regime $q > 4$



Numerical results in $2D$: Regime $q > 4$

The dynamics of MC simulations leads to compatible conclusions: energy autocorrelation time τ_E is exponentially large (with system size) when non vanishing order-disorder interface tension $\sigma_{\mathrm{o.d.}}$ exists,

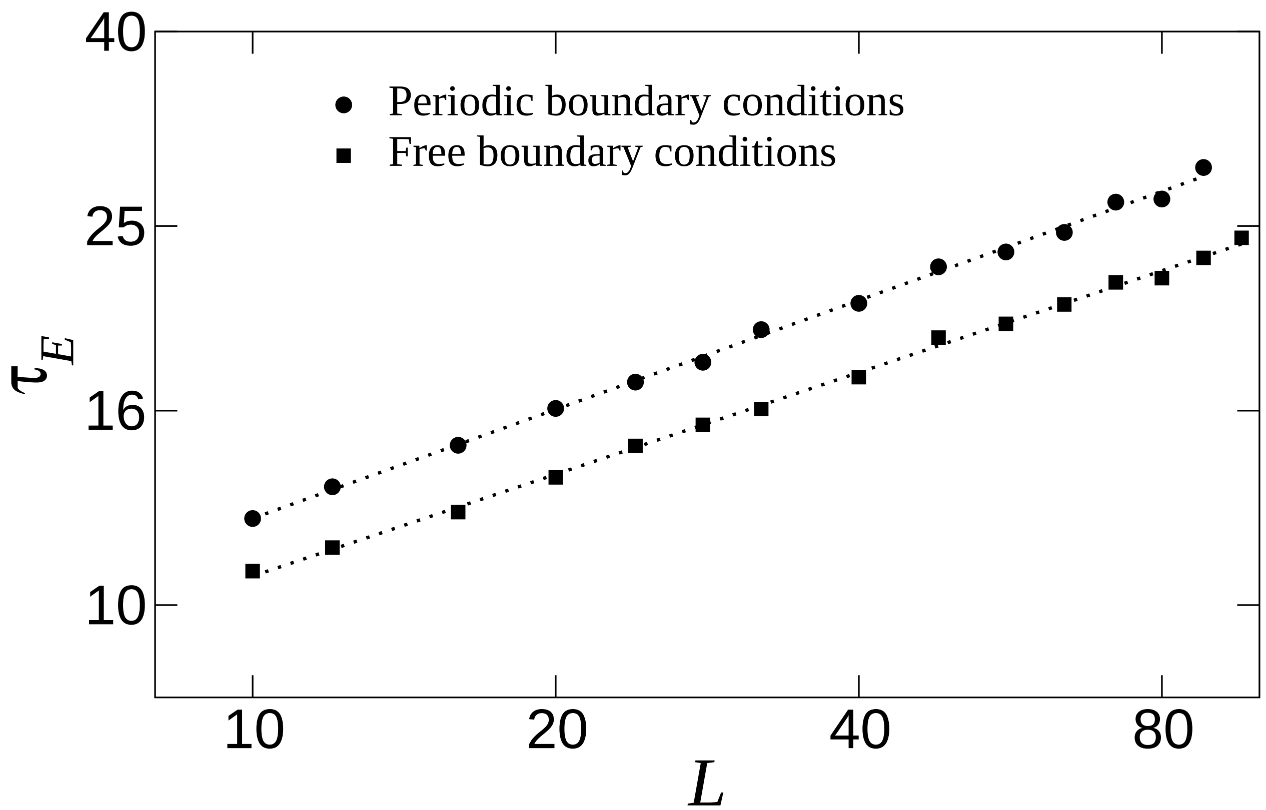
$$\tau_E \sim L^{d/2} \mathrm{e}^{2\sigma_{\mathrm{o.d.}} L^{d-1}},$$

while it is a power law at second-order transitions,

$$\tau_E \sim L^z,$$

dynamical exponent z depends on the algorithm.

Numerical results in $2D$: Regime $q > 4$



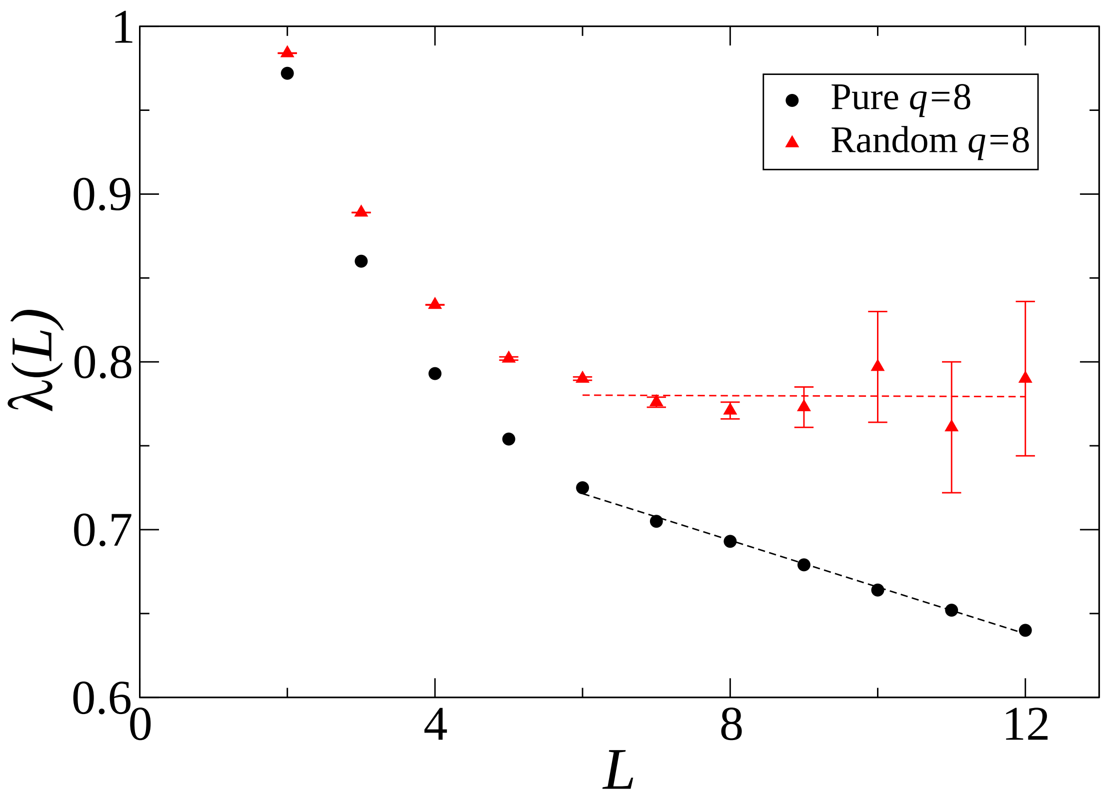
Numerical results in $2D$: Regime $q > 4$

In strip geometry, free energy density $\bar{f}_L$ has corrections to scaling

$$\bar{f}_L \sim f_\infty + O(L^{-d} \mathrm{e}^{-L/\xi})$$

at fisrt-order transitions. Plotting $\lambda(L) = \ln(\bar{f}_L - f_\infty) + d \ln L$ vs strip width L should give asymptotically a straight line with slope $1/\xi$. With randomness, the curve corresponding to $8-$state Potts model indicates a diverging correlation length.

Numerical results in $2D$: Regime $q > 4$



Numerical results in $2D$: Regime $q > 4$

Location of the random fixed point

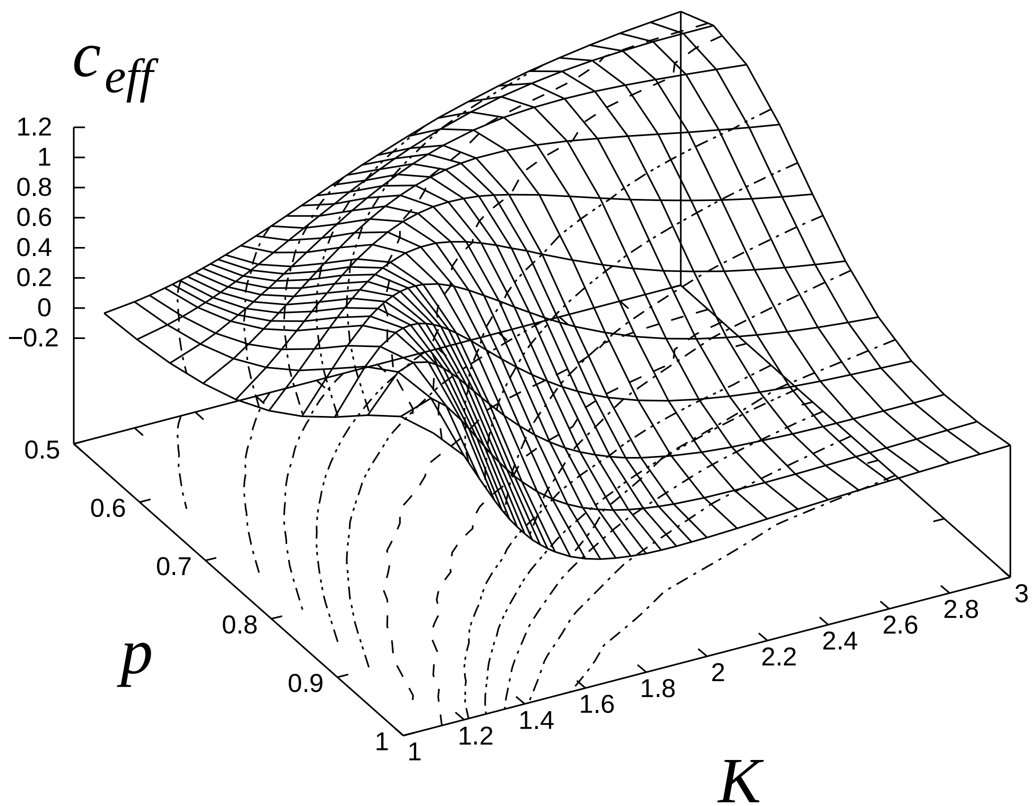
Generically: strong *crossover effects* (competition between disordered FP and pure and percolation FP), or *corrections to scaling* linked to irrelevant scaling variables. These effects are important in random systems and corresponding corrections to scaling can be substantially reduced when one measures critical exponents in the regime of the random FP, expected to be reached at the vicinity of the maximum of the effective central charge.

Numerical results in $2D$: Regime $q > 4$

For a disordered system, c is defined from the finite-size behaviour of the quenched average free energy density $\overline{f_L}$, and depends on disorder strength, $c_{\text{eff}}(g)$,

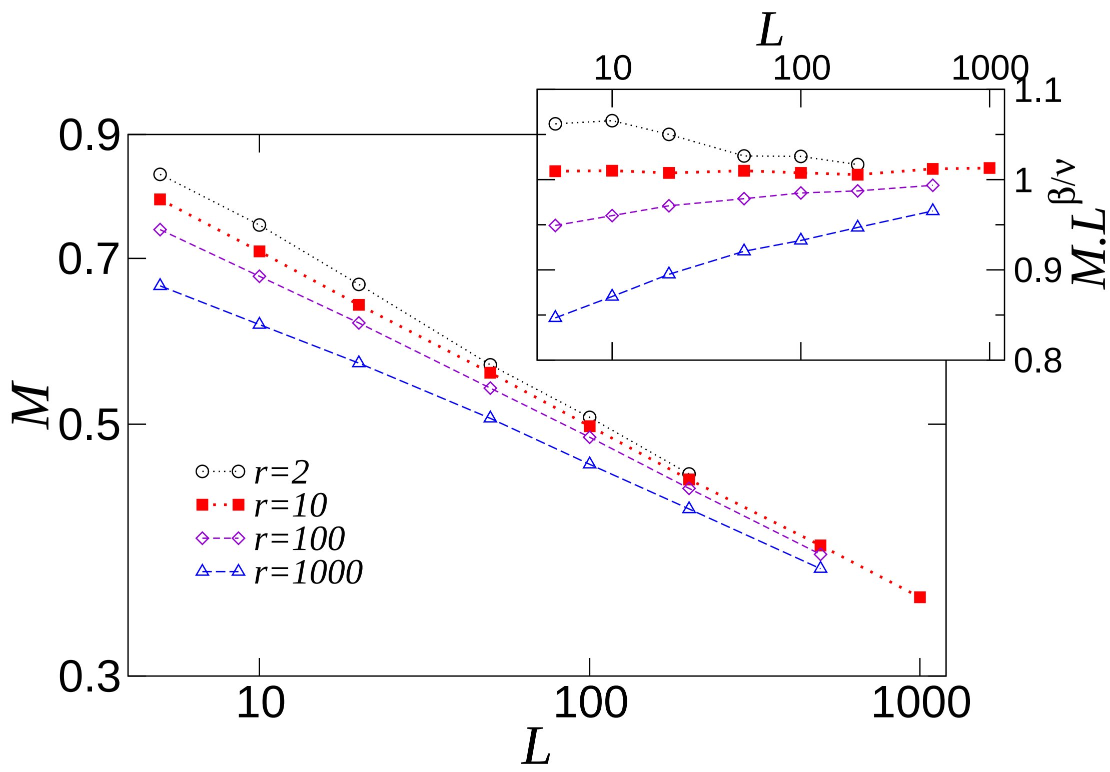
$$\overline{f_L} = f_\infty - \frac{\pi c_{\text{eff}}}{6L^2} + a_4 L^{-4}.$$

Numerical results in $2D$: Regime $q > 4$

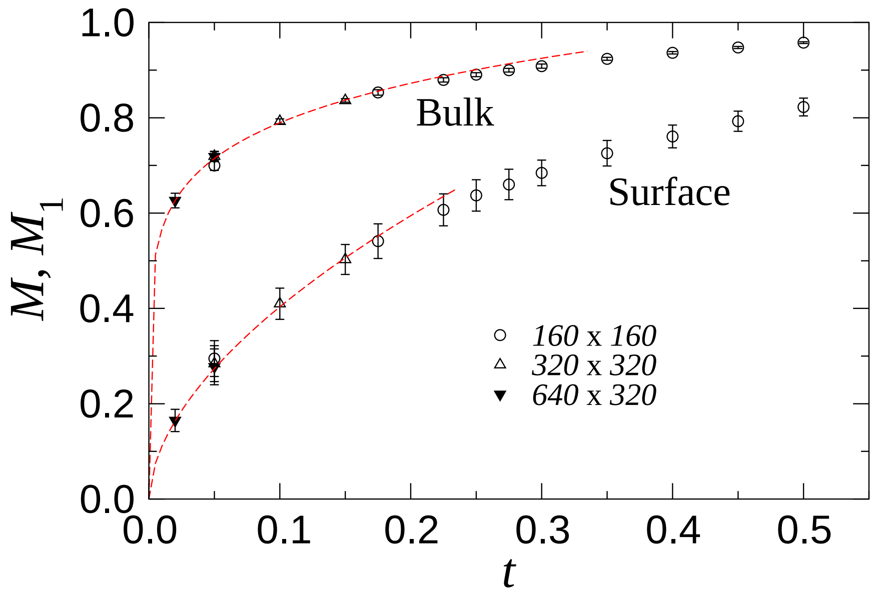


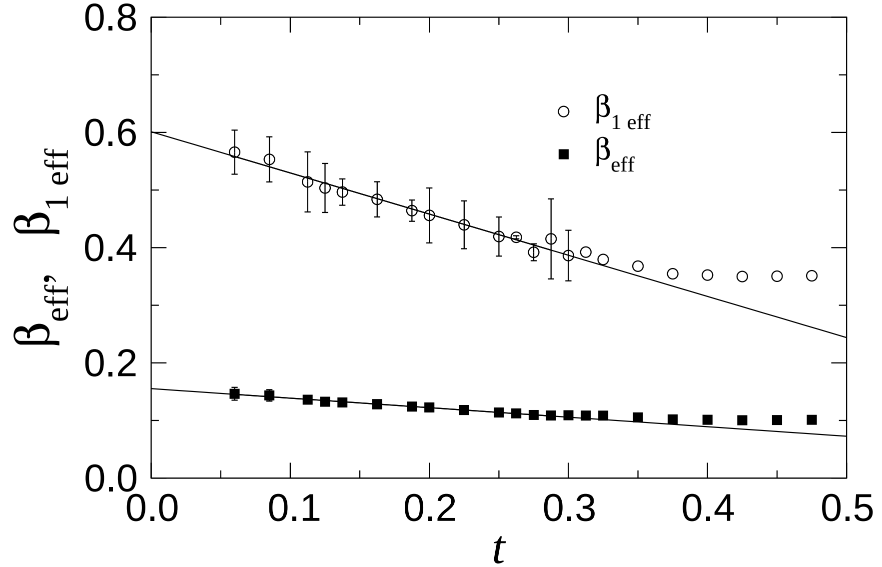
Numerical results in $2D$: Regime $q > 4$

Also standard FSS:



Numerical results in $2D$: Regime $q > 4$

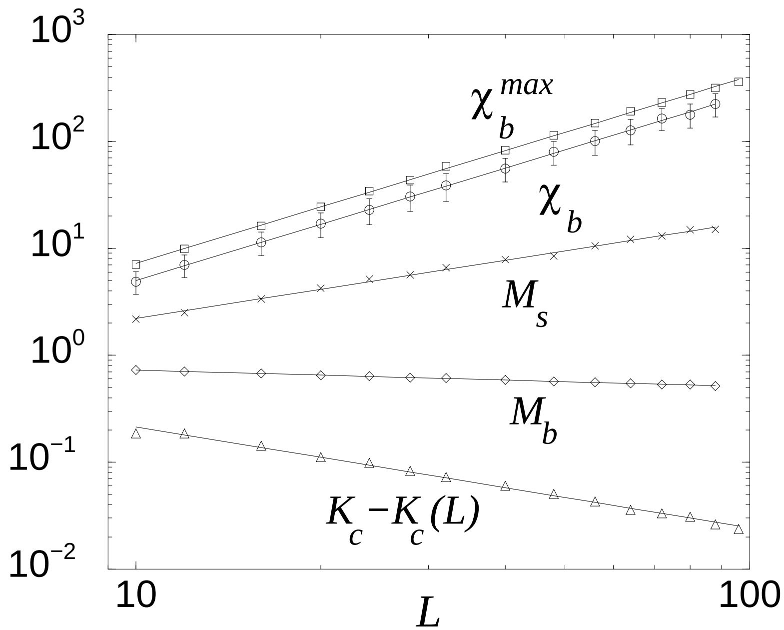




One gets

- $\beta = 0.151(1)$
- $\beta_1 = 0.60(1)$

Numerical results in $2D$: Regime $q > 4$



$8-$state Potts model.

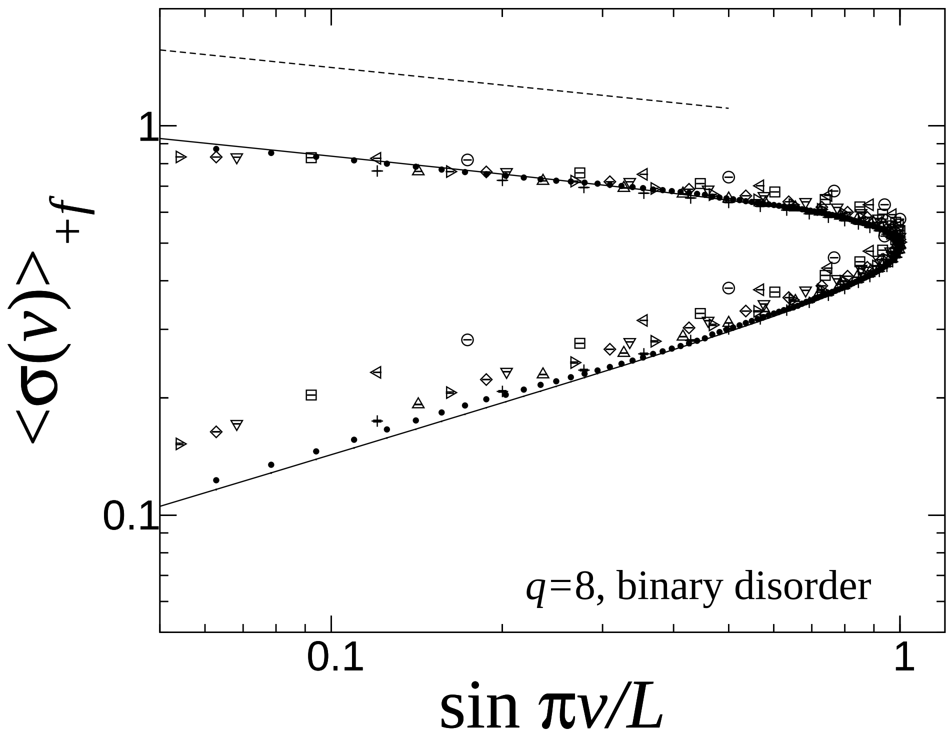
One gets

- $\gamma/\nu = 1.686(17)$,
- $\beta/\nu = 0.152(4)$
- $\nu = 1.005(30)$

Numerical results in $2D$: Regime $q > 4$

Conformal mappings versus *FSS*

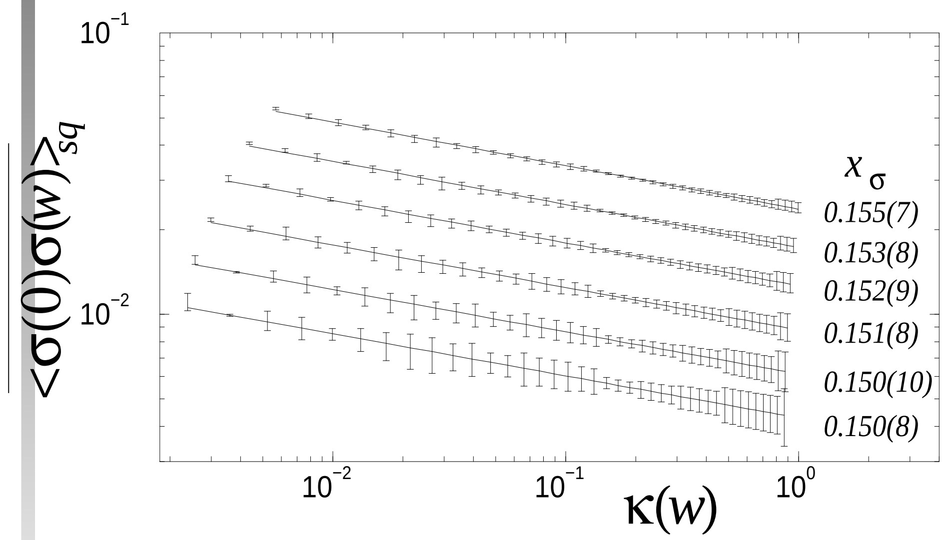
$$\langle\sigma(v)\rangle_{+f} = \text{const} \times \left[\frac{L}{\pi}\sin\left(\frac{\pi v}{L}\right)\right]^{-x'_\sigma} \left[\cos\left(\frac{\pi v}{2L}\right)\right]^{x'^{1}_\sigma},$$

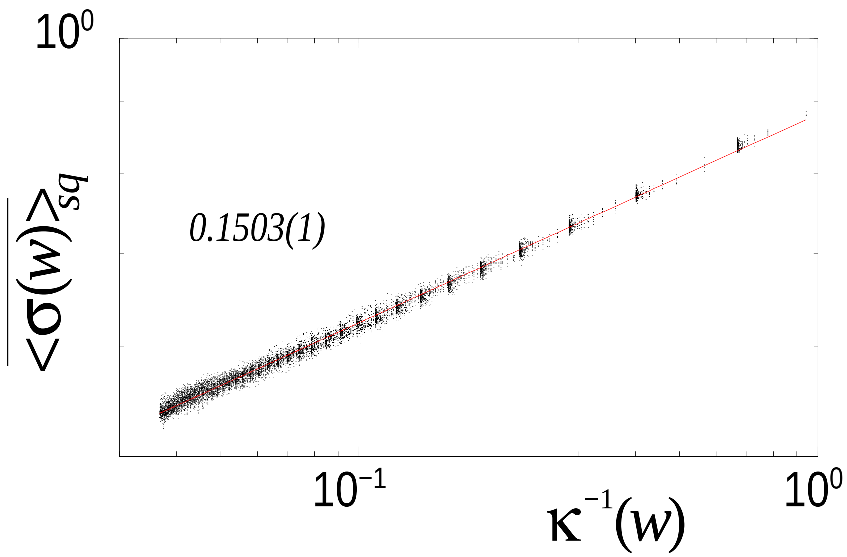


Numerical results in $2D$: Regime $q > 4$

In the square geometry,

$$\overline{\langle\sigma(w_1)\sigma(w)\rangle}_{\rm sq} \sim A_\omega|\kappa(w)|^{-x'_\sigma}, \ \overline{\langle\sigma(w)\rangle}_{\rm sq} \sim \mathrm{const} \times |\kappa(w)|^{-x'_\sigma},$$





Numerical results in $2D$: Regime $q > 4$

x'_σ for the $8-$state Potts model with binary disorder			
Technique	Quantity	x'_σ	Ref.
Standard techniques			
$t-$dependence	$\overline{M_b(t)}$	0.151(1)	Palàgyi et al
FSS	$\overline{M_b(K_c)}$	0.153(1)	Picco, Chatelain and Berche
FSS	$\overline{\langle\sigma(0)\sigma(L/2)\rangle}$	0.159(3)	Olson and Young
Short-time dynamics	$\overline{M_b(\tau)}$	0.151(3)	Ying and Harada
Conformal mappings			
Periodic strip	$\overline{\langle\sigma(0)\sigma(u)\rangle}_{\rm st}$	0.1505(3)	Chatelain and Berche
Free BC square	$\overline{\langle\sigma(0)\sigma(w)\rangle}_{\rm sq}$	0.152(3)	Chatelain and Berche
Fixed-free strip	$\overline{\langle\sigma(v)\rangle}_{\rm st}$	0.150(1)	Palàgyi et al
Fixed BC square	$\overline{\langle\sigma(w)\rangle}_{\rm sq}$	0.1503(1)	Chatelain and Berche

Numerical results in $3D$: Regime $q = 4$

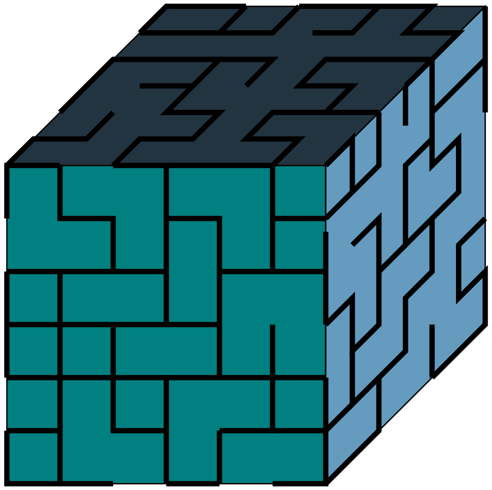
- Implementation of the simulations
- Typical/rare samples - 1st-2nd order regimes
- Phase diagram and critical exponents

Numerical results in $3D$: Regime $q = 4$

Bond-diluted 4-state Potts model on simple cubic lattice:

$$-\beta\mathcal{H} = K \sum_{(i,j)} \varepsilon_{ij} \delta_{\sigma_i,\sigma_j}$$

$$P[\varepsilon_{ij}] = \prod_{ij} [p\delta(\varepsilon_{ij} - 1) + (1-p)\delta(\varepsilon_{ij})]$$



Numerical results in $3D$: Regime $q = 4$

The system is characterized by the values of:

- size L^3
- temperature T
- dilution p and more precisely distribution of couplings on the lattice, $\{K_{ij}\}$.

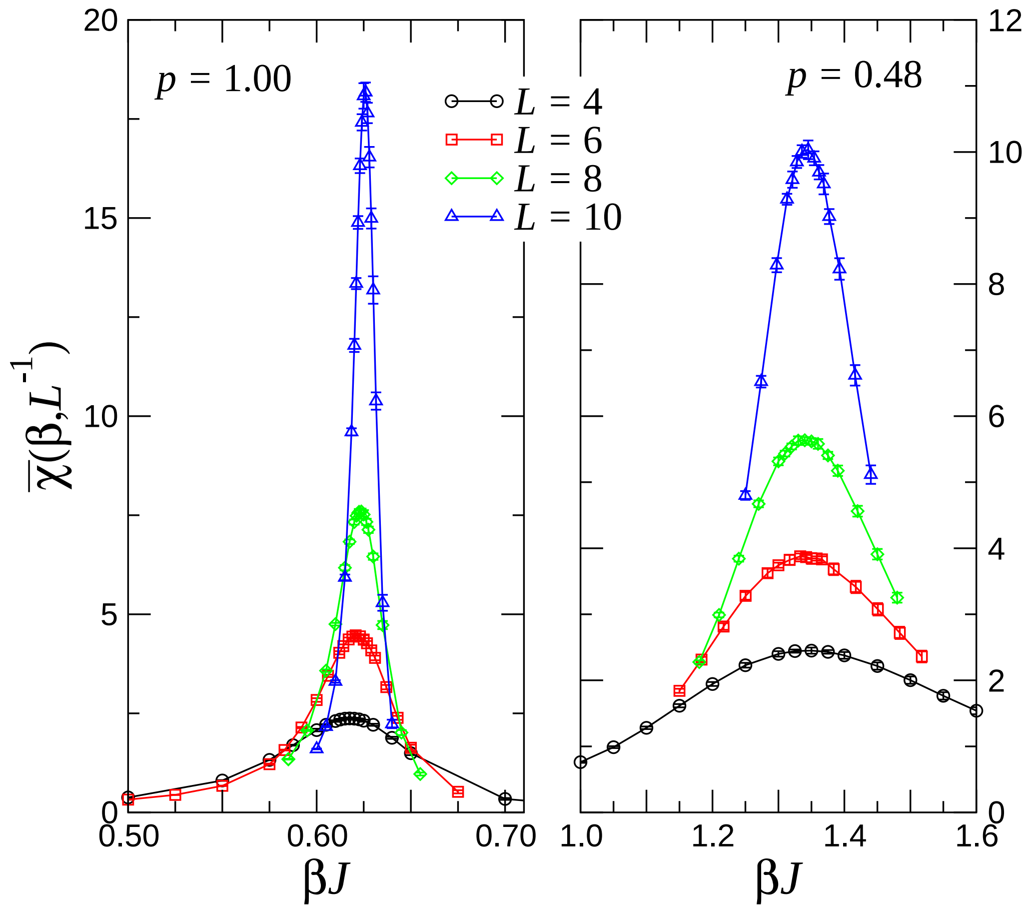
For each disorder realization, simulations of the system consist in storing the time series $E_{[K]}(\mathtt{t})$, $M_{[K]}(\mathtt{t})$ for each MC iteration $\mathtt{t}$ of an update algorithm (Swendsen-Wang or multicanonical, depending on the case considered).

Numerical results in $3D$: Regime $q = 4$

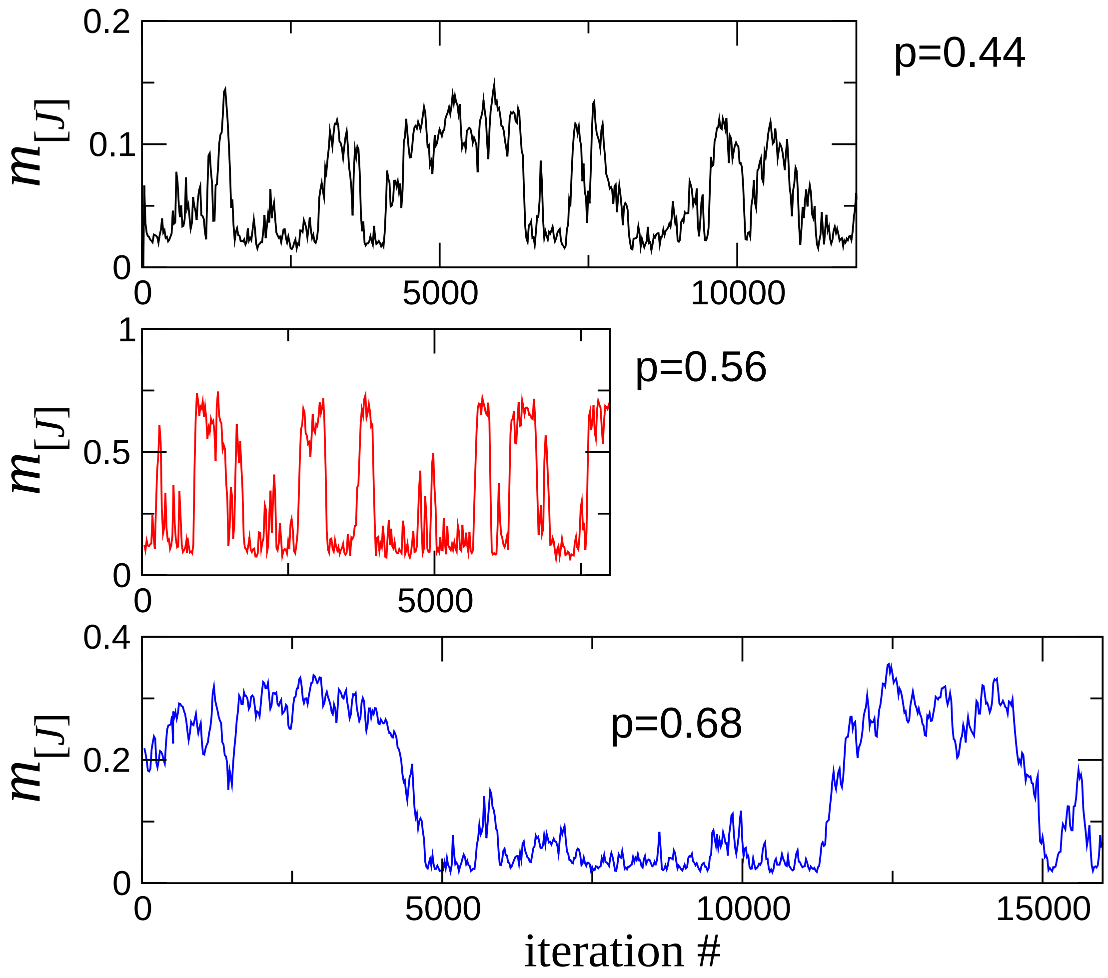
MCS	E	M
	$[K] = [\#1]$	
1	$E_{[\#1]}(1)$	$M_{[\#1]}(1)$
2	$E_{[\#1]}(2)$	$M_{[\#1]}(2)$
$\dots$	$\dots$	$\dots$
	$[K] = [\#2]$	
1	$E_{[\#2]}(1)$	$M_{[\#2]}(1)$
2	$E_{[\#2]}(2)$	$M_{[\#2]}(2)$
$\dots$	$\dots$	$\dots$

Done at a given value of p, for several sizes L, each size simulated at several temperatures T. Other input parameters are $\#\mathrm{MCS}$, $\#[K]$.

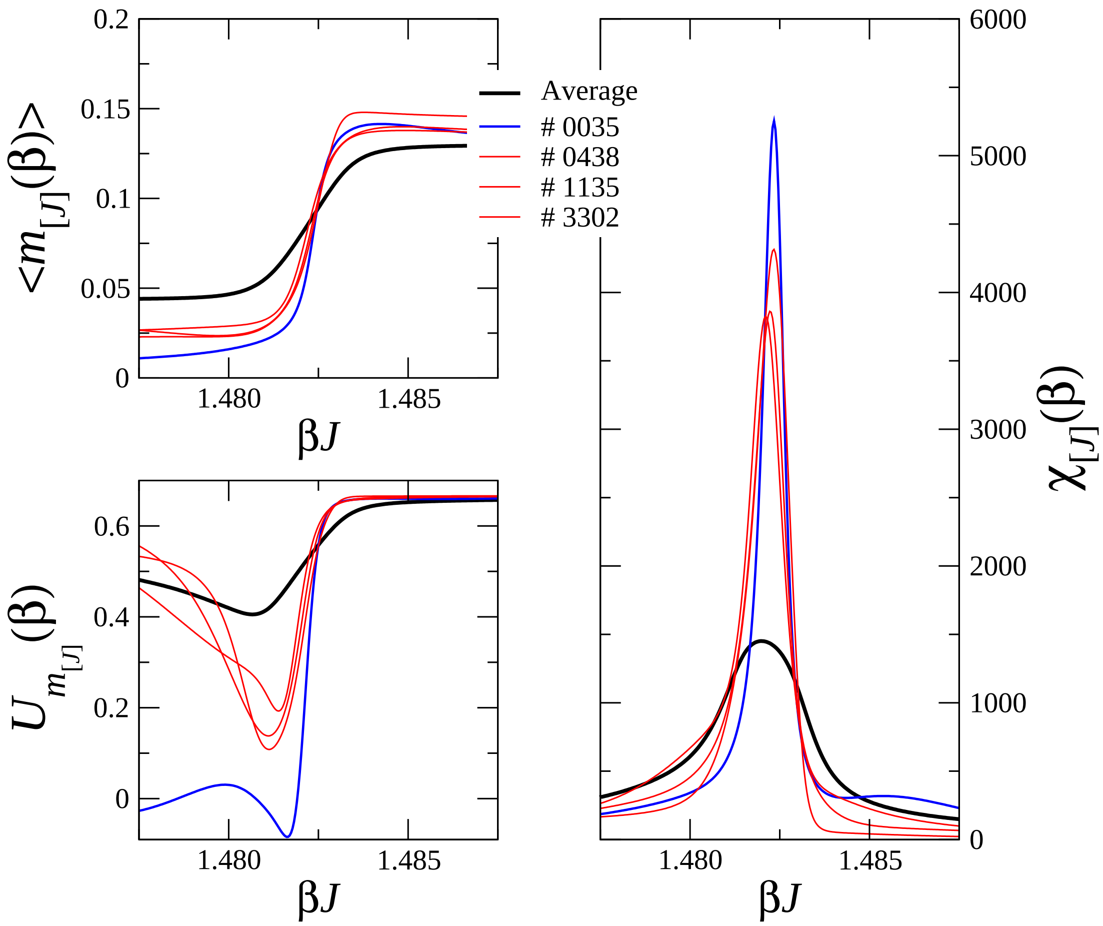
First versus second order



Influence of # MC iterations

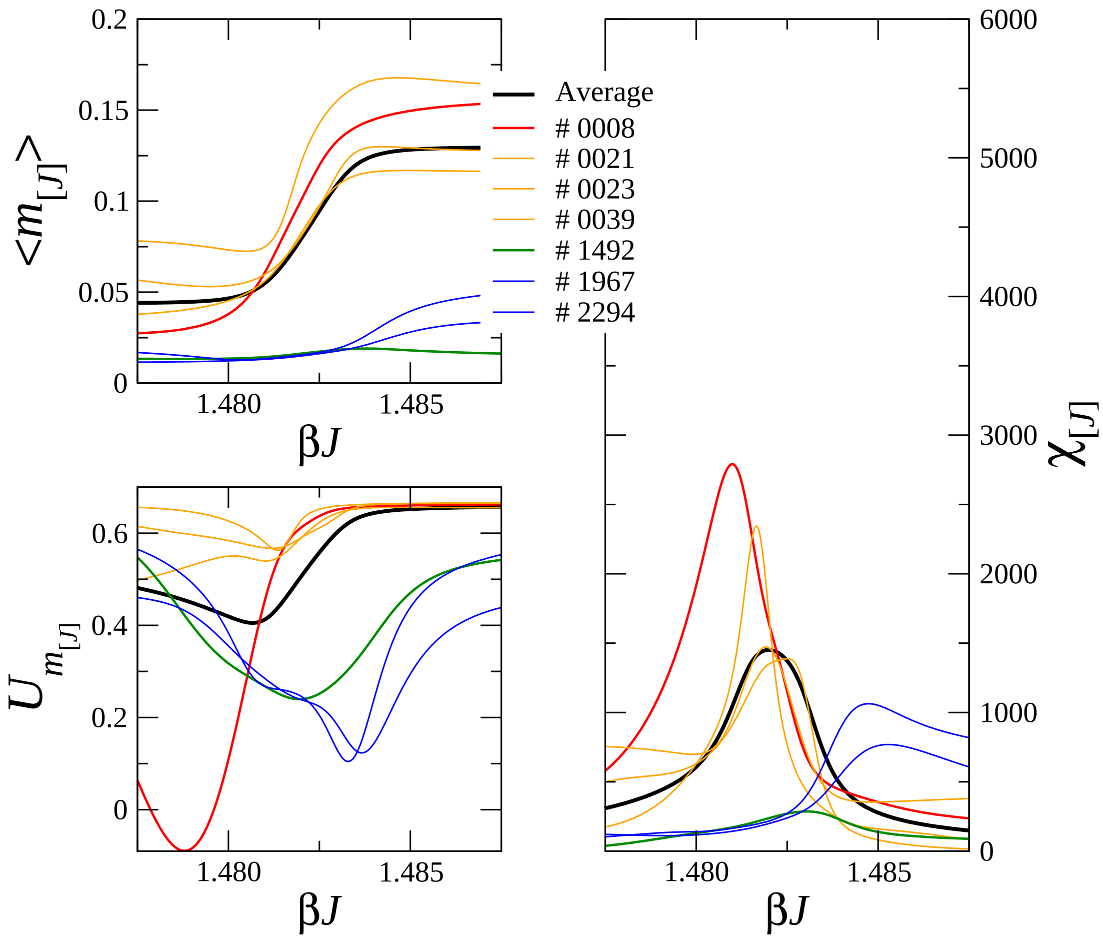


Rare events

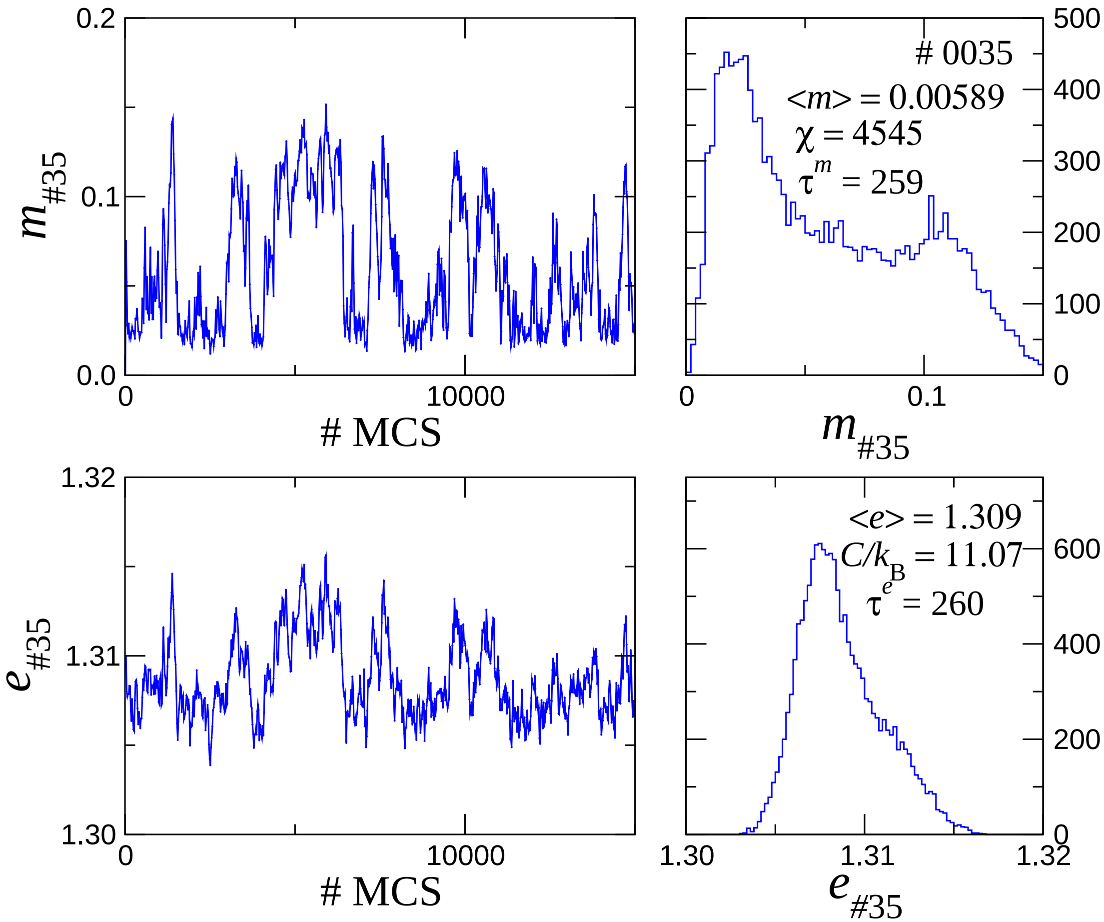


0.2
0.15
0.1
0.05
0
1.480
1.485
βJ
<m[J](β)>
Average
0035
0438
1135
3302
0.6
0.4
0.2
0
1.480
1.485
βJ
U m[J](β)
6000
5000
4000
3000
2000
1000
0
1.480
1.485
βJ
χ[J](β)

Typical events

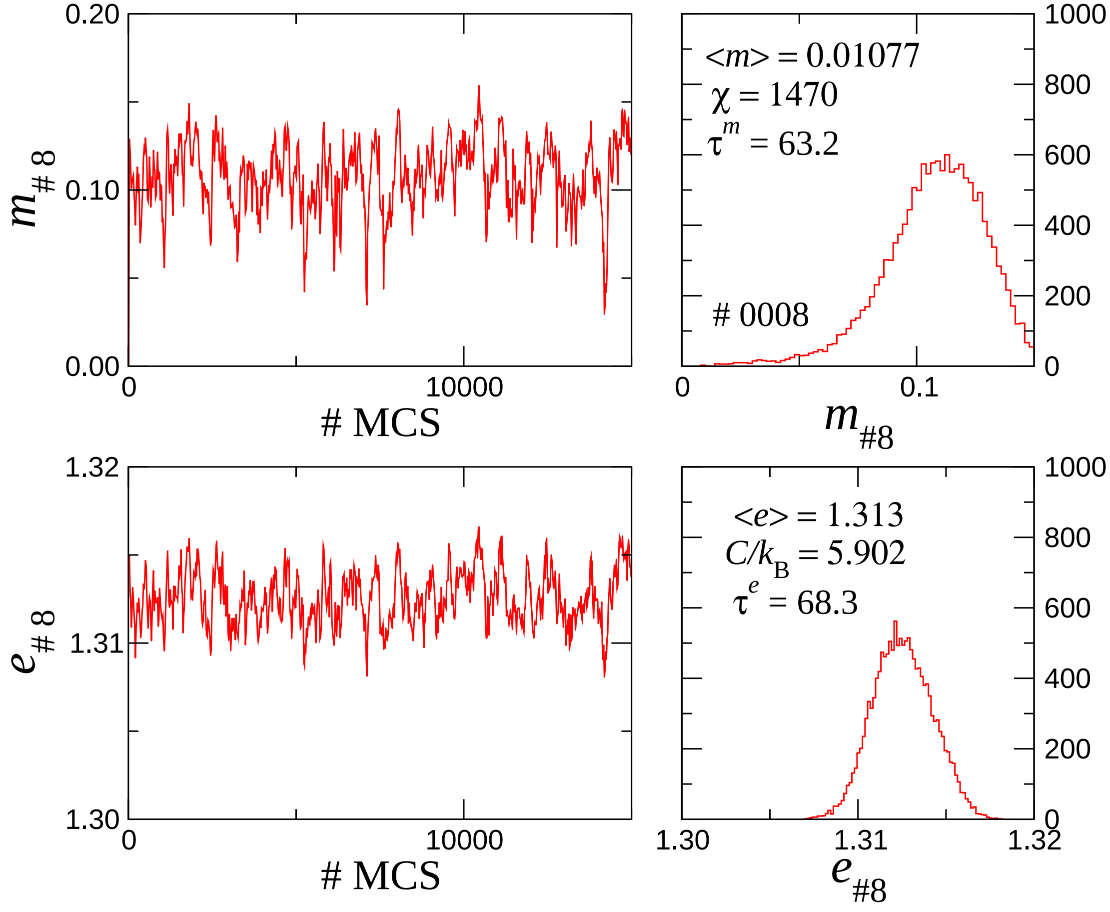


Rare event

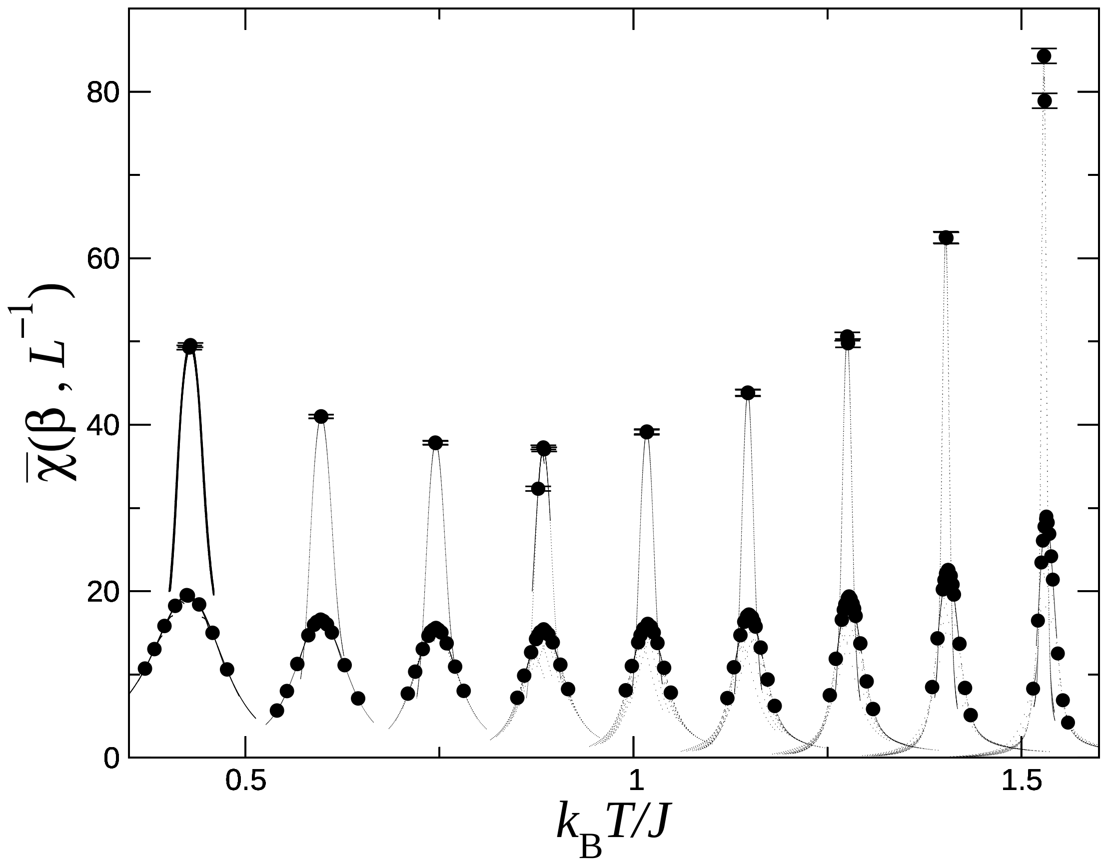


0.2
0.1
0.0
$m_{\#35}$
0
10000
MCS
0035
<m> = 0.00589
χ = 4545
τ^m = 259
500
400
300
200
100
0
0.1
$m_{\#35}$
1.32
1.31
1.30
$e_{\#35}$
MCS
<e> = 1.309
C/k_B = 11.07
τ^e = 260
600
1.32

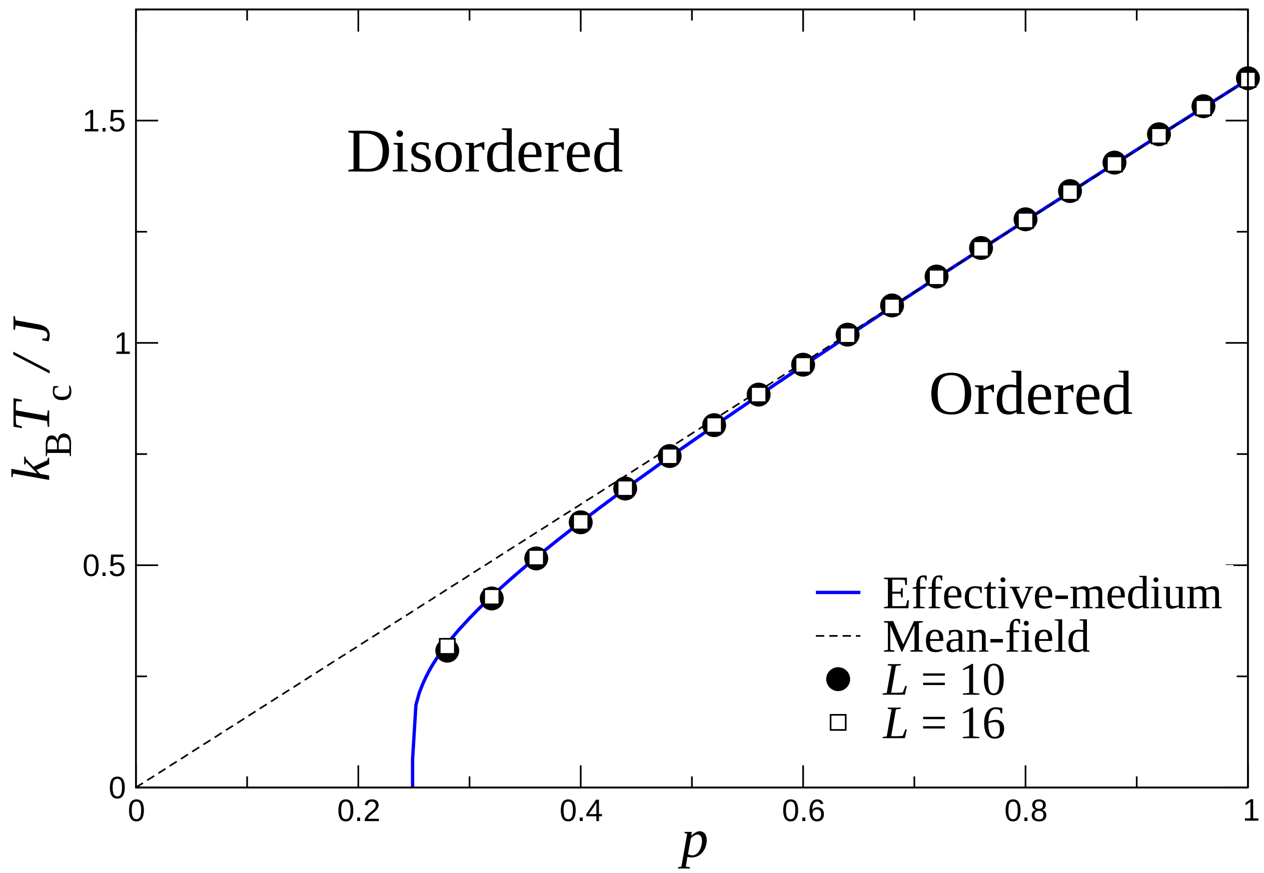
Typical event



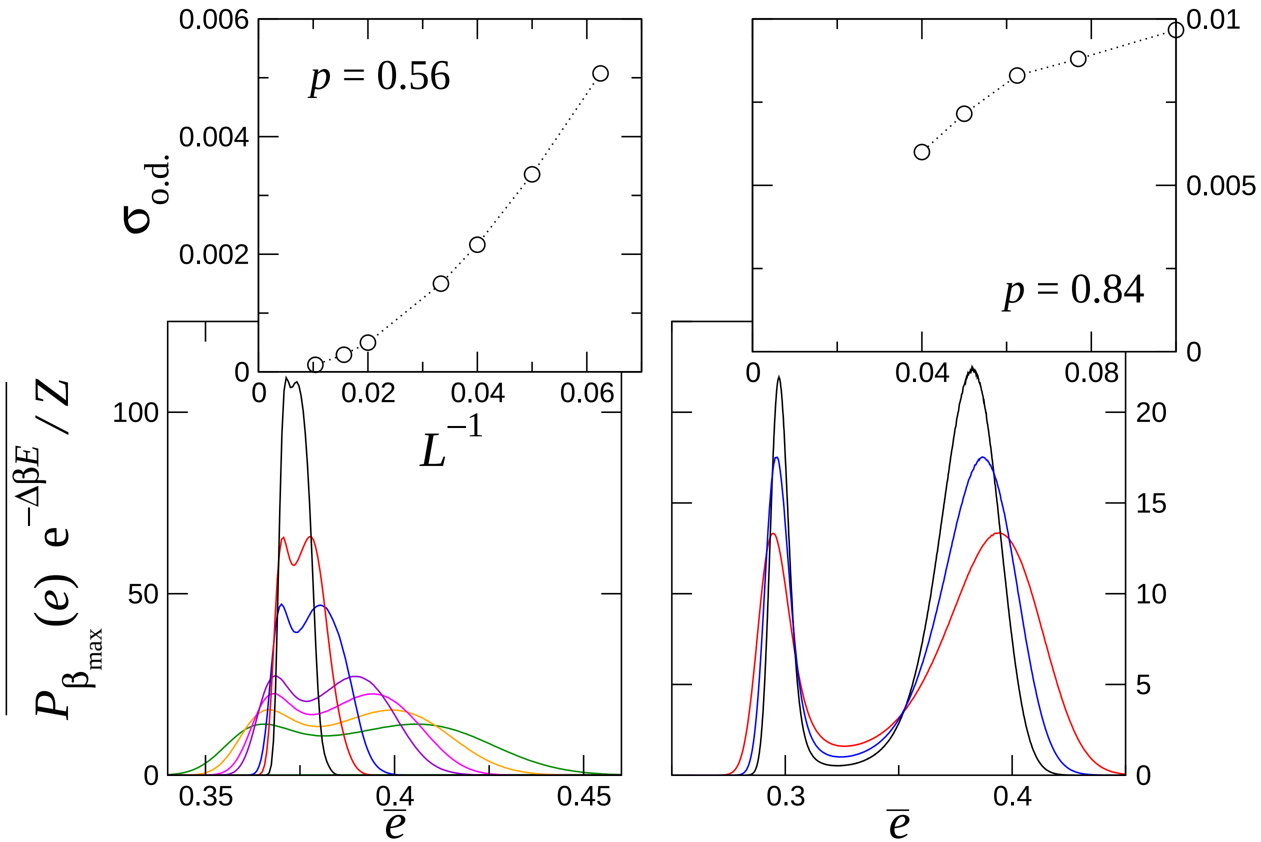
Phase diagram



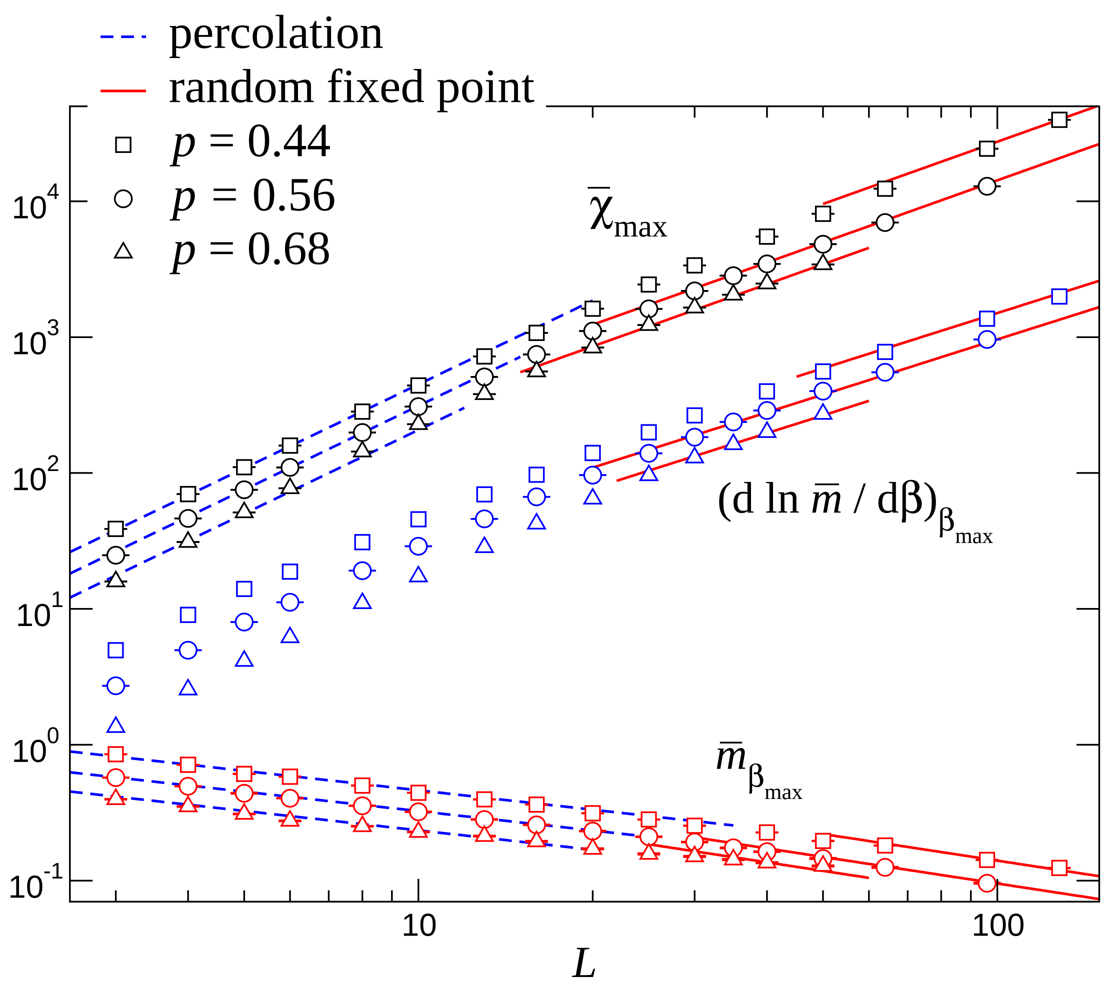
Phase diagram



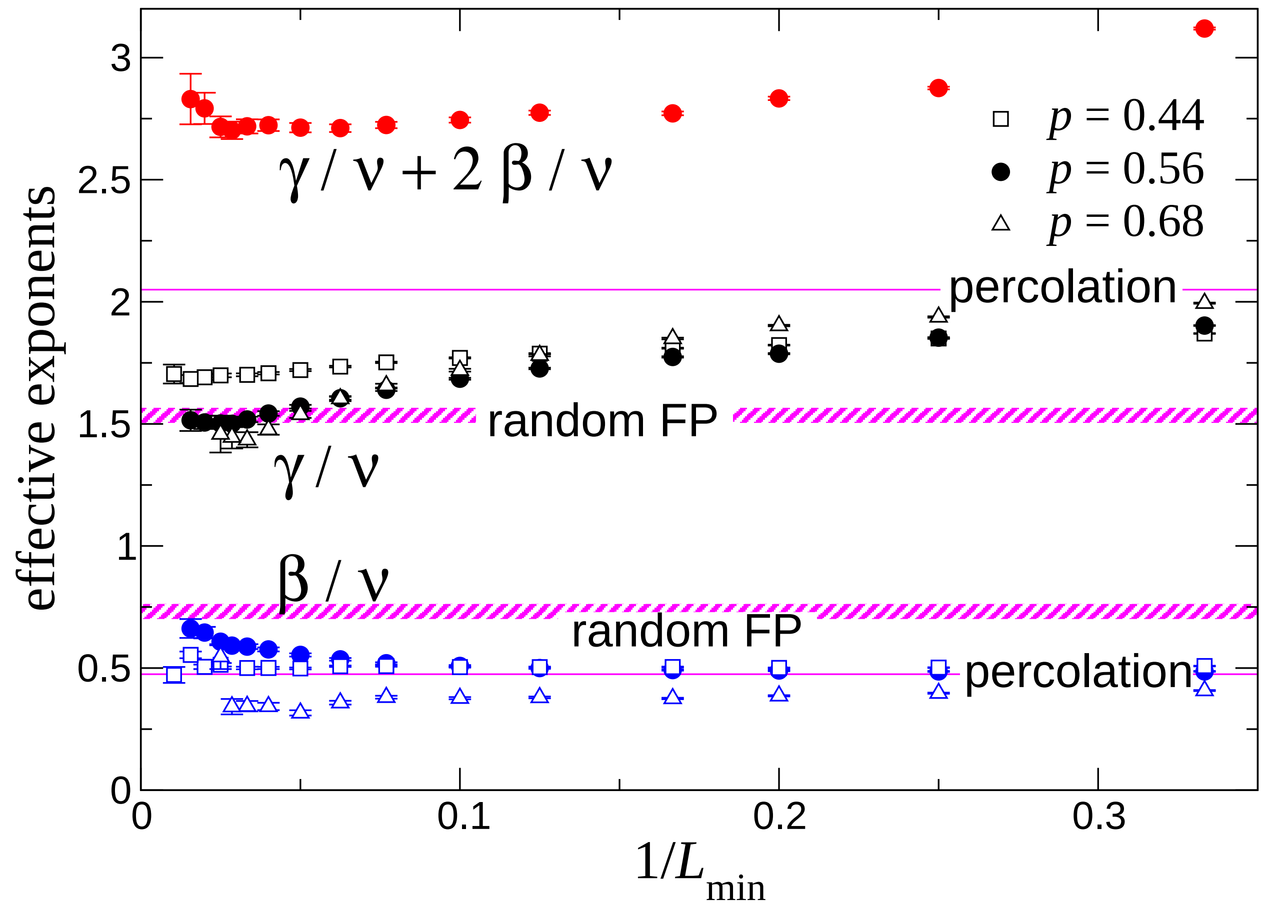
Tricritical point



Finite-Size Scaling



Critical exponents



Conclusions in 2D

The two-dimensional Potts model is ideal framework to test influence of quenched randomness on phase transitions.

- It exhibits second-order transition completely characterised by conformal invariance when $q \leq 4$ and a first-order transition above.
- The transition line is exactly known, and it is easy to build, in the random case, probability distributions of coupling strengths which preserve the self-duality relation.
- Many results concerning the effect of a weak disorder are known using perturbations expansions around the pure fixed point.
- Numerical studies were performed from different sides: Monte Carlo simulations coupled to finite-size scaling analysis, transfer matrices and sophisticated graph and loop algorithms coupled to extensive use of conformal mappings.
- The regime $q > 4$ was extensively studied, but did not display any particular features compared to the regime $q \leq 4$ in the presence of quenched randomness.

Results and conclusions in 2D

At the 2nd order induced FP:

γ/ν	β/ν	ν	α
1.51 ± 0.03	0.64 ± 0.03	0.74 ± 0.02	-0.22 ± 0.06

Results and conclusions in 3D

Open problems:

- Precise location of the tricritical point ($p_{TCP} \simeq 0.68 - 0.84$)
- Corrections to scaling
- Crossover phenomena and influence of the percolation FP (pb with ν)