High-Temperature Series Expansions for Disordered Systems

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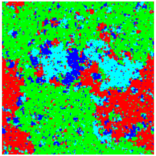
- The q-state Potts model: Phase transitions, Quenched disorder
- Series expansions
  - General remarks
  - Extrapolation techniques
  - Star graph expansion
  - Embedding numbers
- Examples
  - Bond-diluted Ising model in 3,4,5 dimensions
  - Percolation: $q \to 1$ Potts model
  - Tree percolation: $q \to 0$ Potts model

The q-state Potts model

- *Potts* 1952
- Graph $G = (V, E),\ E \subseteq V \times V$: vertices and edges
- Edges define "nearest neighbours"
- Parameter $q = 2, 3, \ldots$; Ising model: $q = 2$
- discrete local degrees of freedom (spins) $s_i \in \{1, \ldots, q\}$ on vertices

$$Z = \sum_{\{s_i\}} e^{-\beta H}, \quad H = -\sum_{e \in E} \delta(s_{e_1}, s_{e_2})$$



$q = 4$ Potts configuration

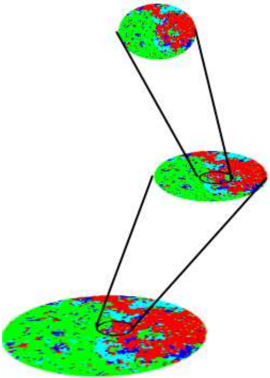
Phase transitions

Infinite volume limit $G \to \mathbb{Z}^d$

Sharp phase transition between an ordered low-T and a disordered high-T phase at some critical value β_c

This phase transition is

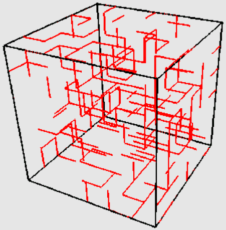
- First order for large q
- Second order for $q \leq 4$ in $d = 2$ and $q \leq 2$ in $d > 2$
  - diverging correlation length, universal critical exponents
  - self-similarity, fixed point of the renormalization group
  - correlation length $\xi \sim |\beta - \beta_c|^{-\nu}$
  - susceptibility $\chi \sim |\beta - \beta_c|^{-\gamma}$
  - continuum limit can be described by an euclidean quantum field theory



Quenched disorder

$$\mathcal{Z}(\{J_{ij}\}) = \mathrm{Tr}\, \exp\left(-\beta \sum_{<ij>} J_{ij}\delta(S_i, S_j)\right)$$

$$-\beta F = [\log \mathcal{Z}(\{J_{ij}\})]_{P(J)}$$



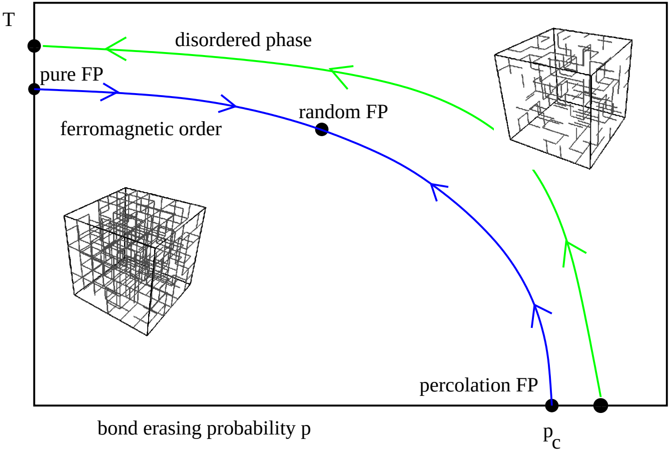
- random couplings: J_{ij} chosen according to some probability distribution $P(J)$
  - spin glasses: $J = \pm 1$
  - random bond models: $J = +1/+5$
  - correlated disorder
- geometric disorder: random graphs, site dilution, we look at bond dilution:

$$P(J_{ij}) = (1-p)\,\delta(J_{ij}-J_0)+p\,\delta(J_{ij})$$

in a ferromagnet $J_0 > 0$

Effect of quenched disorder on critical behaviour:

Bond-diluted Ising model



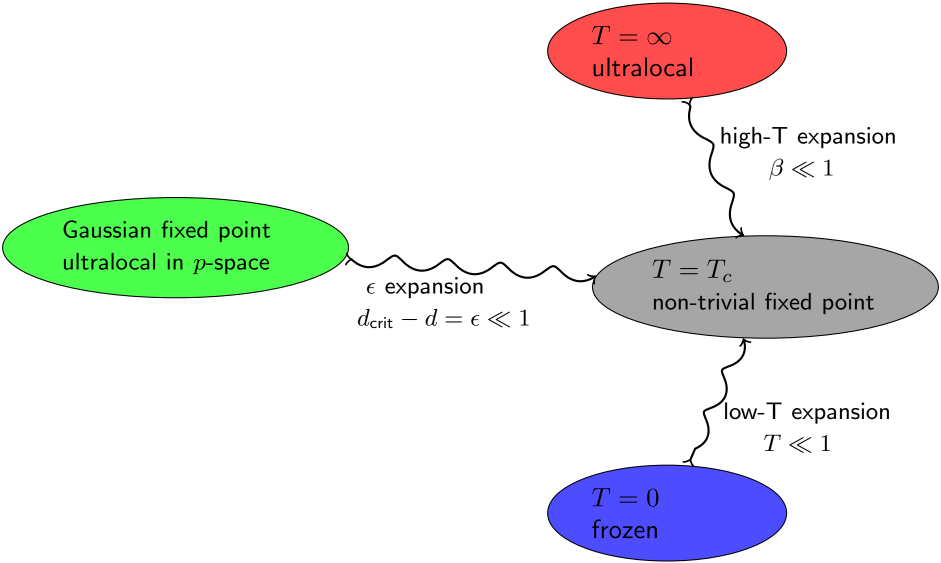
$q = 2$

Harris criterion:

- 3D: relevant $\longrightarrow$ new fixed point
- 4D: marginal $\longrightarrow$ log corrections
- 5D: irrelevant $\longrightarrow$ only non-universal quantities (T_c) change

$q > 2$: effect on first order phase transition: softening to second order

Renormalization group fixed points and expansions



High-temperature Series Expansions

I. Calculate quantities on subgraphs of the lattice and put them together in a systematic way ... series in β

for physical quantities like free energy, susceptibility,...

- Linked cluster expansion: **pure** 3D Ising model:

Sykes et al.	1973	13. order
Nickel, Rehr	1990	21. order
Butera, Comi	2000	23. order
Campostrini et al.	2000	25. order

- Finite lattice methods: **pure** 3D Ising model:

Arisue et al.	2004	32. order

- Star graph expansion: **disordered** models:

Singh, Chakravarty	1987	15	3D Ising glass
Schreider, Reger	1993	10	q-Potts glass
Roder, Adler, Janke	1998	11	2D RB Ising
Hellmund, Janke	2001	17	bond-diluted Potts, all D
Hellmund, Janke	2004	19	bond-diluted Potts, $D < 6$
Hellmund, Janke	2005	21	bond-diluted Ising, $D = 3$
Hellmund, Janke	2005	20	pure Potts,all q, $D = 3$

Set $\{G_i\}$ of subgraphs of a lattice is a partially ordered set

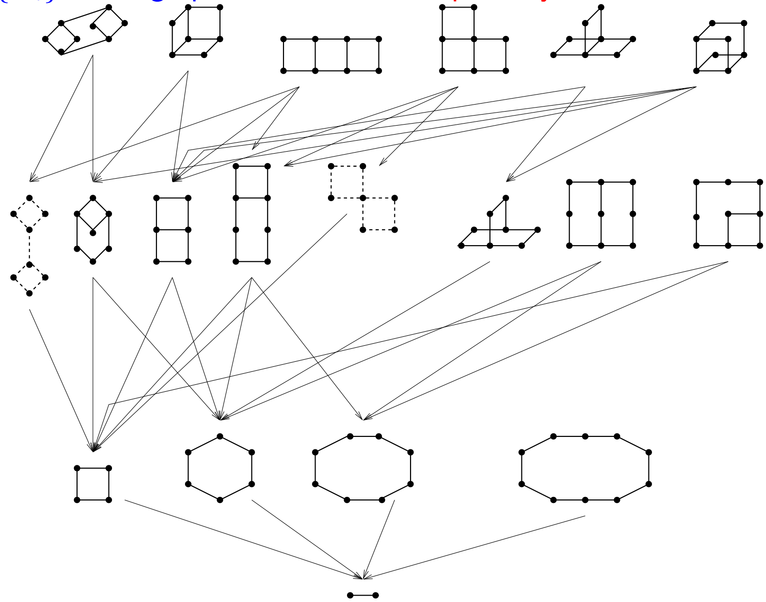


Fig: all bipartite connected no-free-end graphs up to 10 edges

Star graph expansion

I. $F(G)$ function on set of graphs $\{G_i\} \Longrightarrow \exists$ function $W_F(G)$:

$$\begin{aligned} F(G) &= \sum_{g\subseteq G} W_F(g) \\ W_F(G) &= F(G) - \sum_{g\subset G} W_F(g) \\ \Rightarrow \quad F(\mathbb{Z}^d)/V &= \sum_{G} E(G:\mathbb{Z}^d)\, W_F(G) \end{aligned}$$

(with weak embedding number $E(G:\mathbb{Z}^d)$)

II. Consider operation $\#$ on $\{G\}$:

$$G = G_1 \# G_2$$

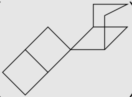
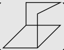
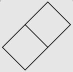
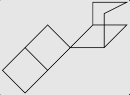
such that $g \subseteq G$ implies either $g \subseteq G_1$ or $g \subseteq G_2$ or $g = g_1 \# g_2$ with $g_1 \subseteq G_1, g_2 \subseteq G_2$.
Theorem: If $F(G)$ has the property

$$G = G_1 \# G_2 \quad \Longrightarrow \quad F(G) = F(G_1) + F(G_2)$$

then $W_F(G)$ vanishes on every graph G reducible under $\#$.

Applications:

- $\#$ = disjoint union of graphs $\Longrightarrow$ reduction to connected graphs.
- $\#$ = glueing of graphs at one node $\Longrightarrow$ reduction to star graphs

$F\Big($  $\Big) = F\Big($  $\Big) + F\Big($  $\Big) \Longrightarrow W_F\Big($  $\Big) = 0$

We need to consider only graphs without articulation points, i.e.,

"star graphs" $\equiv$ biconnected graphs.

For the q-state Potts model with uncorrelated disorder,

$[\log Z]$ and $1/[\chi]$ have star graph expansions.

Embedding numbers

Definition

Embedding: map of the graph G into the lattice (e.g., $\mathbb{Z}^d$), which maps vertices to vertices and edges to edges.

Embedding number: count possible embeddings modulo translations

- **free embeddings:** the map needs not to be injective

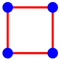
is allowed

  - used in linked cluster expansion, fast counting algorithms exist,
  - but not suitable for disorder averaging

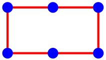
- **weak embeddings:** only injective maps allowed $\Rightarrow$ collision tests,
  - difficult to count
  - used in star graph expansion

Examples for weak embedding numbers in $\mathbb{Z}^d$

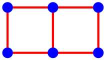
$$d$$



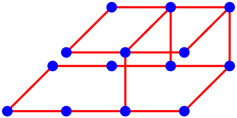
$$\binom{d}{2}$$



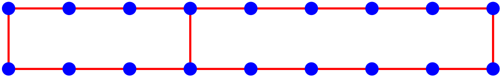
$$2\binom{d}{2} + 16\binom{d}{3}$$



$$2\binom{d}{2} + 12\binom{d}{3}$$



$$12048\binom{d}{3} + 396672\binom{d}{4} + 2127360\binom{d}{5} + 2488320\binom{d}{6}$$



$$8\binom{d}{2} + 275184\binom{d}{3} + 18763392\binom{d}{4} + 208611840\binom{d}{5} + 645442560\binom{d}{6} + 559964160\binom{d}{7}$$

Series generation techniques - Star graph expansion

- Construct all star graphs embeddable in $\mathbb{Z}^D$ up to a given order (number of edges E):

order E	8	9	10	11	12	13	14	15	16	17	18	19	20	21
#graphs	2	3	8	9	29	51	142	330	951	2561	7688	23078	55302	165730

  - number of graphs $\sim \exp(E)$
  - for each generated graph: isomorphism test (P or NP?)

- Count the (weak) embedding numbers $E(G; \mathbb{Z}^D)$
  - for each graph: backtracking algorithm $\sim \exp(E)$

- Calculate Z and correlations $G_{ij} = \langle \delta_{s_i, s_j} \rangle$ for every graph with symbolic couplings $J_1, ..., J_B$ (using a cluster representation)
  - NP hard

- Calculate disorder averages $[\log Z]$, $C_{ij} = [G_{ij}/Z]$ up to $O(J^N)$
- Inversion of correlation matrix and subgraph subtraction
  $W_\chi(G) = \sum_{i,j} (C^{-1})_{ij} - \sum_{g \subset G} W_\chi(g)$
- Collect the results from all graphs
  $1/\chi = \sum_G E(G; \mathbb{Z}^d)\, W_\chi(G)$

Example: susceptibility of the bond-diluted 3D Ising model

$$\chi(p,v) = 1 + 6pv + 30p^2v^2 + 150p^3v^3 + 726p^4v^4 - 24p^4v^5 + 3534p^5v^5 - 24p^4v^6 - 192p^5v^6 + 16926p^6v^6 - 24p^4v^7 - 192p^5v^7 - 1608p^6v^7 + 81318p^7v^7 - 192p^5v^8 - 1608p^6v^8 - 10464p^7v^8 + 387438p^8v^8 + 24p^4v^9 - 1608p^6v^9 - 10536p^7v^9 - 67320p^8v^9 + 1849126p^9v^9 + 24p^4v^{10} + 192p^5v^{10} - 264p^6v^{10} - 9744p^7v^{10} - 67632p^8v^{10} - 395328p^9v^{10} + 8779614p^{10}v^{10} + 24p^4v^{11} + 192p^5v^{11} + 1080p^6v^{11} - 240p^7v^{11} - 60912p^8v^{11} - 397704p^9v^{11} - 2299560p^{10}v^{11} + 41732406p^{11}v^{11} + 192p^5v^{12} + 1344p^6v^{12} + 8400p^7v^{12} - 1440p^8v^{12} - 339936p^9v^{12} - 2295744p^{10}v^{12} - 12766944p^{11}v^{12} + 197659950p^{12}v^{12} - 24p^4v^{13} + 1608p^6v^{13} + 10296p^7v^{13} + 51480p^8v^{13} + 26544p^9v^{13} - 1886928p^{10}v^{13} - 12680496p^{11}v^{13} - 70404720p^{12}v^{13} + 936945798p^{13}v^{13} - 24p^4v^{14} - 192p^5v^{14} + 264p^6v^{14} + 10032p^7v^{14} + 64560p^8v^{14} + 341568p^9v^{14} + 259656p^{10}v^{14} - 9915696p^{11}v^{14} - 69162048p^{12}v^{14} - 377522064p^{13}v^{14} + 4429708830p^{14}v^{14} - 24p^4v^{15} - 192p^5v^{15} - 1080p^6v^{15} - 1704p^7v^{15} + 60024p^8v^{15} + 427920p^9v^{15} + 2062368p^{10}v^{15} + 2482464p^{11}v^{15} - 51644200p^{12}v^{15} - 367148472p^{13}v^{15} - 2014331904p^{14}v^{15} + 20955627110p^{15}v^{15} - 192p^5v^{16} - 1080p^6v^{16} - 12144p^7v^{16} - 14448p^8v^{16} + 360192p^9v^{16} + 2493600p^{10}v^{16} + 12550416p^{11}v^{16} + 17926128p^{12}v^{16} - 259622976p^{13}v^{16} - 1931961792p^{14}v^{16} - 10550435184p^{15}v^{16} + 98937385374p^{16}v^{16} + 24p^4v^{17} - 1080p^6v^{17} - 13440p^7v^{17} - 80928p^8v^{17} - 132024p^9v^{17} + 1840776p^{10}v^{17} + 14790144p^{11}v^{17} + 73051512p^{12}v^{17} + 126567264p^{13}v^{17} - 1293631728p^{14}v^{17} - 9980137536p^{15}v^{17} - 55050628008p^{16}v^{17} + 467333743110p^{17}v^{17} + 24p^4v^{18} + 192p^5v^{18} - 8544p^7v^{18} - 95040p^8v^{18} - 569760p^9v^{18} - 1214880p^{10}v^{18} + 9797904p^{11}v^{18} + 82573800p^{12}v^{18} + 420942768p^{13}v^{18} + 807789264p^{14}v^{18} - 6273975792p^{15}v^{18} - 51221501136p^{16}v^{18} - 283516855968p^{17}v^{18} + 2204001965006p^{18}v^{18} + 24p^4v^{19} + 192p^5v^{19} + 1080p^6v^{19} + 5832p^7v^{19} - 60888p^8v^{19} - 705216p^9v^{19} - 3910368p^{10}v^{19} - 8858136p^{11}v^{19} + 46862760p^{12}v^{19} + 457439184p^{13}v^{19} + 2361075624p^{14}v^{19} + 5069434800p^{15}v^{19} - 30136593768p^{16}v^{19} - 259361429784p^{17}v^{19} - 1455780298776p^{18}v^{19} + 10398318680694p^{19}v^{19} + 192p^5v^{20} + 1080p^6v^{20} + 18912p^7v^{20} + 36720p^8v^{20} - 437952p^9v^{20} - 4512600p^{10}v^{20} - 25012512p^{11}v^{20} - 63580104p^{12}v^{20} + 220823568p^{13}v^{20} + 2449336680p^{14}v^{20} + 13097561328p^{15}v^{20} + 30177202248p^{16}v^{20} - 141380350848p^{17}v^{20} - 1306684851840p^{18}v^{20} - 7403140259952p^{19}v^{20} + 48996301350750p^{20}v^{20} - 24p^4v^{21} + 1080p^6v^{21} + 24744p^7v^{21} + 129816p^8v^{21} + 283752p^9v^{21} - 2272584p^{10}v^{21} - 28419456p^{11}v^{21} - 158605280p^{12}v^{21} - 422656608p^{13}v^{21} + 936811968p^{14}v^{21} + 12971851368p^{15}v^{21} + 71258617752p^{16}v^{21} + 177314558064p^{17}v^{21} - 655481735280p^{18}v^{21} - 6514909866600p^{19}v^{21} - 37556614417032p^{20}v^{21} + 230940534213046p^{21}v^{21} + O(v^{22})$$

- 21th order in $3D$
- 19th order in $\geq 4D$ – This extends known series for Ising model without disorder.

II. Extrapolate critical behaviour

Series $\chi(\beta) = 1 + 6v + 30v^2 + 150v^3 + 726v^4 + 3510v^5 + \cdots, \quad v = \tanh(\beta)$

- We expect finite radius β_c of convergence
- Smallest singularity at real axis corresponds to critical behaviour $\chi(\beta) \sim (\beta_c - \beta)^{-\gamma}$
- DLog Padé approximants:

  If $F(z) = \sum a_n z^n \sim A(z_c - z)^{-\gamma} + \ldots$

  then $\frac{d}{dz} \log F(z) \sim \frac{\gamma}{z_c - z} + \ldots$

  Compute $[M|N]$ Padé approximant

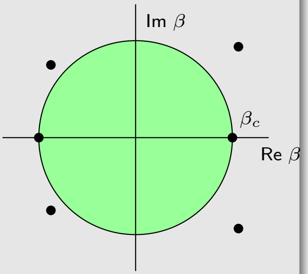
  $\mathcal{P}(z|M,N) = \frac{P_M(z)}{Q_N(z)} = \frac{p_0 + p_1 z + \ldots p_M z^M}{1 + q_1 z + \ldots q_N z^N}$

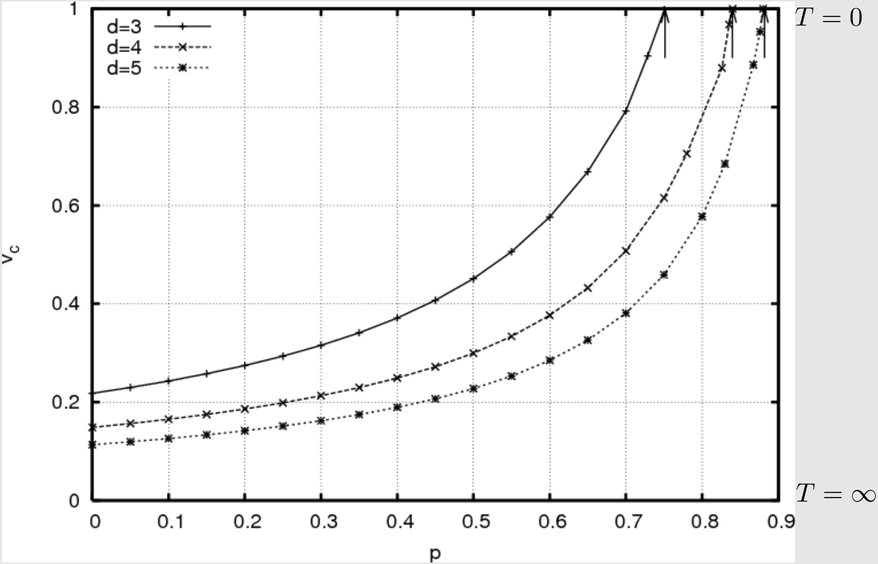
  and analyse poles and their residues
- Inhomogeneous differential approximants

  $P_1(z)\frac{\partial^2 F}{\partial z^2} + P_2(z)\frac{\partial F}{\partial z} + P_3(z)F(z) + P_4(z) = 0$

  allows for correction terms

  $\chi \sim \frac{A_0}{(\beta_c - \beta)^\gamma}\left[1 + A_1(\beta_c - \beta)^\Delta + A_2(\beta_c - \beta) + \cdots\right]$





Critical coupling v_c as function of p for $D = 3, 4, 5$.
The arrows indicate the percolation thresholds in $D = 3, 4$ and 5, resp.

Bond-diluted Ising model in 5 Dimensions

- Critical point is a Gaussian fixed point: $\gamma{=}1$
- Disorder irrelevant
- Corrections to scaling: $\chi \sim (t-t_c)^{-\gamma}(A_0 + A_1(t-t_c)^{\Delta_1} + \ldots$

Results from 19th order high-temperature series for the susceptibility χ:

- without disorder:

$$\begin{aligned} \gamma &= 1 \\ v_c &= .113425(3) \\ \Delta_1 &= 0.50(2) \end{aligned}$$

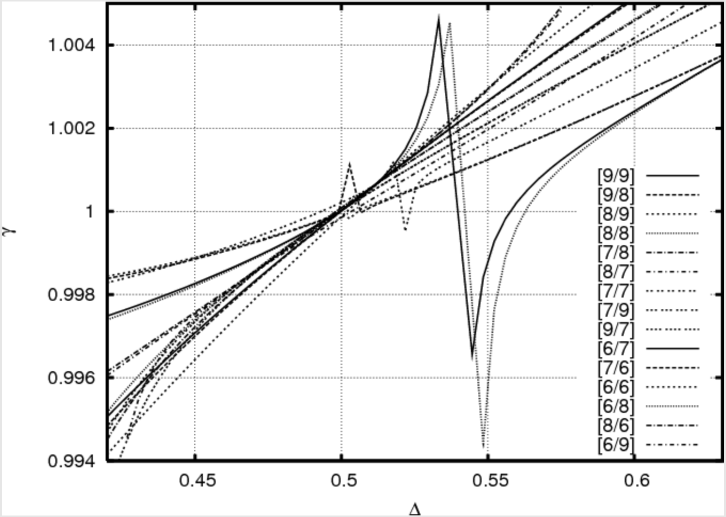
(compare MC data (*Binder et al.* 99): $v_c = 0.1134250(4)$)

- with disorder:

$$\begin{aligned} \gamma &= 1 \\ \Delta_1 &= 0.50(5) \end{aligned}$$

for large range of dilutions $p = 0 \ldots 0.7 \quad (p_c = 0.8818)$

M2 analysis



γ as function of Δ_1 for the $p = 0.5$ diluted 5D Ising model at $v_c = .227498$

Bond-diluted Ising model in 4 Dimensions

Aharony 1976:

$$\chi \sim t^{-1} |\log t|^{\frac{1}{3}} \quad \xrightarrow{\text{disorder}} \quad \chi \sim t^{-1} \exp\left(\zeta \sqrt{|\log t|}\right), \;\; \zeta = \sqrt{\frac{6}{53}} \approx 0.3364$$

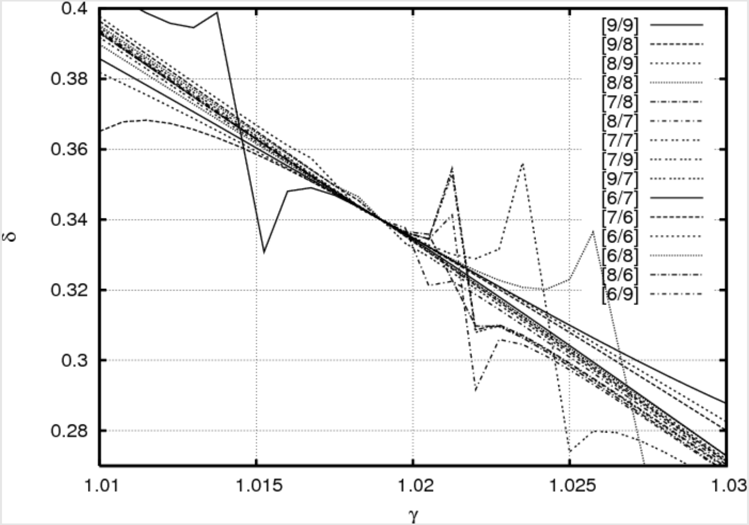
- pure case: We determine log correction (difficult to determine in MC simulations):

$$\begin{aligned} \delta &= 0.34(1) \\ v_c &= 0.148583(3) \end{aligned}$$

MC simulations (*Bittner* et al.): $v_c = 0.148589(2)$

- disordered case:

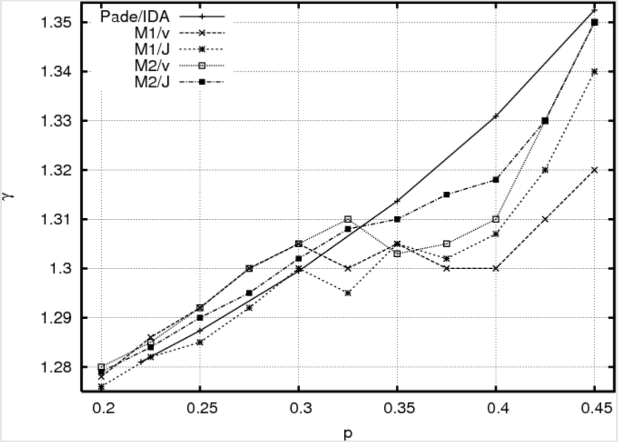
  successful fit with $t^{-1} \exp\left(\zeta \sqrt{|\log t|}\right)$ with p-dependent $\zeta = 0.2 \ldots 0.6$



$$\chi \sim t^{-\gamma} |\log t|^{\delta}$$

δ as function of γ for the pure 4D Ising model via M3 approximants at $v_c = 0.148607$

Bond-diluted Ising model in 3 Dimensions



dilution range
$p \approx 0.3 \ldots 0.4$:

$\gamma \approx 1.305$

- strong crossover effects
- slightly smaller than MC results $\gamma \approx 1.34$

Ballesteros et al. (1998): site dil.
Berche et al. (2004): bond dil.

q-state Potts model without disorder

Fortuin-Kasteleyn cluster representation

$$\mathcal{Z} = \mathrm{Tr}\,\exp\left(-\beta J \sum_{<ij>} \delta(S_i, S_j)\right)$$
$$= \sum_{\text{cluster } C} q^{\#\text{conn. comp.}(C)} (e^{\beta J} - 1)^{\#\text{edges}(C)}$$

$q \to 1$ limit describes bond percolation with $p = 1 - e^{-\beta J}$.
Scaling near p_c:

- Cluster size distribution

$$n(s,p) \sim s^{-\tau} f((p_c - p) s^{\sigma})$$

- mean cluster size

$$\left\langle \sum_s s^2 n(s,p) \right\rangle \sim (p_c - p)^{-\gamma}, \qquad \gamma = \frac{3-\tau}{\sigma}$$

Percolation thresholds (bond percolation on $\mathbb{Z}^d$) and critical exponents

Dim.	Methods	p_c	σ	τ	$\gamma = \frac{3-\tau}{\sigma}$
2	exact, CFT	$\frac{1}{2}$	$\frac{36}{91}$	$\frac{187}{91}$	$\frac{43}{18}$
3	MC (Lorenz and Ziff 1998)	$0.248\,812(2)$	$0.453(1)$	$2.189(1)$	$1.795(5)$
	HTS (Adler *et al.* 1990)	$0.248\,8(2)$			$1.805(20)$
	MCS (Ballesteros *et al.* 1999)		$0.4522(8)$	$2.18906(6)$	$1.7933(85)$
	MCS (Deng and Blöte 2005)		$0.4539(3)$	$2.18925(5)$	$1.7862(30)$
	present work	$0.248\,91(10)$			$1.804(5)$
4	HTS (Adler *et al.* 1990)	$0.160\,05(15)$			$1.435(15)$
	MCS (Ballesteros *et al.* 1997)				$1.44(2)$
	MC (Paul *et al.* 2001)	$0.160\,130(3)$		$2.313(3)$	
	MC (Grassberger 2003)	$0.160\,131\,4(13)$			
	present work	$0.160\,08(10)$			$1.435(5)$
5	HTS (Adler *et al.* 1990)	$0.118\,19(4)$			$1.185(5)$
	MC (Paul *et al.* 2001)	$0.118\,174(4)$		$2.412(4)$	
	MC (Grassberger 2003)	$0.118\,172(1)$			
	present work	$0.118\,170(5)$			$1.178(2)$
6	RG (Essam *et al.* 1978)		$\frac{1}{2}$	$\frac{5}{2}$	$\chi \sim t^{-1}\lvert\ln t\rvert^{\delta}$ $\delta = \frac{2}{7}$
	HTS (Adler *et al.* 1990)	$0.094\,20(10)$			
	MC (Grassberger 2003)	$0.094\,201\,9(6)$			
	present work	$0.094\,202\,0(10)$			$\delta = 0.40(2)$
> 6	RG		$\frac{1}{2}$	$\frac{5}{2}$	1

MC=Monte Carlo, MCs = Monte Carlo, site percolation, HTS= High-temperature series

Large dimension expansion for q-state Potts model

Critical point equation $1/\chi(D, v_c) = 0$ can be iteratively solved:
Large-D expansion for v_c in terms of $\sigma = 2D - 1$

$$v_c(q,\sigma) = \frac{1}{\sigma}\Bigg[1 + \frac{8-3q}{2\sigma^2} + \frac{3(8-3q)}{2\sigma^3} + \frac{3\left(68-31q+q^2\right)}{2\sigma^4} + \frac{8664-3798q-11q^2}{12\sigma^5}$$

$$+ \frac{78768-36714q+405q^2-50q^3}{12\sigma^6}$$

$$+ \frac{1476192-685680q-2760q^2-551q^3}{24\sigma^7}$$

$$+ \frac{7446864-3524352q-11204q^2-6588q^3-9q^4}{12\sigma^8} + \cdots\Bigg]$$

Percolation thresholds p_c for hypercubic lattices

Dim.	Series exp.	MC data (Grassberger 2002)	$1/D$-expansion
5	0.118165(10)	0.118172(1)	0.118149
6	0.0942020(10)	0.0942019(6)	0.0943543
7	0.078682(2)	0.0786752(3)	0.0786881
8	0.067712(1)	0.06770839(7)	0.0677080
9	0.059497(1)	0.05949601(5)	0.0594951
10	0.0530935(5)	0.05309258(4)	0.05309213
11	0.0479503(1)	0.04794969(1)	0.04794947
12	0.0437241(1)	0.04372386(1)	0.04372376
13	0.0401877(1)	0.04018762(1)	0.04018757
14	0.0371838(1)		0.03718368

Spanning forests

The limit $q \to 0$ of the q-state Potts model describes an ensemble of spanning forests, i.e., tree-like clusters covering the lattice.

- Equivalent to bond percolation with the nonlocal constraint that clusters are free of loops: tree percolation
- $d > 2$: phase transition at some v_c:
  - $v < v_c$: forests consist of small trees
  - at v_c: one component of the forest percolates
  - $v > v_c$: ensemble is dominated by configurations where a single infinite tree covers a finite fraction of the lattice
  - $v \to 1$: this fraction approaches 1: spanning trees
- $d = 2$: phase transition only in the antiferromagnetic regime $v_c < 0$.
- Fermionic field theory with $OSp(1|2)$ supersymmetry:

$$\mathcal{L} = \int \mathcal{D}(\psi, \bar{\psi}) \exp\left[\bar{\psi}\Delta\psi + t\sum_i \bar{\psi}_i\psi_i - t\sum_{\langle i,j\rangle} \bar{\psi}_i\psi_i\bar{\psi}_j\psi_j\right]$$

Critical properties of spanning forests

Table: Critical points for hypercubic lattices $\mathbb{Z}^D$ for dimensions $D \geq 3$.

	MC (Deng, Garoni, Sokal 2007)		HT series	
D	v_c	γ	v_c	γ
3	0.433 65(2)	2.77(10)	0.433 33(5)	2.785(5)
4	0.210 302(10)	1.73(3)	0.209 97(3)	1.71(1)
5	0.140 36(2)	1.22(6)	0.140 31(3)	1.31(1)
6			0.106 68(3)	1.0(1)
7			0.086 74(1)	1.00(2)

- Upper critical dimension is $d = 6$ with logarithmic corrections $\chi \sim (v_c - v)^{-1}(\log(v_c - v))^{\delta}$, $\delta = 0.65(5)$

Conclusions

- Series expansion techniques are an interesting mixture of combinatorics, graph theory, computer algebra . . .
- Quenched disorder average can be treated exactly
- Easily extendable to different dimensions
- Large parameter spaces $(d, q, p, ...)$ can be scanned
- But need sophisticated extrapolation techniques to get critical behaviour
- ...and higher-order expansions are not really straightforward to generate