Fortuin-Kasteleyn Versus Geometrical Clusters — Fractal Dimensions and Critical Exponents

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Workshop
Statistical Geometry and Field Theory
KITP, UC Santa Barbara, California, USA
6 September 2006
Motivation

- Understand ("picture") phase transitions in terms of geometrical objects:
  - spin clusters in simple magnets
  - vortex lines in superfluid helium
  - dislocation and disclination lines in crystals
  - surfaces of evolving strings
  - ...
- Does their proliferation and percolation behaviour encode the standard critical behaviour?
- Use simple models (Ising, Potts, XY, ...) to highlight the basic features
- In 2D, rich interplay between numerical analysis and theoretical predictions (conformal field theory, Coulomb gas mappings, ...) ...
- ...and, more recently, even mathematically rigorous statements via SLE (= Stochastic Loewner Evolution)

Geometric vs. Stochastic Clusters

$100 \times 100$ Ising model: black = spin “up”, white = spin “down”

HOT

$T = 2T_c$

CRITICAL

$T = 1.02 \ T_c$

Which type of cluster do we “see” (and intuitively interprete)?
Clearly, these are geometric clusters which

- in 2D have their percolation point at the thermodynamically determined $T_c$
- show fractal behaviour and critical scaling . . .
Clearly, these are geometric clusters which

- in 2D have their percolation point at the thermodynamically determined $T_c$
- show fractal behaviour and critical scaling . . .
- . . . but do not encode the proper (thermodynamic) critical exponents
- in 3D do not start percolating at $T_c$ ($T_p < T_c$)
Stochastic clusters: Fortuin-Kasteleyn cluster representation of the Ising model:

\[
Z = \sum_{\{\sigma_i\}} \exp \left( \beta \sum_{\langle ij \rangle} \sigma_i \sigma_j \right) = \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} e^{\beta \left( (1 - p) + p \delta_{\sigma_i \sigma_j} \right)}
\]

\[
= \sum_{\{\sigma_i\}} \sum_{\{n_{ij}\}} \prod_{\langle ij \rangle} e^{\beta \left( (1 - p) \delta_{n_{ij},0} + p \delta_{\sigma_i \sigma_j} \delta_{n_{ij},1} \right)}
\]

\[ p = 1 - e^{-2\beta} \]

\[ \rightarrow \] Bonds between like spins are stochastically broken with probability \( p = 1 - e^{-2\beta} \)

(basis for Swendsen-Wang and Wolff cluster update algorithms)
Fortuin-Kasteleyn Coniglio Klein Stochastic Clusters
Fractal structure of spin clusters and domain walls

From general percolation theory: Distribution of spin clusters and their boundaries can be parameterized as ($n = \text{mass of cluster, size of boundary}$):

$$\ell_n \sim n^{-\tau} e^{-\theta n}$$

with

$$\theta \propto |T - T_p|^{1/\sigma}$$

(i) Entropy factor governed by exponent $\tau$

(ii) Boltzmann weight governed by exponent $\sigma$; suppresses large clusters when $\theta$ is non-zero

2D Ising model at criticality ($\theta = 0$), stochastic Fortuin-Kasteleyn clusters:

$$\tau = 31/15$$
Percolation Observables

- Percolation strength (magnetization) $P_\infty$: fraction of sites in the largest cluster

- Average cluster size (susceptibility): $\chi = \sum_n n^2 \ell_n / \sum_n n \ell_n$

Finite-size scaling close to percolation threshold:

$$P_\infty = L^{-\beta/\nu} P(L/\xi), \quad \chi = L^{\gamma/\nu} \chi(L/\xi)$$

$$\frac{\beta}{\nu} = d \frac{\tau - 2}{\tau - 1}, \quad \frac{\gamma}{\nu} = d \frac{3 - \tau}{\tau - 1}$$

This gives:

$$\tau = \frac{3 \beta + 2 \gamma}{\beta + \gamma}$$

2D Ising model: $\beta = 1/8$, $\gamma = 7/4 \Rightarrow \tau = 31/15$
Fractal Dimension

Radius of gyration (cf. polymer physics):

\[ R_n^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2 \sim n^{2/D} \]

- \( \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \)
- **\( D \): Hausdorff or fractal dimension**
  (random walk: \( D = 2 \))

\( R_n \) related to correlation length \( \xi \):

\[ \xi \sim |T - T_c|^{-\nu} \quad \Rightarrow \quad \sigma = \frac{1}{\nu D} \quad \text{also} \quad \tau = \frac{d}{D} + 1 \]

Scaling laws \( \Rightarrow \) all critical exponents from cluster distribution

\[ l_n(T) \propto n^{-\tau} e^{-\theta n}, \quad \theta \propto |T - T_p|^{1/\sigma} \]
Monte Carlo Simulations (SW Cluster Update)

2D Ising model, cluster mass $C$:

**Stochastic** clusters: $P_\infty$ and $\chi$ standard improved estimators; finite-size scaling fits at criticality ($L = 64 - 512$) yield (the expected results):

$$\gamma_{FC} / \nu = 1.7505(12) \approx 7/4 \, , \, \beta_{FC} / \nu = 0.1248(8) \approx 1/8$$

**Geometric** clusters: Finite-size scaling fits at criticality ($L = 64 - 512$) yield:

$$\gamma_{GC} / \nu = 1.8951(5) \approx 91/48 = 1.8958 \, , \, \beta_{GC} / \nu = 0.0527(4) \approx 5/96 = 0.0521$$

![Graph showing $\chi$ vs. $L$ for different cluster types]

Straight lines $\propto L^{91/48}$

Where are these strange exponents coming from?
Conformal Field Theory in a Nut-Shell

2D $q$-state Potts model parametrization (SLE notation) [Nienhuis, Duplantier, Saleur, Schramm]:

$$\sqrt{q} = -2 \cos(\pi/\bar{\kappa}), \quad 2 \geq \bar{\kappa} \geq 1$$

Central charge:

$$c = 1 - 6(1 - \bar{\kappa})^2/\bar{\kappa}$$

Critical exponents:

$$\nu = \frac{2}{32 - 3\bar{\kappa}}, \quad \eta_C = 2 - 1/\bar{\kappa} - 3\bar{\kappa}/4, \quad \sigma_C = \frac{12\bar{\kappa}(2 - \bar{\kappa})}{3\bar{\kappa}^2 + 8\bar{\kappa} + 4}, \quad \tau_C = \frac{3\bar{\kappa}^2 + 24\bar{\kappa} + 4}{3\bar{\kappa}^2 + 8\bar{\kappa} + 4}$$

Fractal dimension:

$$D_C^{FK} = 1 + 1/2\bar{\kappa} + 3\bar{\kappa}/8$$

This describes the fractal and scaling properties of stochastic Fortuin-Kasteleyn clusters.

Special cases:

$$\bar{\kappa} = 2 \Rightarrow q = 0 \text{ (tree percolation)}, \quad \bar{\kappa} = 3/2 \Rightarrow q = 1 \text{ ((uncorrelated) percolation)}, \quad \bar{\kappa} = 4/3 \Rightarrow q = 2 \text{ (Ising model)}, \quad \bar{\kappa} = 6/5 \Rightarrow q = 3, \quad \bar{\kappa} = 1 \Rightarrow q = 4$$
For a given central charge $c$, there are two solutions for $\kappa$:

$$\kappa_{\pm} = \frac{13 - c \pm \sqrt{(c - 25)(c - 1)}}{12}$$

with $\kappa_+\kappa_- = 1$

where $\kappa \equiv \kappa_+ \geq 1$ (and hence $\kappa_- \leq 1$). The substitution ("duality map") [Duplantier]

$$\kappa \rightarrow 1/\kappa$$

in the various critical exponent expressions yields the corresponding critical exponents for the geometric clusters, e.g.

$$D_{FK}^C = 1 + 1/2\kappa + 3\kappa/8 \rightarrow D_{C}^G = 1 + \kappa/2 + 3/8\kappa$$

$\kappa_- = 1/\kappa_+$ describes the tri-critical branch for the same value of $c$ (but, in general, another value of $q$). In the Ising case, the tri-critical model is realized by the diluted $q = 1$ Potts model [Vanderzande, Coniglio, . . . ].

**2D Ising model:**

$q = 2 \Rightarrow \kappa = 4/3 \Rightarrow D_{C}^G = 187/96 \Rightarrow \gamma_{C}^G/\nu = 2D_{C}^G - 2 = 91/48$
Hull & External Perimeter

Part of a single stochastic Fortuin-Kasteleyn cluster of nearest-neighbour sites (filled circles) connected by bonds (black links):

Sites belonging to the hull (blue filled circles) are found by allowing the random walker tracing out the boundary to move only over set bonds.

Sites belonging to the external perimeter (blue filled circles) are found by allowing the random walker to move to a nearest neighbor on the cluster irrespective whether the connecting bond is set or not.

The external perimeter, which contains two sites less than the hull for this boundary segment, is therefore a smoother version of the hull.
Conformal Field Theory Predictions

Stochastic Fortuin-Kasteleyn clusters:

\[ D_{\text{H}}^{\text{FK}} = 1 + \frac{\kappa}{2}, \quad D_{\text{EP}}^{\text{FK}} = 1 + \frac{1}{2\bar{\kappa}} \]

satisfying

\[ (D_{\text{H}}^{\text{FK}} - 1)(D_{\text{EP}}^{\text{FK}} - 1) = \frac{1}{4} \]

and implying

\[ \gamma_{\text{H}}^{\text{FK}} / \nu = \bar{\kappa}, \quad \gamma_{\text{EP}}^{\text{FK}} / \nu = 1/\bar{\kappa} \]

Geometric clusters:

Distinction between hull and external perimeter is non-sensical,

\[ D_{\text{EP}}^{\text{G}} = D_{\text{H}}^{\text{G}} \]

Duality map \( \bar{\kappa} \rightarrow 1/\bar{\kappa} \) yields

\[ D_{\text{H}}^{\text{G}} = D_{\text{EP}}^{\text{FK}}, \quad \gamma_{\text{H}}^{\text{G}} / \nu = \gamma_{\text{EP}}^{\text{FK}} / \nu = 1/\bar{\kappa} \]

Recall: 2D Ising model has \( \bar{\kappa} = 4/3 \)
Monte Carlo Simulations (SW Cluster Update)

Stochastic clusters

Fit \((L = 8 - 48)\): \(0.310L^{1.329}\) – but problems asymptotically (exponent too small)

Geometric clusters

Straight line: \(\propto L^{3/4}\) – but strong corrections to scaling

\(\Rightarrow\) All numerical data compatible with theoretical conjectures

Fit \((L = 64 - 512)\): \(1.388L^{0.736}\)
Distributions

\[ \ell_n \sim n^{-\tau} \]

Spin Clusters on Dynamical Triangulations

Use standard KPZ formula for dressing of conformal weights $\Delta$:

\[
\tilde{\Delta} = \frac{\sqrt{1 - c + 24\Delta} - \sqrt{1 - c}}{\sqrt{25 - c} - \sqrt{1 - c}}
\]

Relation with fractal dimension of clusters:

\[
\Delta_C = \beta / d\nu = 1 - D_C / d
\]

Explicitly for the Ising model (with $d = 2$, $c = 1/2$):

\[
\begin{align*}
D_C^{FK} / d &= 15/16 \quad \text{Fortuin-Kasteleyn clusters} \\
D_C^G / d &= 187/192 \quad \text{geometric clusters}
\end{align*}
\]

such that ($d_h \approx 4$)

\[
\begin{align*}
\tilde{D}_C^{FK} / d_h &= 5/6 \quad \text{Fortuin-Kasteleyn clusters} \\
\tilde{D}_C^G / d_h &= 11/12 \quad \text{geometric clusters}
\end{align*}
\]
Monte Carlo Simulations

Non-degenerate dynamical triangulations with \( N_2 \) Ising spins on the faces (corresponding to dual one-point irreducible \( \phi^3 \) Feynman diagrams with Ising spins on the vertices):

\[
\beta_c = \frac{1}{2} \ln \frac{108}{23} \approx 0.7733
\]

Measuring average cluster sizes in a Swendsen-Wang cluster simulation, i.e., the susceptibility \( \chi \), and performing a finite-size scaling analysis at \( \beta_c \):

\[
\chi \propto N_2^{\gamma/d_h \nu} = N_2^{2 \tilde{D}_C/d_h - 1}
\]

Result (\( N_2 = 8192, \ldots, 65536 \)):

\[
\begin{align*}
\tilde{D}_C^{\text{FK}}/d_h &= 0.84301(93) \approx 5/6 = 0.83333 \ldots \\
\tilde{D}_C^{\text{G}}/d_h &= 0.92220(55) \approx 11/12 = 0.91666 \ldots
\end{align*}
\]
Large fractal dimension $d_h \approx 4 \Rightarrow$ small effective linear extent $L = N_2^{1/d_h} \Rightarrow$ strong corrections to scaling: Use ansatz

$$L_{\text{eff}}(N_2) = L_0 N_2^{1/d_h} + L_1 + L_2 N_2^{-1/d_h} + \ldots$$

and fit

$$\chi = [L_{\text{eff}}(N_2)]^{\gamma/\nu}$$

Fixing $d_h = 4$ and using only $L_1$-term, i.e., $L_2 \equiv 0$ ($N_2 = 1024, \ldots, 65536$):

$$\tilde{D}_C^{\text{FK}} / d_h = 0.8291(19) \approx 5/6 = 0.8333 \ldots \quad \text{Fortuin-Kasteleyn clusters}$$

$$\tilde{D}_C^{G} / d_h = 0.9132(12) \approx 11/12 = 0.9166 \ldots \quad \text{geometric clusters}$$

$\Rightarrow$ statistically fully consistent

Generalization to $q$-state Potts model and cluster boundaries possible. Duality relation $\kappa \to 1/\kappa$ between Fortuin-Kasteleyn and geometric clusters lost after “dressing” for Ising spins coupled to dynamical triangulations.

High-Temperature Representation MC Simulations

\[ Z = (\cosh \beta)^{2N} e^{2N \sum_{\text{closed graphs}} v^n}, \quad e^{\beta S_i S_j} = \cosh \beta (1 + v S_i S_j) \]

w/ \( v = \tanh \beta \), \( n \): \# links in graph

Monte Carlo

- Plaquette \( \square \) update
- Acceptance rate: \( p_{HT} = \min \left( 1, v^{n'-n} \right) \)

Phase transition: Proliferation of high-temperature graphs

Monte Carlo Results

Percolation strength

Average graph size

\[ \therefore \beta_G = 0.627(8) \approx \frac{5}{8} \]

\[ \therefore \gamma_G = 0.748(6) \approx \frac{3}{4} \]
Outlook

Collapsing planar loops (2D $O(N)$ models):

Include vacancies: tend to compress loops ($\bowtie$ attraction between monomers)

- High-temperature graphs proliferate @ tri-critical point ($\Theta$ point of polymers)
- High-temperature graphs of tri-critical $O(N)$ model $\bowtie$
  Hulls of critical Potts (Fortuin-Kasteleyn) clusters
- Predictions:

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<td>$\frac{1}{4}$</td>
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<td>$\frac{3}{2}$</td>
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[Guo, Blöte & Liu, 2004]
**Vortex loops** in 3D $|\phi|^4$ theory:

$T < T_c$

$T > T_c$

Spanning probability

\[ L = 22 \quad L = 24 \quad L = 26 \quad L = 28 \quad L = 32 \quad L = 36 \quad L = 40 \]

\[ \therefore \text{Vortex proliferation } @ \; T_p \]

Scaled spanning probability

\[ \therefore \; \nu = \nu_{XY} \]

Loop-length distribution

\[ \therefore \text{Power law } @ \; T_p \]

- Very similar concepts employed
- (Stochastic) vortex connectivity definition such that percolation point does coincide with thermodynamic \( T_c \) ?
Monopoles, anti-monopoles and vortex lines in 3D compact Abelian Higgs model:

Euclidean lattice action $S = S_g + S_\phi$ with

$$S_g = \beta \sum_{x, \mu < \nu} [1 - \cos \theta_{\mu \nu}(x)]$$

$$S_\phi = -\kappa \sum_{x, \mu} \rho(x) \rho(x + \mu) \cos [\Delta_\mu \varphi(x) - q\theta_\mu(x)] + \sum_x \left\{ \rho^2(x) + \lambda \left[ \rho^2(x) - 1 \right]^2 \right\}$$

$\beta = 1.1$ → Kertesz line

(Point-like) monopoles and anti-monopoles connected by vortex lines

Work partially supported by Deutsche Forschungsgemeinschaft (DFG) under grant JA483/17-3 and the EU RTN-Network ‘ENRAGE’: *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics* under grant No. MRTN-CT-2004-005616.

THANK YOU!