Critical geometry approach to three-dimensional percolation

Alessandro Galvani
with Giacomo Gori and Andrea Trombettoni

May 6, 2021

- Uniformization hypothesis for bounded domains
- Yamabe equation
- Correlation functions
- Fractional Yamabe equation
  - Computing the fractional Laplacian
  - Ising and XY models
- Percolation
- Conclusions and work in progress

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Bounded critical systems

Why study critical systems with boundaries?

- Important to compare with experiments
- Bulk universal quantities can be computed from them
- Many interesting phenomena are observed in bounded systems at criticality
- Necessary to interpret numerical simulations

We will focus on systems with **Fixed** Boundary Conditions: aligned spins on the boundaries, e.g on the edges of a slab $\rightarrow$ diverging order parameter *after rescaling*

Uniformization hypothesis

Introducing a boundary breaks translational and conformal invariance

Is there a way to put bulk and boundary on the same footing?

Uniformization hypothesis

Introducing a boundary breaks translational and conformal invariance

Is there a way to put bulk and boundary on the same footing?

1. A metric with negative curvature sets the boundary infinitely far away
2. Requiring homogeneity in the system means the curvature must be constant
3. The system has to be locally euclidean

[Giacomo Gori and Andrea Trombettoni. Geometry of bounded critical phenomena. JSTAT, 2020]

Metric and curvature

- To preserve local properties, a natural way is to pick a metric in the same conformal class as the euclidean metric

$$\delta_{ij} \to g_{ij} = \frac{\delta_{ij}}{\gamma(x)^2}, \qquad i, j = 1, \ldots, d$$

  $\gamma(x)$ is a point-dependent scale factor
- From g we can compute the Christoffel symbols, the Ricci tensor and then the Ricci scalar

$$\Gamma^i_{jk} = \frac{1}{2} g^{il} \left(\partial_k g_{lj} + \partial_j g_{lk} - \partial_l g_{jk} \right)$$
$$R_{ij} = \partial_l \Gamma^l_{ji} - \partial_j \Gamma^l_{li} + \Gamma^l_{lm} \Gamma^m_{ji} - \Gamma^l_{jm} \Gamma^m_{li}$$
$$R = R_{ij} g^{ij}$$

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Yamabe problem

- The requirement of uniform curvature, written for $\gamma(x)$, gives us the Yamabe equation:

$$\boxed{(-\triangle)\gamma(x)^{-\frac{d-2}{2}} = -\frac{d(d-2)}{4}\gamma(x)^{-\frac{d+2}{2}}}$$

- The problem can be framed more generally:
  given a smooth manifold with a Riemann metric g, is it always possible to find a metric in the same conformal class as g with constant scalar curvature?

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- The problem can be framed more generally:
  given a smooth manifold with a Riemann metric g, is it always possible to find a metric in the same conformal class as g with constant scalar curvature?

- **Yes**, provided the manifold is compact
  [Hidehiko Yamabe. On a deformation of riemannian structures on compact manifolds. Osaka Mathematical Journal, 1960]

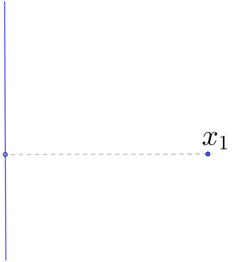
Solutions of the Yamabe equation: half-space

Exact solutions are available in a few interesting cases

- For a half space, $x_1 > 0, x_2 \ldots x_d \in \mathbb{R}^{d-1}$: γ only depends on the transverse coordinate x_1

$$\triangle \gamma(x)^{-\frac{d-2}{2}} \to \frac{d^2}{dx_1^2}\gamma(x_1)^{-\frac{d-2}{2}}$$

$$\gamma(x) = x_1$$



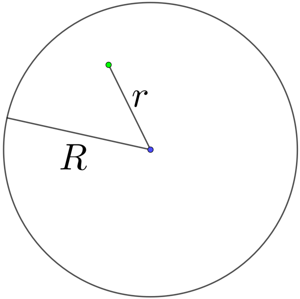
[John M Lee, Thomas H Parker, The Yamabe problem. Bulletin of the American Mathematical Society, 1987]

Solutions of the Yamabe equation: ball

- For a ball of radius R in any d

$$\gamma(r) = \frac{R^2 - r^2}{2R}$$

Notice that $\gamma = 0$ on the boundary



The half-space and ball solutions actually construct the hyperbolic space $\mathbb{H}^d$ [John M Lee, Thomas H Parker,The Yamabe problem.

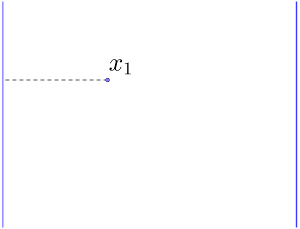
Bulletin of the American Mathematical Society, 1987]

Solutions of the Yamabe equation: slab

- For a slab $-1 < x_1 < 1, x_2 \cdots x_d \in \mathbb{R}^{d-1}$, a solution for any d is found in the inverse function $x_1(\gamma)$.

$$\pm x_1(\gamma) = 1 - {}_2F_1\left(\frac{1}{2}, \frac{1}{d}; 1 + \frac{1}{d}; \left(\frac{\gamma}{\gamma_0}\right)^d\right)$$

$$\gamma_0 = \frac{\Gamma(\frac{1}{2} + \frac{1}{d})}{\sqrt{\pi}\Gamma(1 + \frac{1}{d})}$$



For $d = 2, 3, 4, 6$ it can be inverted
[Alessandro Galvani, Giacomo Gori, and Andrea Trombettoni. Magnetization profiles at the upper critical dimension as solutions of the integer Yamabe problem, arXiv:2103.12449]

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Correlation functions

- For a rescaling of the domain $\Omega \to \lambda\Omega$, $\gamma(x)$ and one-point functions of scaling fields at the critical point are required to transform as

$$\gamma_{\lambda\Omega}(\lambda x) = \lambda\gamma_{\Omega}(x), \qquad \langle\varphi_{\lambda\Omega}(\lambda x)\rangle = \lambda^{-\Delta_\varphi} \langle\varphi_{\Omega}(x)\rangle$$

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Main (naïve) conjecture:
Correlation functions can be expressed through $\gamma(x)$

$$\langle\varphi(x)\rangle = \frac{\alpha}{\gamma(x)^{\Delta_\varphi}}$$

$$\langle\varphi(x)\varphi(y)\rangle = \gamma(x)^{-\Delta_\varphi}\gamma(y)^{-\Delta_\varphi}\mathcal{F}\left(\mathcal{D}_g(x,y)\right)$$

- $\mathcal{F}\left(\mathcal{D}_g(x,y)\right)$ is an unknown function of the distance computed with the metric $g_{ij} = \delta_{ij}/\gamma^2(x)$.

But...

Yamabe equation as mean field of $O(N)$ theories

- At the upper critical dimension $d = d_c$, the anomalous dimension vanishes, that is $\Delta_\phi = \frac{d-2}{2}$. Of course, for $d = 4$, $\Delta_\phi = 1$
- The Yamabe equation in this case can be seen as the mean field equation for an $O(N)$ theory

$$m(x) = \langle \phi(x) \rangle = \alpha \gamma(x)^{-\frac{d-2}{2}}$$

$$\triangle \gamma(x)^{-\frac{d-2}{2}} \propto \gamma(x)^{-\frac{d+2}{2}} \rightarrow \triangle m(x) \propto m(x)^{\frac{d+2}{d-2}}$$

- The (integer) Yamabe equation, then, cannot describe models at $d < d_c$!

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Fractional Yamabe equation

- We can try and modify the exponent of $\gamma(x)$ to include the anomalous dimension

$$(-\triangle)\gamma(x)^{-\Delta_\phi} = k\gamma(x)^{\Delta_\phi - d} \qquad ?$$

- Now, however, the equation does not scale correctly
- A way out is to change the exponent of the Laplacian as well, turning it into a fractional Laplacian

$$\boxed{(-\triangle)^{\frac{d}{2}-\Delta_\phi}\gamma_{(\Delta_\phi)}(x)^{-\Delta_\phi} = k\gamma_{(\Delta_\phi)}(x)^{\Delta_\phi - d}}$$

$$k = \frac{\Upsilon(\Delta_\phi)}{\Upsilon(d-\Delta_\phi)}, \qquad \Upsilon(x) = \Gamma(1-x)\cos(\pi x/2)$$

Fractional Yamabe equation (II)

$$\boxed{(-\triangle)^{\frac{d}{2}-\Delta_\phi}\gamma_{(\Delta_\phi)}(x)^{-\Delta_\phi} = k\gamma_{(\Delta_\phi)}(x)^{-d+\Delta_\phi}}$$

- This corresponds to making the so-called fractional Q-curvature constant
- Not discussed in the following:
  - For any d, Cardy's results for the half-space are retrieved [John Cardy. Conformal invariance and surface critical behavior. Nuclear Physics B, 1984]
  - In the $d = 2$ case the structure of correlators is reproduced

    [Giacomo Gori and Andrea Trombettoni. Geometry of bounded critical phenomena. JSTAT, 2020]

Fractional Laplacian

- $(-\triangle)^s$ is a non-local operator
- It has many definitions, which are equivalent in $\mathbb{R}^d$

$$(-\triangle)^s f(x) = \int \tilde{f}(k) e^{ikx} |k|^{2s} d^d k$$

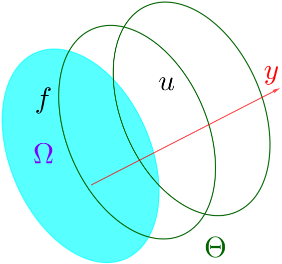
$$(-\triangle)^s f(x) = c_{d,s} \int \frac{f(x) - f(y)}{|x-y|^{d+2s}} d^d y$$

[Mateusz Kwaśnicki, Ten equivalent definitions of the fractional laplace operator. Fractional Calculus and Applied Analysis, 2017]

... however, they are not equivalent in bounded domains

Fractional Laplacian as an extension problem

- We want to compute $(-\triangle)^{1/2} f(x)$, for $x \in \Omega$
- Define a $d+1-$dimensional space $\Theta = \Omega \times \mathbb{R}^+$ by adding an auxiliary coordinate y, so that for $y = 0$ we recover Ω
- Define a harmonic function u on Θ, with f as its boundary condition



Fractional Laplacian as an extension problem

$$\triangle_{(d+1)} u(x,y) = \triangle_{(d)} + \partial_y^2 u = 0, \qquad u(x,0) = f(x)$$

Then,

$$(-\triangle)^{1/2} f(x) = -\partial_y u(x,0)$$

Because

$$(-\triangle)^{1/2}(-\triangle)^{1/2} f(x) = \partial_y^2 u(x,0) = -\triangle_{(d)}\, u(x,0) = -\triangle_{(d)}\, f(x)$$

- $(-\triangle)^{1/2}$ is a Dirichlet to Neumann operator

[Luis Caffarelli and Luis Silvestre. An extension problem related to the fractional laplacian. Comm. in PDE, 2007]

Fractional Laplacian in bounded domains

- The bounded space Ω has metric g
- Define g_+ on Θ such that $g_+ \approx g/y^2$ as $y \to 0$
- Solve the eigenvalue problem for $U \in \Theta$

$$\begin{cases} (-\triangle_{g_+})U = \Delta_\varphi(d-\Delta_\varphi)U \\ U = y^{\Delta_\varphi} F_I + y^{d-\Delta_\varphi} F_O \end{cases}$$

- $\triangle_{g_+}$ is the Laplace-Beltrami operator for the metric g_+

$$\triangle_{g_+} U = \frac{1}{\sqrt{|g_+|}} \partial_i \left(\sqrt{|g_+|} g_+^{ij} \partial_j \right)$$

If $\quad \lim_{y\to 0} F_I = f_I, \quad \lim_{y\to 0} F_O = f_O,$

$$(-\triangle)^{\frac{d}{2}-\Delta_\varphi} f_I = k\, f_O$$

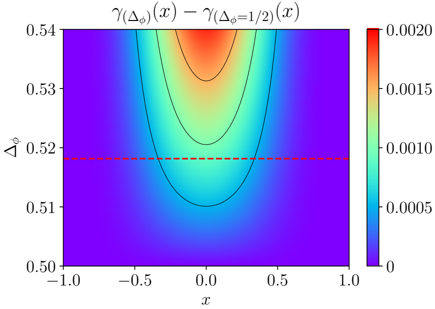
[C. Robin Graham and Maciej Zworski. Scattering matrix in conformal geometry. Inventiones Mathematicae, 2003]

Integer vs fractional Yamabe

$$\boxed{(-\triangle)^s \gamma_{(\Delta_\phi)}(x)^{-\Delta_\phi} = k\gamma_{(\Delta_\phi)}(x)^{-2s-\Delta_\phi}}$$

Currently there is no way to obtain the fractional solution perturbatively, when s is close to 1

For the 3d Ising model, $s = 1 - \frac{\eta}{2} \approx 0.98$
The fractional Yamabe profile is not that different: is it worth the hassle?



We can test the conjecture and the difference between the two with the 3d Ising and XY models
[Giacomo Gori and Andrea Trombettoni. Geometry of bounded critical phenomena. JSTAT, 2020]

Simulation of the Ising model

- Universality allows the choice of a more convenient model in the Ising class
- We use the improved Blume-Capel model

$$\beta H = -\beta \sum_{\langle ij \rangle} s_i s_j + D \sum_i s_i^2, \qquad s_i = \pm 1, 0$$

$$\beta_c = 0.387721735(25), \qquad D = 0.655$$

[Martin Hasenbusch. Finite size scaling study of lattice models in the three-dimensional ising universality class. PRB, 2010]

Testing the conjecture: 3d Ising

- The lattice is a $L \times 6L \times 6L$ slab, with $L = 24, \dots, 192$
- The data for different sizes collapse to

$$\langle \phi(x) \rangle = \alpha \left[L\gamma \left(\frac{x}{1 + a/L} \right) \right]^{-\Delta_\phi}$$

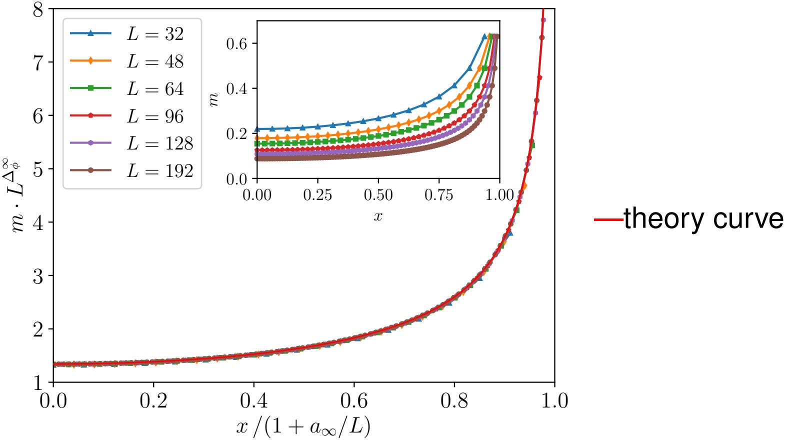
where a is the **extrapolation length**

[H. W. Diehl. The Theory of boundary critical phenomena. Int. J. Mod. Phys., 1997]

- Δ_ϕ can be obtained as a fit parameter, by choosing

$$\gamma = \gamma_{\Delta_\phi}, \qquad \text{(or, as a check} \qquad \gamma = \gamma_{\text{Integer Yamabe}})$$

Ising magnetization profile



[Giacomo Gori and Andrea Trombettoni. Geometry of bounded critical phenomena. JSTAT, 2020]

Δ_ϕ comparison

Linear size L	Δ_ϕ **FYE profile fit**	Δ_ϕ **YE profile fit**
32	0.52287(24)	0.52570(17)
48	0.51955(21)	0.52200(15)
64	0.51812(13)	0.52038(7)
96	0.51812(7)	0.51983(3)
128	0.51811(5)	0.51931(3)
192	0.518150(22)	0.518923(15)

$$\Delta_\phi^{\text{FYE}} = 0.518142(8)$$

$$\Delta_\phi^{\text{Bootstrap}} = 0.5181489(10), \quad \Delta_\phi^{\text{MC}} = 0.51801(35)$$

[Filip Kos, David Poland, David Simmons-Duffin, and Alessandro Vichi. Precision islands in the Ising and O(N) models. JHEP, 2016]
[Alan M. Ferrenberg, Jiahao Xu, and David P. Landau. Pushing the limits of Monte Carlo simulations for the three-dimensional Ising model. PRE, 2018]

Simulation of the XY model

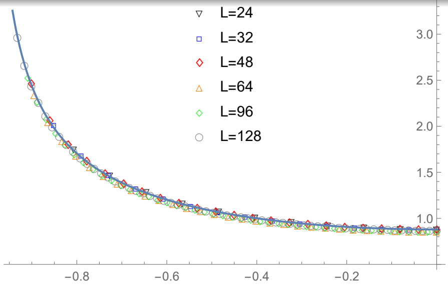
- We again choose a model with vacancies
- Additionally, rather than spins $\in [0, 2\pi)$, we use the $N-$state clock model, with $N = 8$

$$H = -\sum_{\langle ij \rangle} \mu_i \mu_j \cos(\theta_i - \theta_j) - D \sum_i \mu_i^2, \qquad \beta_C = 0.5637963$$

$$\mu_i = 1, \quad \theta_i = \frac{2\pi}{N} p_i, \qquad p_i \in \{1, \cdots, N\}, \qquad \text{or} \quad \mu_i = 0$$

[Martin Hasenbusch. Monte Carlo study of an improved clock model in three dimensions. PRB, 2019]

XY magnetization profile



— theory curve

$$\Delta_\phi^{\text{FYE}} = 0.5192(2)$$

$$\Delta_\phi^{\text{Bootstrap}} = 0.519088(22), \quad \Delta_\phi^{\text{MC}} = 0.519050(40)$$

[Alessandro Galvani, Giacomo Gori, and Andrea Trombettoni, to be submitted]

[S.M. Chester, W. Landry, J. Liu, D. Poland, D. Simmons-Duffin, N. Su, and A. Vichi. Carving out OPE space and precise O(2) model critical exponents. JHEP, 2020]

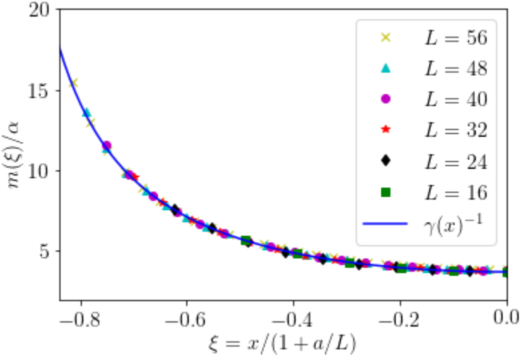
[Martin Hasenbusch. Monte Carlo study of an improved clock model in three dimensions. PRB, 2019]

Four-dimensional Ising model

- Test the validity of the saddle-point equation at $d = d_c$

$$\gamma(x) = \wp_I(x)^{1/2}$$

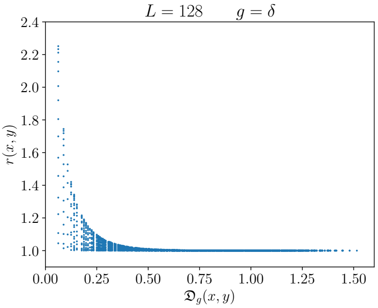
$$m(x) = \alpha\gamma\left(\frac{x}{1 + a/L}\right)^{-1}$$

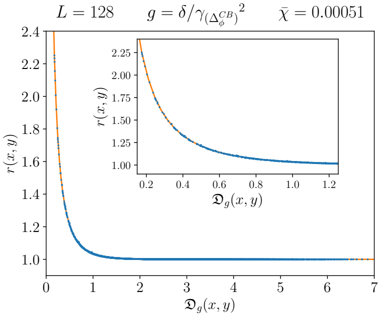


[Alessandro Galvani, Giacomo Gori, and Andrea Trombettoni. Magnetization profiles at the upper critical dimension as solutions of the integer Yamabe problem, arXiv:2103.12449]

Collapse of the Ising correlation functions

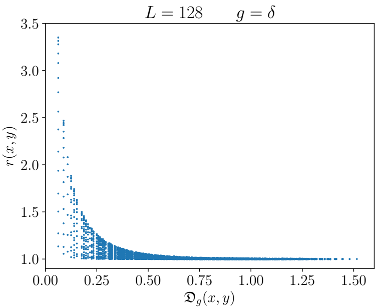
- To test the hypothesis for two-point correlations, we can plot $\frac{\langle\phi(x)\phi(y)\rangle}{\langle\phi(x)\rangle\langle\phi(y)\rangle}$ for the Ising model as a function of the Q-hyperbolic distance and the euclidean distance

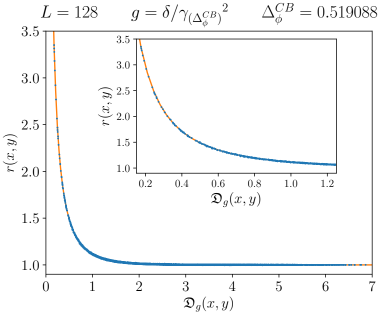




Collapse of the XY correlation functions

- The same can be done for the XY model





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Percolation

- Percolation is the simplest statistical model
- Geometrical in nature, with fractals emerging at the critical point
- Simulations are quick due to lack of weights and acceptance probabilities
- Has nontrivial critical exponents for $2 \leq d < 6$

d	1[7]	2	3	4	5	$6-\varepsilon$ [8][9][10]	$6+$
η	1	5/24	-0.046(8)[20] -0.059(9) [22] -0.07(5)[18] -0.0470[16]	-0.12(4)[18] -0.0944(28) [21] -0.0929(9)[23] -0.0954[16]	-0.075(20)[18] -0.0565[16]	$-\frac{\varepsilon}{21}-\frac{206}{3^3 7^3}\varepsilon^2$	0

From the nice page (mostly curated by R. Ziff)

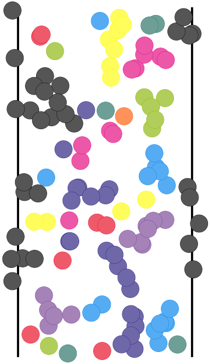
`en.wikipedia.org/wiki/Percolation_critical_exponents`

Continuum percolation

- Discrete lattice percolation is not the best choice for obtaining profiles

Continuum percolation

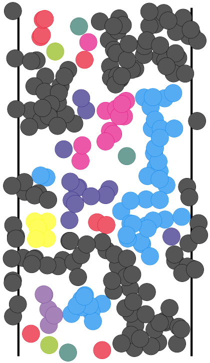
- Discrete lattice percolation is not the best choice for obtaining profiles
- Continuum percolation is in the same universality class
- Ideally suited to the study of the emergence of continuous symmetries



[Giacomo Gori and Andrea Trombettoni. Conformal invariance in three dimensional percolation. JSTAT, 2015]

Continuum percolation

- Spheres are randomly placed throughout the slab up to a critical filling
- Intersecting spheres belong to the same cluster
- Fixed boundary conditions: spheres intersecting a boundary belong to the boundary cluster



Two-dimensional check

- To ensure that our data analysis is sensible, we first test it in $d = 2$, where $\Delta_\phi = 5/48$ is known exactly
- The $d \to 2$ limit of the Yamabe equation gives the Liouville equation:

$$\triangle \log \gamma(x) = k\gamma(x)^{-2}$$

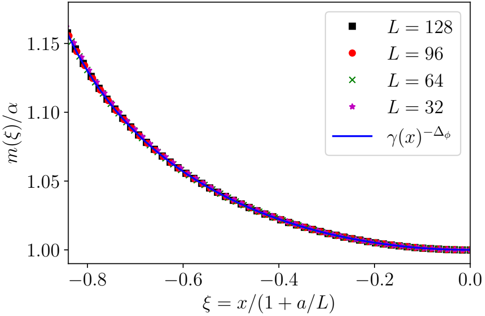
- Fixing the scalar curvature completely determines the metric
- Its solution can be used for any field, even though their dimensions are entirely anomalous
- Solving the Liouville equation is equivalent to finding a map from the upper-half plane to the desired domain

Two-dimensional order parameter profile

- $\langle\phi(x)\rangle$ is the total area of the intersection between balls in the large cluster and a plane through x, parallel to the boundaries

In a slab $-1 < x < 1$,

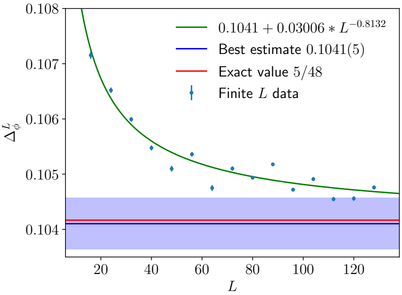
$$\gamma(x) = \frac{2}{\pi}\cos\left(\frac{\pi x}{2}\right)$$



Obtaining Δ_ϕ

- For each L, $\Delta_\phi(L)$ is extracted from the fit
- $\Delta_\phi(L)$ decreases with L as

$$\Delta_\phi(L) = \Delta_\phi + \frac{c}{L^w}$$

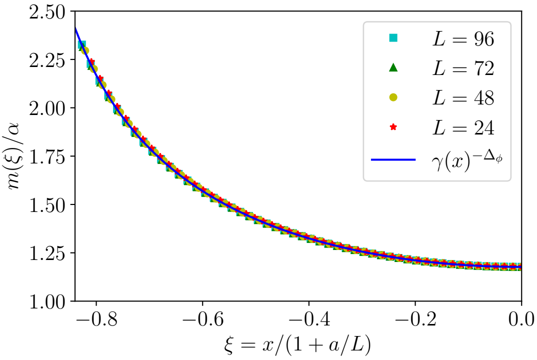


A further fit gives us Δ_ϕ, to compare with the exact value

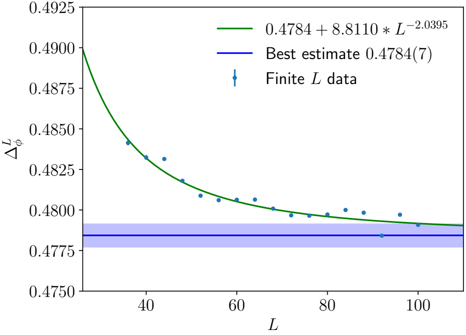
$$\Delta_\phi^{\text{fit}} = 0.1041(5), \qquad \Delta_\phi^{\text{exact}} = \frac{5}{48} \approx 0.10417$$

Three-dimensional percolation

The same procedure can be repeated in three dimensions



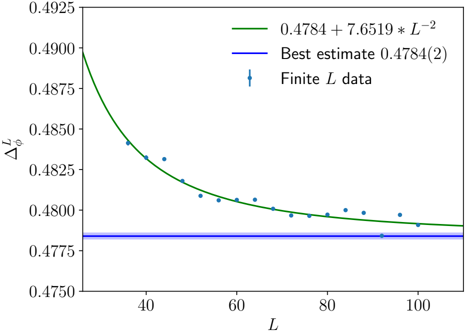
Δ_ϕ for three-dimensional percolation



$$\Delta_\phi = 0.47846(71) \quad \rightarrow \quad \eta = -0.0431(14)$$

Δ_ϕ for three-dimensional percolation (II)

The points decay with a power close to 2: we can get a more precise estimate by fixing the exponent to 2



$$\boxed{\Delta_\phi = 0.4784(2) \quad \rightarrow \quad \eta = -0.0432(4)}$$

Comparison with previous results

Reference	year	Method	η
Adler et al.	1990	Moment expansion	$-0.07(5)$
Lorenz & Ziff	1998	MC, bond percolation	$-0.046(8)$
Jan & Stauffer	1998	MC, site percolation	$-0.059(9)$
Gracey	2015	4-loop RG	-0.0470
This work	2021	Critical geometry	$-0.0432(4)$

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Recap and work in progress

Uniformization hypothesis $\rightarrow$ Yamabe equation

- $d = d_c$: Integer Yamabe equation $\leftrightarrow$ mean field
- $d_c > d > 2$: Fractional Yamabe equation

Results in 3d

- Critical order parameter profiles
- Scaling dimensions:

$$\boxed{\begin{gathered}\Delta_\phi^{\text{Ising}} = 0.518142(8), \quad \Delta_\phi^{\text{XY}} = 0.5192(2), \\ \color{red}{\Delta_\phi^{\text{percolation}} = 0.4784(2)}\end{gathered}}$$

- Ising and XY: two-point correlations satisfy the conjecture

Up next:

- Correlation functions for different fields
- Fractional epsilon expansion

Thank you!