# Self-Avoiding Walks

Gordon Slade
University of British Columbia
http://www.math.ubc.ca/∼slade

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**Abstract**

Random walks are well understood. However, if we require a random walk not to intersect itself, so that it is a self-avoiding walk, then many of the important mathematical problems remain unsolved. This lecture will give an overview of some of what is known about self-avoiding walks, including some old and some more recent results, using methods that touch on combinatorics, probability, and statistical mechanics.

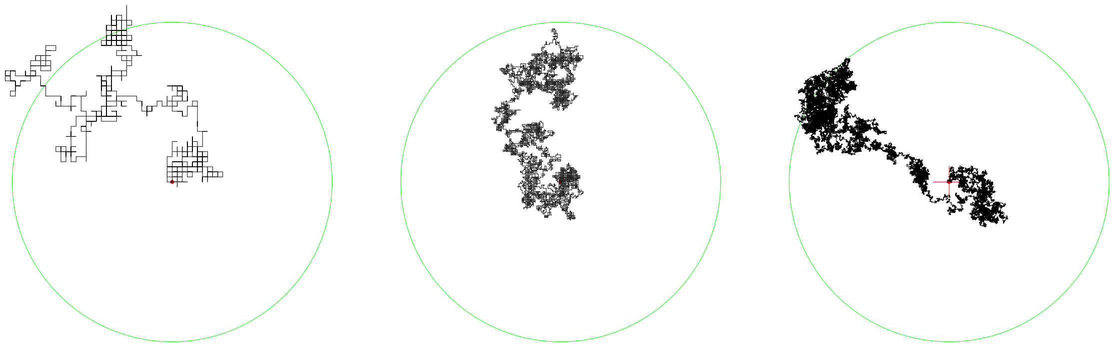
# Simple random walk

Applications: physics, chemistry, biology, finance, ..., everything.

Start at origin of $\mathbb{Z}^d$, take steps to neighbours with equal probability. Markov process.

Scaling limit: Let number of steps $n \longrightarrow \infty$ while shrinking space by $1/\sqrt{n}$. Result is Brownian motion, for any dimension $d$.

Walks with $n = 1,000$, $n = 10,000$ and $n = 60,000$ steps. Circle radius $= \sqrt{n}$.



Brownian paths are two-dimensional.

## Simple random walk

Let $S_n$ be the position after $n$ steps. Let $p_t(x) = \left(\frac{d}{2\pi t}\right)^{d/2} e^{-d|x|^2/2t}$.
Then

$$\lim_{n\to\infty} \mathbb{P}\left(\frac{1}{\sqrt{n}} S_{\lfloor nt \rfloor} \in A\right) = \int_A p_t(x)dx$$

for $A \subset \mathbb{R}^d$ with $\partial A$ of Lebesgue measure zero.
Much more generally, there is convergence to Brownian motion as a process.

Universality.

Let $\omega(n)$ be the position after $n$ steps.
Let $s_n(x)$ be the number of $n$-step SRWs with $\omega(n) = x$.
Let $s_n$ be the number of $n$-step SRWs.

Recursion relation: $s_n(x) = \sum_{y\in\mathbb{Z}^d} s_1(y)s_{n-1}(x-y)$, which can easily be solved.

Sum over $x$: $s_n = 2ds_{n-1}$ which has solution $s_n = (2d)^n$.

Mean-square displacement: $\mathbb{E}|\omega(n)|^2 = n$.

## Self-avoiding walk

According to the poet:

Al andar se hace camino,
y al volver la vista atrás
se ve la senda que nunca
se ha de volver a pisar.

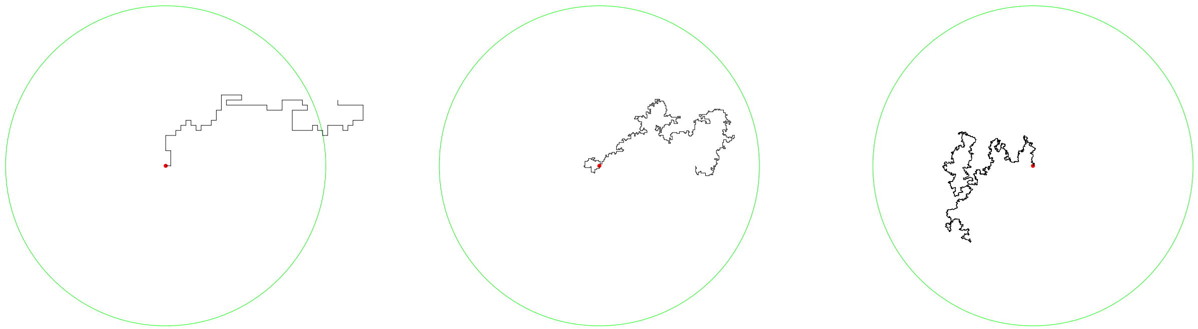
*Antonio Machado*

# Self-avoiding walk

According to the mathematician:

Let $\mathcal{S}_n(x)$ be the set of $\omega : \{0, 1, \ldots, n\} \to \mathbb{Z}^d$ with:
$\omega(0) = 0$, $\omega(n) = x$, $|\omega(i+1) - \omega(i)| = 1$, and $\omega(i) \neq \omega(j)$ for all $i \neq j$.
Let $\mathcal{S}_n = \cup_{x \in \mathbb{Z}^d} \mathcal{S}_n(x)$

Let $c_n(x) = |\mathcal{S}_n(x)|$. Let $c_n = \sum_x c_n(x) = |\mathcal{S}_n|$.
Declare all walks in $\mathcal{S}_n$ to be equally likely: each has probability $c_n^{-1}$.



SAWs on $\mathbb{Z}^2$ taking $n = 100$, 1,000 and 10,000 steps. Circle radius $= n^{3/4}$.

Why?: combinatorics, probability (not a Markov process because not Markovian and not a process!), polymer science, critical phenomena in statistical mechanics.

# The basic questions

Interested in:

$$c_n = \text{number of } n\text{-step SAWs},$$

$$\mathbb{E}|\omega(n)|^2 = \frac{1}{c_n}\sum_{\omega\in\mathcal{S}_n} |\omega(n)|^2 = \frac{1}{c_n}\sum_{x\in\mathbb{Z}^d} |x|^2 c_n(x) = \text{mean-square displacement},$$

what is the scaling limit?

Problem is easy for $d = 1$ (less easy if allow non-nearest-neighbour steps),

unsolved for $d = 2, 3, 4$, and solved for $d \geq 5$.

# Critical exponents

*Connective constant* $\mu = \lim_{n\to\infty} c_n^{1/n}$ exists because $c_{n+m} \le c_n c_m$.
Easy: $d \le \mu \le 2d - 1$.

Conjectured asymptotic behaviour:

$$c_n \sim A\mu^n n^{\gamma-1}, \quad \mathbb{E}|\omega(n)|^2 \sim Dn^{2\nu}$$

with universal critical exponents $\gamma$ and $\nu$ (and $(\log n)^{1/4}$ corrections for $d = 4$).

Problem is solved for $d \ge 5$ (Hara-S 1992):
$\gamma = 1$, $\nu = \frac{1}{2}$, scaling limit is Brownian motion.

Flory values (1949), nonrigorous:
$\nu = \frac{3}{d+2}$ for $1 \le d \le 4$. Correct answers except $d = 3$, where it is close.

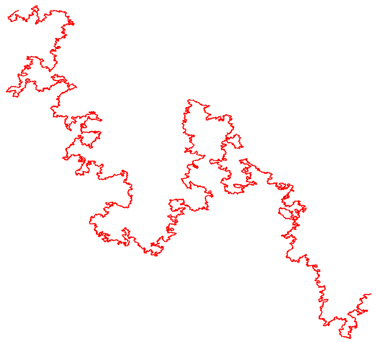
Some embarrassing answers for $d = 2, 3, 4$:

Best bound is $\mu^n \le c_n \le \mu^n e^{Cn^{2/(d+2)} \log n}$.

Not proved that $cn \le \mathbb{E}|\omega(n)|^2 \le Cn^{2-\epsilon}$.

# Two-dimensional self-avoiding walks

Monte-Carlo methods now work with walks of length $10^6$ (perhaps soon $10^9$):



Or, exact enumeration plus series analysis: determine $c_n$ exactly for $n = 1, 2, \ldots, N$ and analyse the sequence to determine $\mu, A, \gamma$.
For $d = 2$ the "finite lattice method" is remarkable (Jensen 2004):
$c_{71} = 4\,190\,893\,020\,903\,935\,054\,619\,120\,005\,916 \approx 4.2 \times 10^{30}$.

Both numerical methods confirm a prediction of Nienhuis (1982): $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$.

Lawler, Schramm, Werner (2004): if the scaling limit exists and has a certain conformal invariance property, then the scaling limit must be $\mathrm{SLE}_{8/3}$. Properties of $\mathrm{SLE}_{8/3}$ would then give $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$.

Existence of the scaling limit (and its conformal invariance) is an open problem.

# Three-dimensional self-avoiding walks

For $d = 3$: no rigorous results.

Three methods to compute the exponents:

1. Field theory (physics)
2. Monte Carlo (walks of length 640,000 have been simulated)
3. Exact enumeration plus series analysis.
   Currently best method for enumeration in dimensions $d \geq 3$ is the lace expansion.

# The lace expansion via inclusion-exclusion

Identifies a function $\pi_m(x)$ such that for $n \geq 1$,

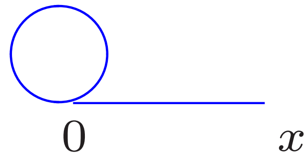
$$c_n(x) = \sum_{y \in \mathbb{Z}^d} c_1(y) c_{n-1}(x-y) + \sum_{m=2}^{n} \sum_{y \in \mathbb{Z}^d} \pi_m(y) c_{n-m}(x-y).$$

Start with

$$c_n(x) = \sum_{y} c_1(y) c_{n-1}(x-y) - R_n^{(1)}(x)$$

where

$$R_n^{(1)}(x) =$$

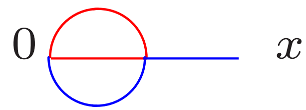



Inclusion-exclusion again:

$$R_n^{(1)}(x) = \sum_{m=2}^{n} u_m c_{n-m}(x) - R_n^{(2)}(x)$$

where

$$R_n^{(2)}(x) =$$

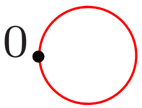
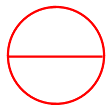
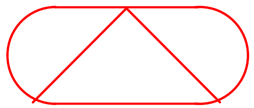


# The lace expansion via inclusion-exclusion

Repetition leads to

$$c_n(x) = \sum_y c_1(y) c_{n-1}(x-y) + \sum_{m=2}^{n} \sum_y \pi_m(y) c_{n-m}(x-y)$$

with

$\pi_m(y) = -\delta_{0,y}$ 0  $+$ 0  $y$ $-$  $+\cdots$

0 $y$

Sum over $x$, with $\pi_m = \sum_y \pi_m(y)$:

$$c_n = 2d c_{n-1} + \sum_{m=2}^{n} \pi_m c_{n-m}.$$

Lace expansion is due to Brydges and Spencer (1985) (with a different formulation).

## Values of $\pi_{m,\delta}$:

| $m$ | $\delta = 2$ | $\delta = 3$ | $\delta = 4$ | $\delta = 5$ | $\delta = 6$ |
|---|---|---|---|---|---|
| 4 | -1 | 0 | 0 | 0 | 0 |
| 5 | 3 | 0 | 0 | 0 | 0 |
| 6 | -8 | -4 | 0 | 0 | 0 |
| 7 | 19 | 15 | 0 | 0 | 0 |
| 8 | -50 | -86 | -27 | 0 | 0 |
| 9 | 121 | 300 | 106 | 0 | 0 |
| 10 | - 305 | -1 511 | -1 340 | - 248 | 0 |
| 11 | 736 | 5 297 | 5 333 | 966 | 0 |
| 12 | -1 853 | -25 566 | -52 252 | -25 020 | -2 830 |
| 13 | 4 531 | 91 234 | 211 403 | 100 988 | 10 755 |
| 14 | -11 444 | - 435 330 | -1 907 566 | -1 850 364 | - 515 509 |
| 15 | 28 294 | 1 586 306 | 7 854 601 | 7 635 822 | 2 029 500 |
| 16 | -71 803 | -7 568 792 | -68 777 498 | - 123 248 980 | -64 816 437 |
| 17 | 179 006 | 28 105 857 | 288 074 727 | 517 006 517 | 260 695 401 |
| 18 | - 455 588 | - 134 512 520 | -2 498 227 824 | -7 899 351 270 | -7 074 329 136 |
| 19 | 1 142 357 | 507 675 751 | 10 626 960 167 | 33 569 520 427 | 28 860 719 280 |
| 20 | -2 914 236 | -2 438 375 322 | -92 047 793 514 | - 500 752 577 733 | - 724 291 034 691 |
| 21 | 7 341 457 | 9 330 924 963 | 396 919 882 288 | 2 150 581 793 271 | 2 984 307 507 943 |
| 22 | -18 768 621 | -44 965 008 206 | -3 445 692 397 195 | -31 789 616 257 271 | -72 005 867 458 629 |
| 23 | 47 466 002 | 174 103 216 625 | 15 035 569 992 917 | 137 713 940 393 321 | 298 797 296 949 195 |
| 24 | - 121 579 349 | - 841 380 441 626 | - 130 974 140 581 412 | -2 032 548 406 479 564 | -7 072 798 632 884 530 |
| 25 | 308 478 355 | 3 290 830 791 268 | | | |
| 26 | - 791 455 148 | -15 941 476 401 251 | | | |
| 27 | 2 013 666 265 | 62 897 919 980 935 | | | |
| 28 | -5 174 044 897 | - 305 298 415 550 796 | | | |
| 29 | 13 195 280 922 | 1 213 812 491 872 081 | | | |
| 30 | -33 949 508 883 | -5 901 490 794 431 276 | | | |

## SAW enumeration using the lace expansion

Clisby–Liang–S (2007):

For $d = 3$:

$c_{30} = 270\,569\,905\,525\,454\,674\,614$

For $d = 4$:

$c_{24} = 124\,852\,857\,467\,211\,187\,784$

For $d = 5$:

$c_{24} = 63\,742\,525\,570\,299\,581\,210\,090$

For $d = 6$:

$c_{24} = 8\,689\,265\,092\,167\,904\,101\,731\,532$

$d = 3$, $c_{30}$ took 15000 CPU hours; *all* $d \geq 2$, $c_{24}$ took 4400 CPU hours.

## Series analysis

Estimates for critical parameters for $d = 3$: $c_n \sim A\mu^n n^{\gamma-1}$, $\mathbb{E}[|\omega(n)|^2] \sim D n^{2\nu}$.

$\mu = 4.684043(12)$

$\gamma = 1.1568(8)$ [Caracciolo et al 1998, MC: 1.1575(6)]

$\nu = 0.5876(5)$ [Prellberg 2001, MC: 0.5874(2)]

$A = 1.216(5)$, $D = 1.220(12)$.

## Self-avoiding walks in dimensions $d > 4$

Theorem (Hara–S 1992). For $d \geq 5$, $\gamma = 1$ and $\nu = \frac{1}{2}$, in the sense that

$$c_n = A\mu^n[1 + O(n^{-\epsilon})],$$
$$\mathbb{E}|\omega(n)|^2 = Dn[1 + O(n^{-\epsilon})],$$

and, moreover,

$$\frac{\omega(\lfloor nt \rfloor)}{\sqrt{Dn}} \Rightarrow B_t.$$

In particular, the central limit theorem holds, and the scaling limit is Brownian motion for $d \geq 5$, with spatial scaling $1/\sqrt{Dn}$.

Proof: Lace expansion. Perturbation of simple random walk.

Upper critical dimension is $4$:

$$4 = 2 + 2$$

Ranges of two independent BMs do not intersect each other iff $d \geq 4$.

# Idea of proof: Simple random walk

Define the generating function:

$$C_z(x) = \sum_{\omega:0\to x} z^{|\omega|} = \sum_{n=0}^{\infty} p_n(x)(2dz)^n,$$

where $p_n(x) = (2d)^{-n}s_n(x)$ is the transition probability. Want asymptotics of $p_n(x)$ for large $x$ and large $n$. Let $D(x) = p_1(x) = \frac{1}{2d}\delta_{|x|,1}$. Then

$$p_n(x) = \sum_y p_1(y)p_{n-1}(x-y) = \sum_y D(y)p_{n-1}(x-y)$$

and hence

$$C_z(x) = \delta_{0,x} + 2dz\sum_y D(y)C_z(x-y).$$

Let

$$\hat{f}(k) = \sum_{x\in\mathbb{Z}^d} f(x)e^{ik\cdot x}, \quad k \in [-\pi,\pi]^d,$$

so $\hat{D}(k) = d^{-1}\sum_{j=1}^{d}\cos k_j$.

# Idea of proof: Simple random walk

Then

$$\hat{C}_z(k) = 1 + 2dz\hat{D}(k)\hat{C}_z(k)$$

and hence

$$\hat{C}_z(k) = \frac{1}{1 - 2dz\hat{D}(k)}.$$

Note singularity of $\hat{C}_z(0)$ at $z_0 = \frac{1}{2d}$.

Behaviour of $p_n(x)$ for large $n$ and large $x$ determined by behaviour of $\hat{C}_z(k)$ for $z \approx z_0$ and $k \approx 0$, namely:

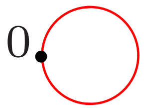
$$\begin{aligned} \hat{C}_z(k) &= \frac{1}{2dz[1 - \hat{D}(k)] + (1 - 2dz)} \\ &\approx \frac{1}{\frac{|k|^2}{2d} + (1 - \frac{z}{z_0})} \quad \text{for } k \approx 0 \text{ and } z \approx z_0. \end{aligned}$$

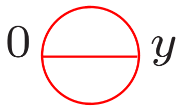
# Idea of proof: Self-avoiding walk

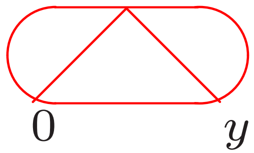
Recall that for $n \geq 1$,

$$c_n(x) = \sum_y c_1(y) c_{n-1}(x-y) + \sum_{m=2}^{n} \sum_y \pi_m(y) c_{n-m}(x-y)$$

with

$\pi_m(y) = -\delta_{0,y}$ 

$+$ 

$-$ 

$+ \cdots$

Let

$$G_z(x) = \sum_{n=0}^{\infty} c_n(x) z^n.$$

Then

$$G_z(x) = \delta_{0,x} + 2dz \sum_y D(y) G_z(x-y) + \sum_y \Pi_z(y) G_z(x-y),$$

where

$$\Pi_z(y) = \sum_{n=2}^{\infty} \pi_n(y) z^n.$$

# Idea of proof: Self-avoiding walk

Fourier transformation gives

$$\hat{G}_z(k) = \frac{1}{1 - 2dz\hat{D}(k) - \hat{\Pi}_z(k)} \equiv \frac{1}{\hat{F}_z(k)}.$$

Critical point: $\hat{G}_z(0) = \sum_n c_n z^n$ has radius of convergence $z_c = \mu^{-1}$ and $\hat{F}_{z_c}(0) = 0$.
Taylor expansion:

$$\hat{F}_z(k) = \hat{F}_z(k) - \hat{F}_{z_c}(0) \approx a\frac{|k|^2}{2d} + b\Big(1 - \frac{z}{z_c}\Big)$$

with $a = \nabla_k^2 \hat{F}_{z_c}(0)$ and $b = -z_c \partial_z \hat{F}_{z_c}(0)$, assuming $a, b$ finite. Then

$$\hat{G}_z(k) \approx \frac{1}{a\frac{|k|^2}{2d} + b(1 - \frac{z}{z_c})}, \quad \text{for } k \approx 0,\ z \approx z_c,$$

which is the approximate generating function for simple random walk.

# Idea of proof: Self-avoiding walk

For this to work, need $z_c \partial_z \hat{\Pi}_{z_c}(k)$ finite. Leading term is

$$\sum_n u_n n z_c^n \leq \sum_x G_{z_c}(x)^2 = \int_{[-\pi,\pi]^d} \hat{G}_{z_c}(k)^2 \frac{d^d k}{(2\pi)^d}.$$

Reason this might work: insert SRW behaviour on RHS:

$$\int_{[-\pi,\pi]^d} \hat{G}_{z_c}(k)^2 \frac{d^d k}{(2\pi)^d} \approx \int_{[-\pi,\pi]^d} \frac{1}{k^4} \frac{d^d k}{(2\pi)^d} < \infty \quad \text{for } d > 4.$$

Proof finds a way to exploit this.

Proof is computer assisted to handle all $d \geq 5$; easier for $d \geq d_0$ for some larger $d_0$.

Method has been extended to several other models:
Percolation ($d > 6$), oriented percolation ($d + 1 > 4 + 1$), contact process ($d > 4$), lattice trees and lattice animals ($d > 8$), Ising model ($d > 4$).

# Four-dimensional self-avoiding walks

Non-rigorous renormalisation group methods predict that

$$c_n \sim A\mu^n (\log n)^{1/4}, \quad \mathbb{E}|\omega(n)|^2 \sim Dn(\log n)^{1/4},$$

and that the scaling limit is again Brownian motion (scale by $(Dn)^{-1/2}(\log n)^{-1/8}$).

Theorem (Brydges–Imbrie 2003): $\mathbb{E}|\omega(n)|^2 \sim Dn(\log n)^{1/4}$ holds for a continuous-time weakly self-avoiding walk on a 4-dimensional *hierarchical* lattice. The latter is a replacement of $\mathbb{Z}^4$ by something with a tree-like recursive structure.

The Green function $G_z(x) = \sum_{n=0}^{\infty} c_n(x) z^n$ has radius of convergence $z_c = \mu^{-n}$. Work in progress with Brydges aims to prove that the critical Green function obeys

$$G_{z_c}(x) \sim \text{const}\frac{1}{|x|^2} \quad \text{as} \quad x \to \infty,$$

for a discrete time strictly self-avoiding walk on $\mathbb{Z}^4$, where the walk is spread out in the sense that it is permitted to take steps not only to nearest neighbours.

# Functional integral representation

In this form, due to Imbrie. (Previous representations for weakly SAW.)

Replace $\mathbb{Z}^4$ by a large box $\Lambda \subset \mathbb{Z}^4$. Fix a positive definite matrix $A : \Lambda \times \Lambda \to \mathbb{R}$ and let $C = A^{-1}$. [Our choice: $A = I - \lambda^{-1}\Delta$ where $0 < \lambda \ll 1$ and $\Delta$ is the lattice Laplacian.] Consider the Green function

$$G_z(x) = \sum_{\omega:0\to x} \left( \prod_{i=1}^{|\omega|} C_{\omega(i-1),\omega(i)} \right) z^{|\omega|},$$

where the sum is over self-avoiding walks on $\Lambda$ taking *arbitrary* steps. Then

$$G_z(x) = z \int_{\mathbb{C}^{|\Lambda|}} e^{-S_A} \bar{\varphi}_0 \varphi_x \prod_{w\neq 0,x} (1 + z\tau_w),$$

where $\varphi : \Lambda \to \mathbb{C}$,

$$\tau_w = \varphi_w \bar{\varphi}_w + d\varphi_w \frac{1}{2\pi i} d\bar{\varphi}_w,$$

$$S_A = \varphi A \bar{\varphi} + d\varphi \frac{A}{2\pi i} d\bar{\varphi} = \sum_{x,y} \left( \varphi_x A_{xy} \bar{\varphi}_y + d\varphi_x \frac{A_{xy}}{2\pi i} d\bar{\varphi}_y \right),$$

the differentials anti-commute, and a function of differentials is defined by its Taylor polynomial.

## Functional integral representation: basic idea of proof

Goal is to show that:

$$z \int e^{-S_A} \bar{\varphi}_0 \varphi_x \prod_{w \neq 0,x} (1 + z\tau_w) = \sum_{\omega:0 \to x} \prod_{i=1}^{|\omega|} C_{\omega(i-1),\omega(i)} z^{|\omega|}.$$

Proof uses the integration by parts formula

$$\int e^{-S_A} \bar{\varphi}_x F = \sum_v C_{xv} \int e^{-S_A} \frac{\partial F}{\partial \varphi_v}$$

and the self-normalising property that for nice $F$

$$\int e^{-S_A} F(\tau) = F(0).$$

Applied to $F = \varphi_x \prod_{w \neq 0,x}(1 + z\tau_w)$, these give

$$z \int e^{-S_A} \bar{\varphi}_0 F = zC_{0,x} + z \sum_v C_{0,v} \int e^{-S_A} z \bar{\varphi}_v \varphi_x \prod_{w \neq 0,x,v} (1 + z\tau_w),$$

and the identity follows by iterating this procedure.

## The renormalisation group

The identity is the point of departure of a renormalisation group analysis of the functional integral representation, based on a major extension of the methods used by Brydges and Imbrie for the hierarchical model.

The starting point is a finite-range self-similar decomposition of the covariance $C$:

$$C = \sum_{j=1}^{N} C_j$$

with corresponding field decomposition

$$\varphi = \sum_{j=1}^{N} \varphi_j,$$

together with the basic fact that

$$\int_{\mathbb{C}^{|\Lambda|}} e^{-S_A} F(\varphi) \equiv \mathbb{E}_C F(\varphi) = \mathbb{E}_{C_N} \circ \cdots \circ \mathbb{E}_{C_2} \circ \mathbb{E}_{C_1} F(\varphi_1 + \cdots + \varphi_N).$$

The iterated integral is then performed inductively.

## Conclusions

- $d = 2$: scaling limit is $\mathrm{SLE}_{8/3}$ and $\gamma = \frac{43}{32}$, $\nu = \frac{3}{4}$, *if* the scaling limit can be proved to exist and to be conformally invariant.

- $d = 3$: only have numerical results: $\gamma \approx 1.157$, $\nu \approx 0.5875$. No idea how to describe the scaling limit.

- $d = 4$: $\gamma = 1$ and $\nu = \frac{1}{2}$ on a hierarchical lattice. Renormalisation group methods offer hope also for results on $\mathbb{Z}^4$ for critical Green function in near future.

- $d \geq 5$: Problem is solved. $\gamma = 1$ and $\nu = \frac{1}{2}$ and scaling limit is Brownian motion.