Self-avoiding walks adsorbed at a surface

Tony Guttmann.
Joint work with Nick Beaton, Mireille Bousquet-Mélou, Jan de Gier and Hugo Duminil-Copin

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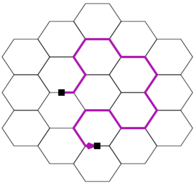
Outline of talk

- In 2010 Duminil-Copin and Smirnov proved Nienhuis's 1982 conjecture that the critical point of the hexagonal lattice SAW generating function is $x_c = 1/\sqrt{2+\sqrt{2}}$.
- In 2012 Beaton, Bousquet-Mélou, de Gier, Duminil-Copin and Guttmann proved the 1995 conjecture of Batchelor and Yung that the critical fugacity for hexagonal lattice SAWs in a half plane, adsorbed onto the surface is $y_c = 1 + \sqrt{2}$.
- Together with Jensen and Beaton we asked to what extent we can extend D-C/S's result to SAWs on other lattices (sq. and tri.)?
- Together with Jensen and Beaton we asked to what extent we can extend the results of Beaton et al. to study surface adsorption (both bond and vertex) on other lattices?
- Together with Elvey-Price, Lee and de Gier we asked if we could extend the D-C/S result off-criticality? In that way we might be able to say something about critical exponents.

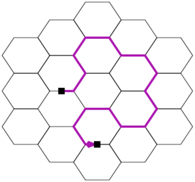
Self-avoiding walks



A self-avoiding walk on the honeycomb lattice, starting and finishing on a mid-edge. (A technical ploy only).

These are known to 105 steps (Iwan Jensen 2006)

SELF-AVOIDING WALKS



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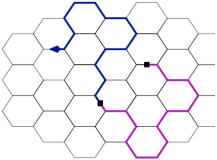
THE (EXPONENTIAL) GROWTH CONSTANT μ.



Concatenate two walks. They either intersect or not. So clearly

$$c_{m+n} \leq c_m c_n$$

Hence $\lim_n c_n^{1/n}$ exists and

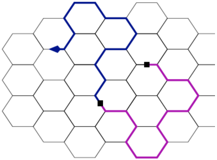
$$\mu := \lim_n c_n^{1/n} = \inf_n c_n^{1/n}.$$

Conjecture: Nienhuis 1982

$$\mu = \sqrt{2+\sqrt{2}}.$$

Proved by Smirnov and Duminil-Copin 2010.

The (exponential) growth constant μ.



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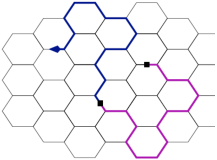

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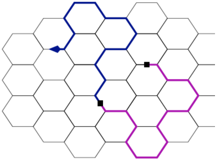

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GENERATING FUNCTIONS AND GROWTH CONSTANTS

c_n is the number of $n-$step SAWs. $C(x)$ is the length ogf:

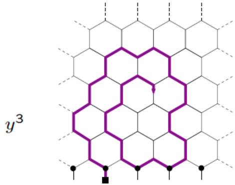
$$C(x) = \sum_{n \geq 0} c_n x^n.$$

The radius of convergence of $C(x)$ is

$$\rho = 1/\mu = x_c,$$

where μ is the growth (connective) constant, and x_c is the critical (length) fugacity.

WALKS IN A HALF-PLANE INTERACTING WITH A SURFACE



Contacts shown as blobs. Fugacity y with each contact of walk γ.

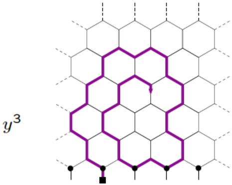
Enumerating by contacts of $n-$step walks:

$$\bar{c}_n(y) = \sum_{\gamma} y^{\text{contacts}(\gamma)}.$$

The full generating function is

$$\bar{C}(x,y) = \sum_{n\geq 0} \bar{c}_n(y) x^n.$$

Walks in a half-plane interacting with a surface



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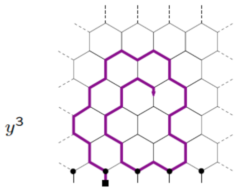

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THE CRITICAL FUGACITY

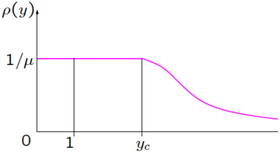
Radius and growth constant: for $y > 0$,

$$\rho(y) = \frac{1}{\mu(y)} = \lim_n \bar{c}_n(y)^{-1/n}$$

Prop: $\rho(y)$ is a continuous, weakly decreasing function of $y \in (0, \infty)$. There exists $y_c > 1$ s.t.

$$\begin{aligned} \rho(y) &= 1/\mu \;\text{ if } y \le y_c, \\ \rho(y) &< 1/\mu \;\text{ if } y > y_c, \end{aligned}$$

where μ is the growth constant.



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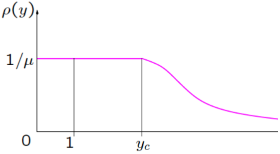

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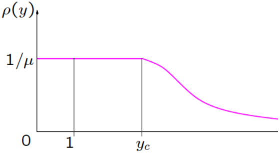
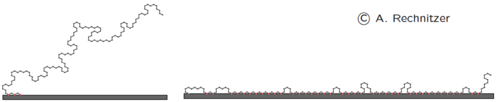


Probabilistic meaning of the critical fugacity

Consider half-space SAWs under a Boltzmann distribution

$$\mathbb{P}_n(\gamma) = \frac{y^{\text{contacts}(\gamma)}}{\bar{c}_n(y)}.$$



Then for $y < y_c$, the walk escapes from the surface. For $y > y_c$, a positive fraction of its vertices lie in the surface.

Theorem [B-BM-dG-DC-G 12]: This phase transition occurs at

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Conjectured by Batchelor and Yung in 1995.

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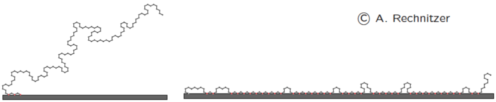

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THE PROOF: THREE INGREDIENTS

- 1. We generalise an identity of Duminil-Copin and Smirnov to the case with an adsorbing surface.
- 2.We give an alternative (equivalent) definition of the critical fugacity.
- 3. Our proof then hinges on proving that a subset of SAWs, called bridges, which are SAWs spanning a strip of width h, have generating function $B_h(x)$, which vanishes for $x \leq x_c$ as $h \to \infty$.
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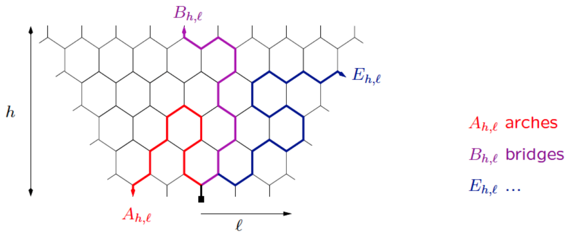
INGREDIENT 1

Duminil-Copin and Smirnov's "global" identity.
Consider the following trapezoidal domain $D_{h,l}$.



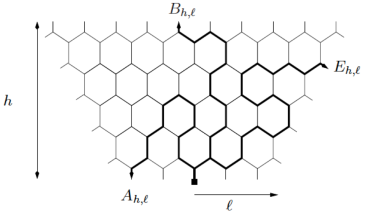
Let $A_{h,l}(x)$ (resp. $B_{h,l}(x)$, $E_{h,l}(x)$) be the length generating function of SAWs starting from the origin and ending at the bottom (resp. top, left/right) border of the domain. (These are polynomials in x.)

Duminil-Copin and Smirnov's "global" identity

For $x = x_c = 1/\sqrt{2+\sqrt{2}}$,

$$\alpha A_{h,l}(x_c) + B_{h,l}(x_c) + \epsilon E_{h,l}(x_c) = 1,$$

where $\alpha = \cos(\pi/8)$ and $\epsilon = \cos(\pi/4)$.



$A_{h,\ell}$ arches
$B_{h,\ell}$ bridges
$E_{h,\ell}$ ...

Remarkable nature of the result

- Letting $l \to \infty$, it follows that $E_h(x_c) = 0$.
- Then in a strip of width h we have

$$\cos(\frac{3\pi}{8})A_h(x_c) + B_h(x_c) = 1.$$

- Consider a strip of width 0, i.e. a spine. Then

$$A_0(x) = \frac{2x^3}{1-x^2}, \;\; B_0(x) = \frac{2x^2}{1-x^2}.$$

- Then solve

$$\cos(\frac{3\pi}{8})A_0(x) + B_0(x) = 1.$$

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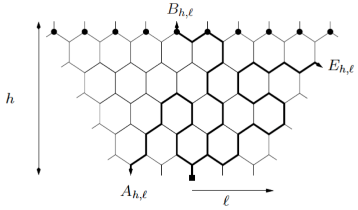
OUR EXTENSION OF DC-S WITH *upper* CONTACTS.

For $x = x_c = 1/\sqrt{2+\sqrt{2}}$, and for any y

$$\alpha A_{h,l}(x_c, y) + \frac{y^* - y}{y(y^* - 1)} B_{h,l}(x_c) + \epsilon E_{h,l}(x_c) = 1,$$

where $\alpha = \cos(\pi/8)$, $\epsilon = \cos(\pi/4)$ and $y^* = 1 + \sqrt{2}$.



$A_{h,\ell}$ arches

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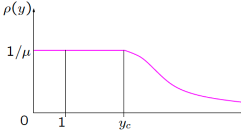
We need to prove that $y_c = y^*$.

The critical fugacity

First, recall that the radius $\rho(y)$ of $\bar{C}(x, y)$ is a continuous, weakly decreasing function of $y \in (0, \infty)$. There exists $y_c > 1$ s.t.

$$\begin{aligned} \rho(y) &= 1/\mu \ \text{ if } y \le y_c, \\ \rho(y) &< 1/\mu \ \text{ if } y > y_c, \end{aligned}$$

where μ is the growth constant of unrestricted SAWs.



We can't use this definition as it stands, as our identity fixes x at x_c.

An alternative description of the critical fugacity

Proposition: Let l, the length of our trapezoid, go to infinity. Then we are in a strip of width h. Let $A_h(x,y)$ be the ogf of arches in a strip of width h, counted by length and number of contacts. Let y_h be the r.c. of $A_h(x,y)$. Then, as $h \to \infty$, $y_h \searrow y_c$.

The same holds for the generating function of bridges, $B_h(x,y)$, and indeed for $C_h(x,y)$, the ogf of all SAWs in the h strip, with the same value of y_h.

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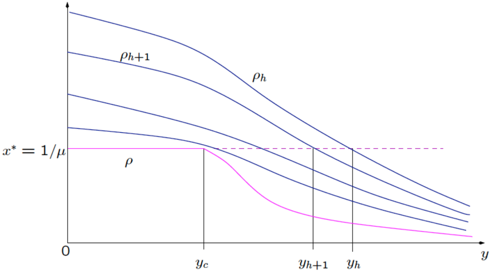
For $y > 0$ fixed, let $\rho_h(y)$ be the r.c. of $A_h(x, y)$ (or $B_h(x, y)$ or $C_h(x, y)$). Then $\rho_h(y)$ decreases to $\rho(y)$ as $h \to \infty$.



INGREDIENT 3. $B_h(x_c, 1) \to 0$ AS $h \to \infty$.

Proposition: The ogf $B_h(x, 1)$ of bridges of height h evaluated at $x_c = 1/\mu$, satisfies $B_h(x_c, 1) \to 0$ as $h \to \infty$.

Remark. The global identity implies that $B_h(x_c, 1)$ converges. The hard part is to show that it converges to zero.

Conjecture: Assuming the scaling limit of SAWs is given by $SLE_{8/3}$,

$$B_h(x_c, 1) \sim c/h^{1/4}.$$

Proof inspired by Duminil-Copin and Hammond (arXiv 2012) *The SAW is sub-ballistic.*

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Putting it all together 1. A lower bound.

Recall that for $x = x_c$ and for any y

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Let $y = y^*$. Then $A_{h,l}(x_c, y^*)$ increases with l but remains bounded. Its limit is $A_h(x_c, y^*)$ (arches in an h-strip), and is finite.

Thus

$$y^* \le y_h,$$

and by taking the limit $h \to \infty$,

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Let $y = y^*$. Then $A_{h,l}(x_c, y^*)$ increases with l but remains bounded. Its limit is $A_h(x_c, y^*)$ (arches in an h-strip), and is finite.

Thus

$$y^* \le y_h,$$

and by taking the limit $h \to \infty$,

$$y^* \le y_c.$$

Putting it all together 1. A lower bound.

Recall that for $x = x_c$ and for any y

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An upper bound on y_c.

Consider arches that fully span the strip. These can be bounded by a product of two bridges. Then by a direct application of our global identity, we readily obtain the bound:

$$\frac{1}{B_{h+1}(x_c, y)} \le \alpha x_c + \frac{1}{B_{h+1}(x_c, 1)} \frac{y^* - y}{y(y^* - 1)}$$

for $0 < y < y_{h+1}$ (and in particular for $y = y_c$). In particular

$$0 \le \alpha x_c + \frac{1}{B_{h+1}(x_c, 1)} \frac{y^* - y}{y(y^* - 1)}.$$

So if $\lim_{h \to 0} B_h(x_c, 1) = 0$, this implies

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PROOF THAT $\lim_{h\to 0} B_h(x_c, 1) = 0$,

This is rather technical. We use renewal theory (following Kesten), to prove the lemma that, as $h \to \infty$

$$B_h(x_c, 1) = \frac{1}{\mathbb{E}_{iB}(H(\gamma))},$$

where $H(\gamma))$ is the height of a bridge γ. We prove by contradiction that this expectation value is infinite.
Proposition: If $\mathbb{E}_{iB}(H(\gamma)) < \infty$, then $\mathbb{E}_{iB}(W(\gamma)) < \infty$.
Corollary: If $\mathbb{E}_{iB}(H(\gamma)) < \infty$, a random infinite bridge is tall and skinny. Proof follows from the law of large numbers.
Introducing *diamond points* and *a stick-beak operation*, we prove that this is not true. QED.

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Extension to other lattices

- There is no corresponding equation for SAW on other lattices.
- For the square lattice, Cardy and Ikhlef found a similar (parafermionic) observable, but the model describes osculating SAW with asymmetric weights.
- Arguing that the scaling limit of all two-dimensional SAW models should be identical, “something similar" should be true for SAW on other lattices.
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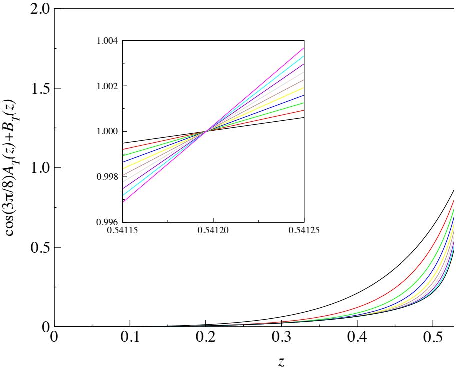

Figure: Bad picture with nice inset of $c_\alpha A_T(x) + B(x)$ for honeycomb lattice walks in a strip of width $1, \cdots, 10$.

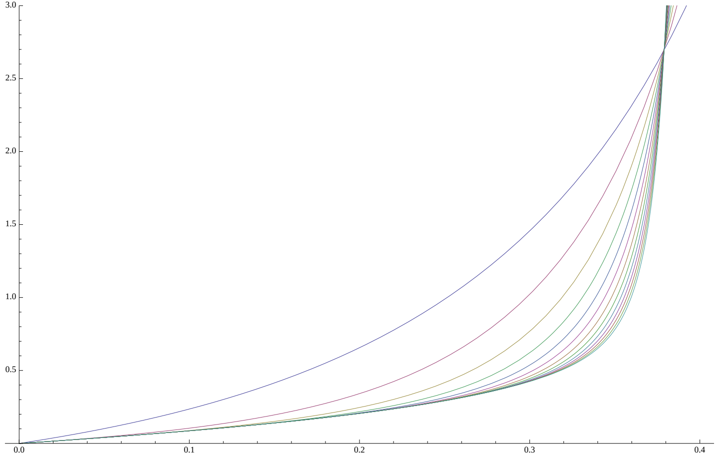

Figure: Square lattice $c_\alpha A_T(x) + B(x)$ for walks in a strip of width $1, \cdots, 15$.

Conjecture (using best estimates of x_c):

$$1 = c_A(T)A_T(x_c) + c_B(T)B_T(x_c),$$

Assume

$$1 = c_A(T)A_{T+1}(x_c) + c_B(T)B_{T+1}(x_c),$$

and solve for $c_A(T)$ and $c_B(T)$.
(Square lattice $T \leq 15$, triangular lattice $T \leq 11$).
Extrapolate:

$$\lim_{T\to\infty} \frac{c_A(T)}{c_B(T)} = \cos\left(\frac{3\pi}{8}\right)$$

to 6 sig. digits. Hence

$$\cos\left(\frac{3\pi}{8}\right) A_T(x_c) + B_T(x_c) = const. + correction$$

In fact $1.02497(1 - 0.14/T^2)$, similarly for the triang. lattice.

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More generally, assume

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Successive triples give

$$c_A(T),\ c_B(T),\ x_c(T).$$

Extrapolate $x_c(T)$ and find
$x_c(sq) = 0.37905228(1)$ and $x_c(tr) = 0.240917575(10)$.

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Surface interaction fugacity for other lattices

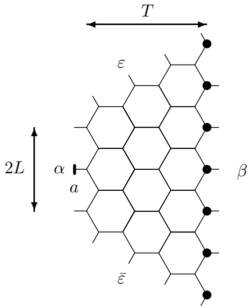

Figure: Finite patch with a boundary. The SAW acquires weights x, y for each step/contact.

For the hexagonal lattice, we have proved that

$$\cos(\frac{3\pi}{8})A_T(x_c, y) + \cos(\frac{\pi}{4}) \left(\frac{y_c - y}{y}\right) B_T(x_c, y) = 1.$$

Repeating,

$$\cos(\frac{3\pi}{8})A_T(x_c, y) + \cos(\frac{\pi}{4})\left(\frac{y_c - y}{y}\right)B_T(x_c, y) = 1.$$

- At $y = y_c$ we have

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- So for the honeycomb lattice $T = 1$ and $T = 2$ results are enough to calculate x_c and y_c!
- Other lattices?
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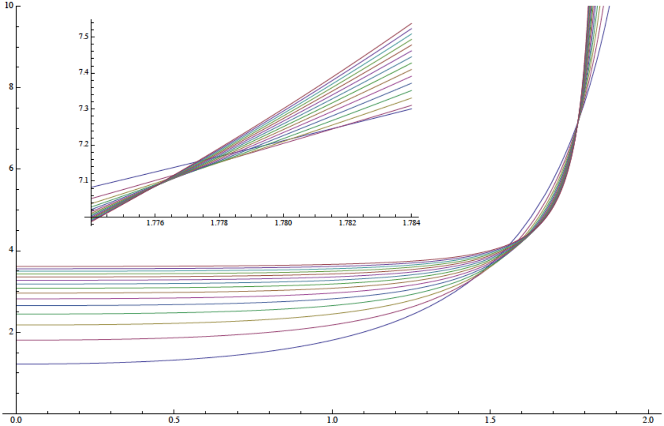

Figure: Square lattice with surface site interactions. $A_T(x_c, y)$ versus y for $T = 1 \ldots 15$. Inset shows the intersection region in finer scale.

- We denote by $y_c(T)$ the point of intersection of $A_T(x_\mathrm{c}, y)$ and $A_{T+1}(x_\mathrm{c}, y)$.
- We observe that the sequence $\{y_c(T)\}$ is a monotone function of T. The argument above implies that $\lim_{T\to\infty} y_c(T) = y_c$.
- This then suggests a new numerical approach to estimating y_c.
- One first calculates the generating function for arches, $A_T(x_\mathrm{c}, y)$, for all strip widths $T = 0, 1, 2, \ldots T_\mathrm{max}$.
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Table: Estimated critical fugacity y_c for surface adsorption.

Lattice	Site weighting	Edge weighting
Honeycomb	1.46767	$\sqrt{1+\sqrt{2}}$
Square	1.77564	2.040135
Triangular	2.144181	2.950026

For the square lattice these are at least 1000 times more accurate than other methods. Other results are new.

EXTEND OFF-CRITICALITY

- We redefine the parafermionic operator ($\bar{\sigma} = 1 + \sigma$) as

$$F(x) = F(a, x, z, \bar{\sigma}) = \sum_{\gamma \subset \Omega : a \to x} e^{i\bar{\sigma} W(\gamma)} z^{|\gamma|}.$$

- In terms of this redefined operator, the D-C/S result is

$$\sum_{\gamma \subset \Omega : a \to x} e^{i\frac{3}{8} W(\gamma)} z_c^{|\gamma|} = 1.$$

  where the sum is over all walks starting at a and ending at x, on the boundary of Ω.

Theorem

For $z \leq z_c$

$$\sum_{\gamma:a\to x\in\partial\Omega} e^{\frac{3i}{8}W(\gamma)} z^{|\gamma|} + (1 - z/z_c) \sum_{\gamma:a\to x\in\Omega\setminus\partial\Omega} e^{\frac{3i}{8}W(\gamma)} z^{|\gamma|} = 1.$$

The first sum is over all walks that finish at the surface of the domain, while the second sum is over all walks that finish strictly in the interior of the domain.

We do this for the n-vector model $n \in [-2, 2]$. The r.h.s. becomes a loop generating function, and F has an extra parameter that counts loops.

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Exponent inequalities

Restricting ourselves to SAWs, in a strip, we obtain

$$\cos(\frac{3\pi}{8})A_T(z) + B_T(z) + (1 - z/z_c)G_T(z) = 1.$$

As $T \to \infty$, $A_T(z) \to \chi_{11}(z)$, $B_T(z) \to 0$, and $G_T(z) \le \chi_1$.

It immediately follows that

$$\gamma_{11} \le \gamma_1 - 1.$$

(Numerically, $\frac{73}{64} \ge 1$.)

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Exponent inequalities

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WINDING ANGLE DISTRIBUTION

We can use this to calculate the winding angle distribution exponent for all O(n) models with $n \in [-2, 2]$ in terms of exponents γ_1 and γ_{11}, subject only to the existence of those exponents.

First conjectured by Duplantier and Saleur for the O(n) model by CFT arguments.

Let $P(x = \theta)$ be the probability density that the winding angle is θ. Then

$$\int_{-\infty}^{\infty} e^{\tilde{\sigma} i\theta} P(\theta) d\theta \propto \ell^{-\omega}, \text{ where}$$

where

$$\omega = \gamma_1 - \gamma_{11} - 1 = \left(\frac{9}{8} \frac{(2-\kappa)^2}{\kappa(4-\kappa)} \right).$$

We prove the first equality. The second assumes scaling relations for these exponents, and that the scaling limit is described by SLE_κ.

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