Partition function zeros of adsorbing walk models

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Introduction: Fisher zeros

For your favourite statistical mechanical model, define the partition function for a size-n system as

$$Z_n(\beta) = \sum_{\omega \in \Omega_n} e^{-\beta E(\omega)}$$

where

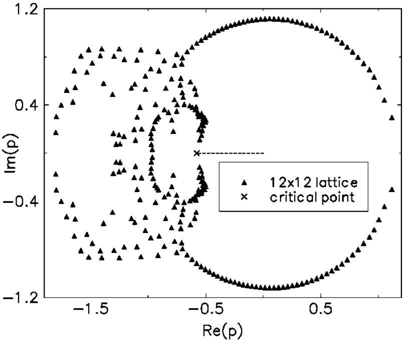
- Ω_n is the set of all size-n configurations
- $E(\omega)$ is the energy of configuration ω
- $\beta = \epsilon / kT$ and ϵ is the energy per interaction

$Z_n(\beta)$ is a polynomial in $e^{-\beta}$ with non-negative coefficients.

The roots of $Z_n(\beta)$ in the complex β-plane are the Fisher zeros.

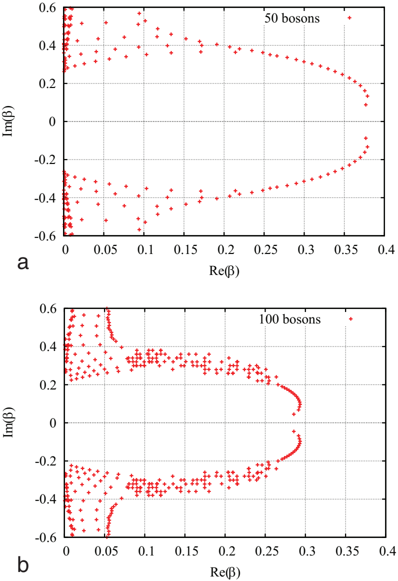
These have been studied for a wide range of models, including

Introduction: Fisher zeros



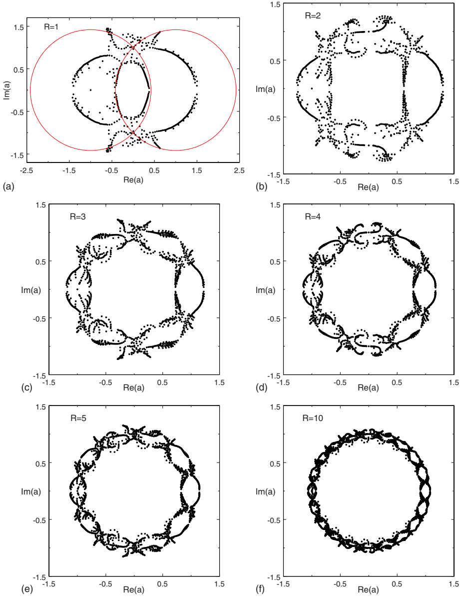
Q-state Potts model

[S.-Y. Kim & R.J. Creswick, Phys. Rev. E **63** (2001), 066107]



Models of trapped ideal bosons

[W. van Dijk, C. Lobo, A. MacDonald & R.K. Bhaduri, Can. J. Phys. **93** (2015), 830–835]



The Ising model (with nearest-neighbour and next-nearest-neighbour interactions)

[S.-Y. Kim, Phys. Rev. E **81** (2010), 031120]

The Fisher zeros can give information about the critical behaviour of the model.

For example, because $Z_n(\beta)$ is polynomial with non-negative coefficients, there are no zeros on the real axis. But as n gets large, the zeros closest to the real axis approach the critical point β_c.

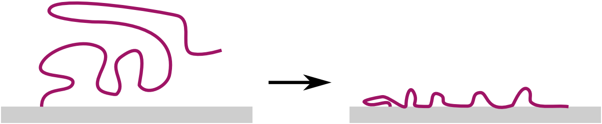
Moreover, if we sort the zeros according to their (positive) argument, then the k-th zero $\beta_{n,k}$ is expected to behave as

$$\beta_{n,k} \sim \beta_c + c_k n^{-\phi} + o(n^{-\phi})$$

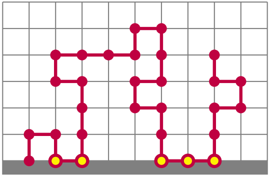
where ϕ is the crossover exponent and $c_k \in \mathbb{C}$ is a constant.

These have been used in the past to estimate β_c and ϕ, among other things.

Linear polymers in a good solvent, terminally attached to an impenetrable surface, can undergo an adsorption phase transition at a critical temperature.



These can be studied using various lattice and off-lattice models. In particular, self-avoiding walks on a half-space of the square or cubic lattices:



In this case, $E(\omega)$ is the number of vertices in the surface (except the initial one), and the partition function can be written as

$$Z_n(a) = \sum_{|\omega|=n} a^{E(\omega)} \qquad \text{where} \qquad a = e^{-\beta}$$

The free energy is

$$\kappa(a) := \lim_{n\to\infty} \frac{1}{n} \log Z_n(a).$$

This exists for all $a \geq 0$, is continuous and almost-everywhere differentiable, and has a point of non-analyticity at a critical point a_c. This is estimated to be

$a_c \approx 1.775615$ (2D) [Guttmann, Jensen & Whittington 2014]

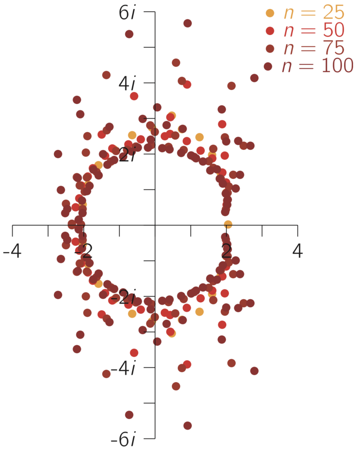
$a_c \approx 1.306$ (3D) [Janse van Rensburg 2016]

The behaviour near a_c is (expected to be) governed by the crossover exponent ϕ:

$$\kappa(a) - \kappa(a_c) \sim (a - a_c)^{\frac{1}{\phi}}, \qquad a \to a_c^+$$

In 2D ϕ is predicted to be exactly $\frac{1}{2}$; it has been proposed that ϕ may be $\frac{1}{2}$ in all dimensions, but (some) numerical evidence in 3D disputes this...

Janse van Rensburg [2017] used Monte Carlo methods (namely flatGAS) to estimate $c_n(v)$, the number of SAWs of length n with v visits to the surface, on the square and cubic lattices. This then gave estimates of the partition functions $Z_n(a)$. The locations of the zeros in the complex a-plane were then computed. In the square lattice:



It was found that

- a positive density of zeros appear to accumulate on a circle of radius a_c centred at 0
- there are other zeros which appear to "drift" away from the origin
- all zeros lie in a vertical strip of slowly increasing width
- the zeros are "pinching" the positive real axis at a point close to the critical point a_c

[Janse van Rensburg, J. Stat Mech. (2017) 033208]

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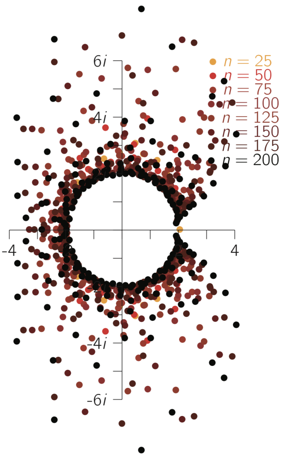

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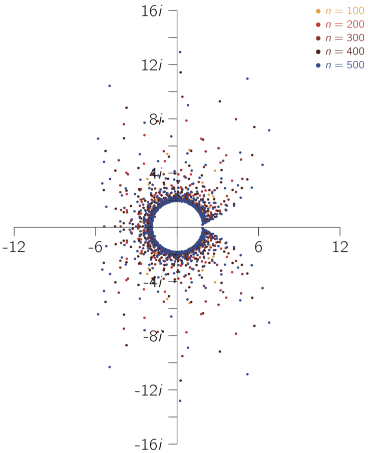

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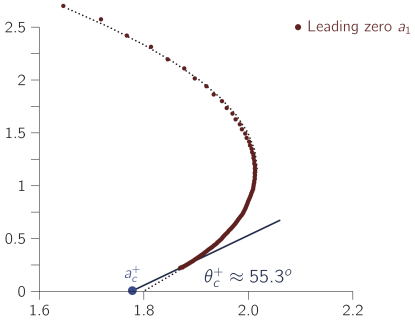
Fisher zeros for adsorbing SAWs

An examination of the leading zero as n gets large produced mixed results:



While the approach to the real axis does match a crossover exponent $\phi = \frac{1}{2}$, fitting to a quadratic gives the estimate $a_c \approx 1.8049$, a fair way off the current best estimate $a_c = 1.775615$.

[Janse van Rensburg, J. Stat Mech. (2017) 033208]

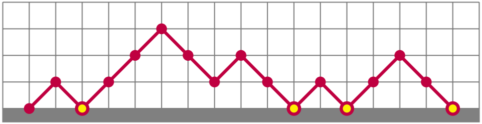
Similar results were found for the cubic lattice.

Fisher zeros for adsorbing directed walks

We then decided to take a completely different approach: what happens for a solvable model? Can we "go backwards" and prove things about the zeros?

eg. For the 2D Ising model (with only nearest-neighbour interactions), the zeros all accumulate on two circles of radius $\sqrt{2}$ centered on ± 1 [Fisher 1965] (see earlier figure).

The simplest model of polymer adsorption uses interacting Dyck paths:



The partition functions $D_n(a)$ of $2n$-step paths satisfy a two-term recurrence

$$2a^2(2n+1)D_n(a) - [2(a-1)(2n+1) + a^2(n+2)]D_{n+1}(a) + (a-1)(n+2)D_{n+2}(a) = 0$$

with solution

$$D_n(a) = \sum_{\ell=0}^{n} \frac{2\ell+1}{n+\ell+1}\binom{2n}{n+\ell}(a-1)^\ell.$$

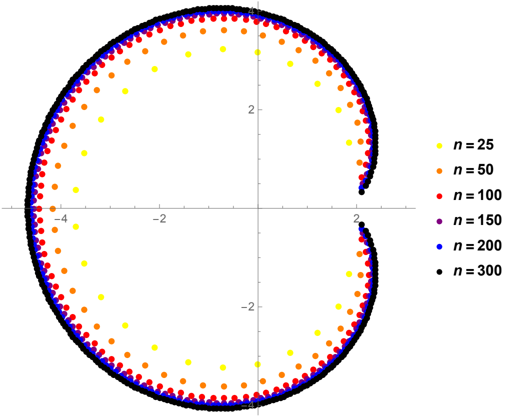
and generating function

$$D(z;a) = \sum_{n=0}^{\infty} D_n(a) z^n = \frac{2}{2 - a(1-\sqrt{1-4z})}.$$

Fisher zeros for adsorbing directed walks

With an exact solution to $D_n(a)$, the zeros can be computed exactly for large n.

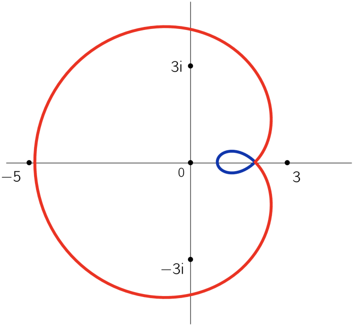
They behave quite differently to adsorbing SAWs:



This curve looks a bit like a cardioid...

The limiting curve

... but in fact it is not a cardioid – it is the outer lobe of a limaçon:



This curve is the locus of points satisfying

$$\left|\frac{a^2}{a-1}\right| = 4$$

and is parametrised by $a = x + iy$ with

$$x = 2 + \left(2\sqrt{2} - 4\cos\phi\right)\cos\phi$$
$$y = \left(2\sqrt{2} - 4\cos\phi\right)\sin\phi$$

for $\phi \in [0, 2\pi)$.

Why? The generating function has two singularities in the complex z-plane, depending on the value of a. They lead to the asymptotic growth rate

$$\lim_{n\to\infty} D_n(a)^{\frac{1}{n}} = \mu(a) = \begin{cases} 4, & \text{if } \left|\frac{a^2}{a-1}\right| \le 4 \text{ or } |a-1| < 1; \\ \frac{a^2}{a-1}, & \text{if } \left|\frac{a^2}{a-1}\right| > 4 \text{ and } |a-1| \ge 1. \end{cases}$$

The outer lobe is exactly the boundary between the two different growth regimes of $D_n(a)$.

The limiting curve

If $|a-1| \geq 1$ then the two singularities contribute to the asymptotics of $D_n(a)$. Roughly,

$$D_n(a) \sim C_1 \left(\frac{a^2}{a-1}\right)^n + C_2 n^{-\frac{3}{2}} 4^n (1 + O(n^{-1}))$$

for constants C_1, C_2.

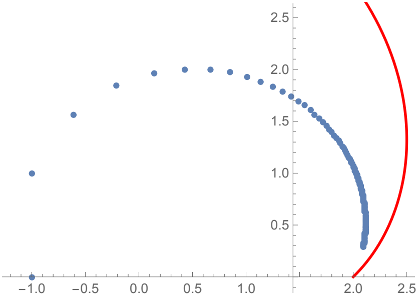
If $D_n(a_n^*) = 0$ then these two terms must cancel. As $n \to \infty$ the two exponential terms must balance, so $\left|\frac{(a_n^*)^2}{a_n^*-1}\right| \to 4$.

With more work, can show that the zeros become dense on the limaçon, ie. for any point $p \neq 2$ on the limaçon and $\epsilon > 0$, there is an N such that $D_n(a)$ has a zero inside the ball $|p-a| \leq \epsilon$ for all $n \geq N$.

Dyck paths undergo an adsorption transition at $a = a_c = 2$.

The limaçon meets the real axis here at an angle of 45°. $D_n(a)$ has no positive real zeros, but the zeros "pinch" the real axis at $a = 2$.

However the first (or k-th) zero does not approach $a = 2$ along the limaçon:



So how does it behave?

The leading zero

The crossover exponent for Dyck paths is $\phi = \frac{1}{2}$, so take $D_n(2 + \frac{c}{\sqrt{n}})$:

$$D_n(2 + \tfrac{c}{\sqrt{n}}) = \sum_{k=0}^{n} \sum_{\ell=k}^{n} \frac{2\ell+1}{n+\ell+1} \binom{2n}{n+\ell} \binom{\ell}{k} \frac{c^k}{n^{k/2}}$$

Using Stirling's approximation etc. this can be (carefully) approximated with an integral, which can be evaluated. The result is

$$D_n(2 + \tfrac{c}{\sqrt{n}}) \sim \frac{4^n}{2\sqrt{\pi n}} \left(2 + c\sqrt{\pi}\, e^{\frac{c^2}{4}} (1 + \operatorname{erf}(\tfrac{c}{2})) \right). \qquad (\star)$$

The leading zero then behaves like $2 + \frac{c_0}{\sqrt{n}}$, where $c_0 \in \mathbb{C}$ is the root of $(\star)$ closest to 0. Approximately

$$c_0 = 2.450314191845586... + 5.094256056412729... \times i$$

Further terms in the approximation can be obtained by setting $a = 2 + \frac{c_0}{\sqrt{n}} + \frac{c_1}{n}$ etc.

SAWs vs. Dyck paths

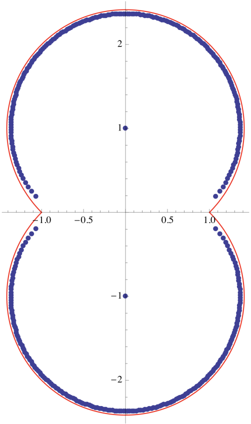
Why the big difference between SAWs and Dyck paths?

The Dyck path generating function has only two singularities, and the zeros are drawn to the region in $\mathbb{C}$ where the exponential contributions of these two singularities balance, ie. the limaçon.

More generally, for a g.f. with $s < \infty$ singularities, the complex a-plane ($\approx$ complex T plane) can be partitioned into regions determined by which singularity is dominant. The zeros are then drawn to the boundaries of these regions.

But the g.f. for SAWs is believed to have infinitely many singularities, or even uncountably many. So the partition function zeros may not be drawn to well-defined curves.

There are lots of other solvable models, e.g. pulled ballot paths,



adsorbing and/or self-interacting partially directed walks, staircase polygons, prudent walks, etc etc. What other pictures can emerge?

References

E.J. Janse van Rensburg, *Partition and generating function zeros in adsorbing self-avoiding walks,* J. Stat. Mech. (2017) 033208.

NRB & E.J. Janse van Rensburg, *Partition function zeros of adsorbing Dyck paths* (2017), to appear in J. Phys A.

Thank you!