Partition function zeros of adsorbing self-avoiding walks

EJ Janse van Rensburg

Department of Mathematics & Statistics, York University, Toronto, Ontario, M3J 1P3, Canada

E-mail: rensburg@yorku.ca

Abstract. Partition function or Fisher zeros play a fundamental role in the theory of phase transitions in models in classical statistical mechanics. In this paper the properties of partition function zeros in a square lattice self-avoiding walk model of polymer adsorption are presented. Some results constraining the distribution of zeros in the complex plane, based on mathematical results on the distribution of polynomial zeros, are presented. Numerical results on the distribution of zeros are shown, based on approximate enumeration of square lattice walks using the GAS algorithm.

1. Introduction

Partition function zeros in the complex plane (also called *Fisher zeros* [4]) provide a mathematical mechanism which explains phase transitions in models in classical statistical mechanics. In the thermodynamic limit, Fisher zeros accumulate in the complex plane in patterns which create an *edge singularity* at the critical point on the real axis where a phase transition occurs.

There is a significant literature devoted to the study of partition function zeros and the edge-singularity in models of lattice spin systems. These models include the Ising model [17, 18], the q-state Potts model [10–13], the van der Waal gas and ideal Bose gas [21]. In contrast, far less is known about the partition function zeros in models of lattice clusters, including models of the self-avoiding walk (see figure 1).

Exact enumeration of self-avoiding walks in the square lattice in reference [14] to lengths $n = 28$ was used to determine partition function zeros, and to study the relation between the leading

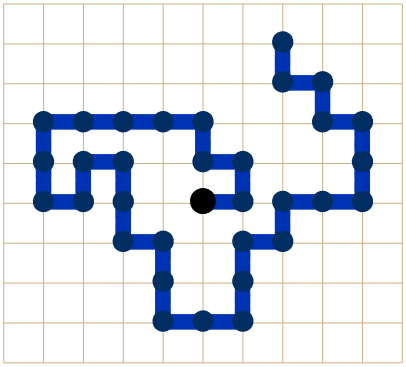

Figure 1: A self-avoiding walk from the origin in the square lattice.

partition function zero and the thermodynamic properties of the model. Similar work in the cubic lattice is reported in references [15, 16]. The partition function zeros in a bond fluctuation model of polymer adsorption was considered in reference [20]. In this last study chains in two dimensions of length up to 1536 were generated and the distribution of partition function zeros was examined.

In this paper a study similar to that of reference [20] is reported. In particular, some theoretical properties of partition function zeros in adsorbing lattice walks in the square lattice are examined, and some numerical data in support of these properties are presented.

2. Adsorbing walks

Denote the d-dimensional hypercubic lattice by $\mathbb{L}^d$ and let c_n be the number of self-avoiding walks from the origin length n in $\mathbb{L}^d$ (see figure 1). Since $d^n \leq c_n \leq 2d(2d-1)^{n-1}$ in $\mathbb{L}^d$, it follows that c_n grows exponentially with n, and it is known that the limit

$$\lim_{n\to\infty} \tfrac{1}{n} \log c_n = \log \mu_d \tag{1}$$

exists [5]. The number $\kappa_d = \log \mu_d$ is the *connective constant* of the lattice $\mathbb{L}^d$, and μ_d is the hypercubic lattice *growth constant* of c_n, namely $c_n = \mu_d^{n+o(n)}$ [2].

The half lattice $\mathbb{L}^d_+$ is defined by

$$\mathbb{L}^d_+ = \{\vec{v} \in \mathbb{L}^d \mid v_d \geq 0\}, \tag{2}$$

where $\vec{v} = (v_1, v_2, \ldots, v_d)$ is a vertex in $\mathbb{L}^d$. A self-avoiding walk from the origin in the half lattice $\mathbb{L}^d_+$ is a *positive walk*. The number of positive walks of length n is denoted by c_n^+. Naturally, $c_n^+ \leq c_n$. It is known that

$$\lim_{n\to\infty} \tfrac{1}{n} \log c_n^+ = \lim_{n\to\infty} \tfrac{1}{n} \log c_n = \log \mu_d. \tag{3}$$

See, for example, reference [6].

The boundary of the half lattice $\mathbb{L}^d_+$ is the $(d-1)$-dimensional hypercubic lattice given by

$$\partial\mathbb{L}^d_+ = \{\vec{v} \in \mathbb{L}^d_+ \mid v_d = 0\}, \tag{4}$$

and it is equivalent to $\mathbb{L}^{d-1}$. A model of *adsorbing (positive) walks* is obtained by weighing vertices of a positive walk with the weight or *activity* a whenever the walk returns to or visits the boundary $\partial\mathbb{L}^d_+$. This assigns a weight a^v to each positive walk making v visits to $\partial\mathbb{L}^d_+$. Notice that, by convention, the first vertex at the origin is not a visit. A *positive* or *adsorbing walk* with visits weighted by a^v is shown in figure 2.

If $c_n^+(v)$ is the number of positive walks of length n and with v visits in the adsorbing boundary $\partial\mathbb{L}^d_+$, then the partition function and limiting free energy of adsorbing walks are given by

$$A_n^+(a) = \sum_{v=0}^{n} c_n^+(v)\, a^v \quad \text{and} \quad \mathcal{A}^+(a) = \lim_{n\to\infty} \tfrac{1}{n} \log A_n^+(a). \tag{5}$$

Existence of the limiting free energy $\mathcal{A}^+(a)$ was shown in reference [6], and it is known that $\mathcal{A}^+(a)$ is a non-decreasing convex function of $\log a$. Moreover, there is a critical point a_c^+ in the model, defined by $\mathcal{A}^+(a) = \log \mu_d$ if $a \leq a_c^+$ and $\mathcal{A}^+(a) > \log \mu_d$ if $a > a_c^+$. The critical point a_c^+ is the *adsorption critical point* in the model, and it is a singular point in the free energy $\mathcal{A}^+(a)$.

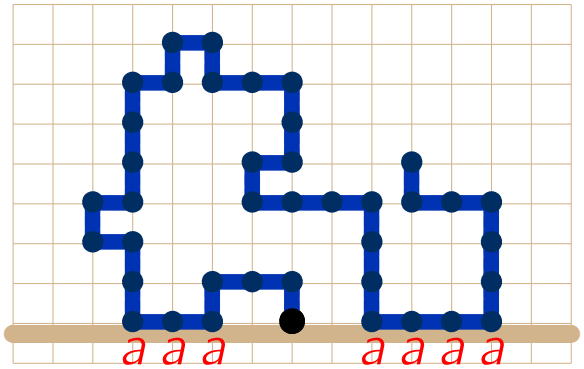

Figure 2: A positive or adsorbing self-avoiding walk in the half square lattice. This positive walk steps from the origin (in the boundary of the half lattice), and each vertex (other than the first vertex at the origin) where the walk returns to or visits the boundary is weighted by an activity a.

3. Partition function zeros

Partition function zeros are the (complex valued) roots of $A_n^+(a)$. Since $A_n^+(a)$ is a polynomial of degree n, there are n zeros $\{a_j\}$, and $A_n^+(a)$ factors as

$$A_n^+(a) = C_n \prod_{j=1}^{n} (a - a_j) \tag{6}$$

where C_n is the (positive) coefficient of a^n in equation (5) (it depends on n). Notice that C_n is the number of walks in $\mathbb{L}^{d-1}$, since the coefficient of a^n is the number of walks with every vertex in $\partial\mathbb{L}_+^d$. Taking logarithms and dividing by n, and letting $n \to \infty$, gives the limiting free energy of the model, namely

$$\mathcal{A}^+(a) = \lim_{n\to\infty} \tfrac{1}{n} \log A_n^+(a) = \log \mu_{d-1} + \lim_{n\to\infty} \tfrac{1}{n} \sum_{j=1}^{n} \log(a - a_j), \tag{7}$$

in particular since $\log \mu_{d-1} = \lim_{n\to\infty} \frac{1}{n} \log C_n$. Taking derivatives to $\log a$ gives the *energy density* and *specific heat* of the adsorbing walk.

3.1. The distribution of partition function zeros

The distribution of partition function zeros may be examined by defining the functions

$$\begin{aligned} \nu_n(\rho) &= \#\{\mathcal{A}^+(a) \text{ zeros } a_k \mid (1-\rho) \le |a_k| \le \tfrac{1}{1-\rho}\} \\ \alpha_n(\theta,\phi) &= \#\{\mathcal{A}^+(a) \text{ zeros } a_k \mid \theta < \mathfrak{Arg}\, a_k \le \phi\}. \end{aligned} \tag{8}$$

That is, $\nu_n(\rho)$ is the number of zeros of $\mathcal{A}^+(a)$ in the annulus $(1-\rho) \le |a| \le \frac{1}{1-\rho}$ in the a-plane (where $\rho \in (0,1)$), and $\alpha_n(\theta,\phi)$ is the number of zeros a_k with complex principal arguments $\mathfrak{Arg}\, a_k$ greater than θ and less than or equal to ϕ.

The theorem by Hughes and Nikeghbali [7] is useful in providing bounds on $\nu_n(\rho)$, while the angular distribution of zeros can be examined using the classical theorem of Erdös and Turán [3]. Let $\zeta_d = \log \frac{\mu_d}{\mu_{d-1}}$, then, if $\zeta_d < \rho < 1$, then Hughes and Nikeghbali's theorem implies that

$$0 < 1 - \tfrac{1}{\rho}\,\zeta_d \le \liminf_{n\to\infty} \tfrac{1}{n}\,\nu_n(\rho) \le \limsup_{n\to\infty} \tfrac{1}{n}\,\nu_n(\rho) \le 1. \tag{9}$$

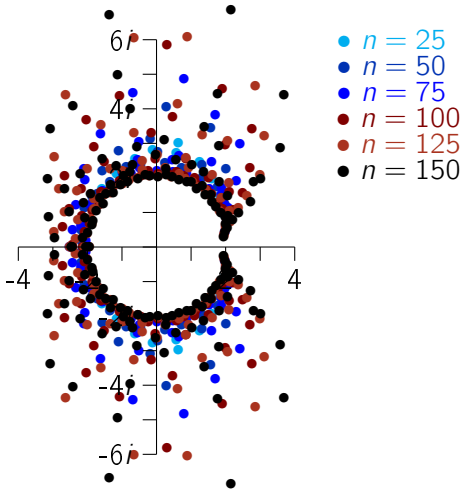

Figure 3: Partition function zeros of the partition function $A_n^+(a)$ of adsorbing self-avoiding square lattice walks. The data shown are for walks of length $n \in \{25, 50, 75, 100, 125, 150\}$.

The theorem by Erdös and Turán similarly shows that there is a constant C_0 so that, if $\zeta_d < \rho < 1$, then

$$\limsup_{n\to\infty} \left| \tfrac{1}{2\pi}(\phi-\theta) - \tfrac{1}{n}\,\alpha_n(\theta,\phi) \right| \le \sqrt{\tfrac{1}{2} C_0 \zeta_d}. \tag{10}$$

These results strongly suggest that partition function zeros are distributed in an annular region in the complex plane, and that the angular distribution is asymptotically fairly even.

3.2. Numerical results

Numerical data were collected on adsorbing walks using the GAS algorithm [9] which was implemented for adsorbing walks in reference [8]. These simulations produced estimates of $c_n^+(v)$ for $0 \le v \le n \le 500$ in the microcanonical ensemble. Combining these data as in equation (5) produces estimates of the partition function $A_n^+(a)$. Zeros of $A_n^+(a)$ were obtained to high accuracy by deflating the polynomials in Maple 17 [19]. In figure 3 the partition function zeros for adsorbing square lattice walks are shown.

Finite size approximations to the free energy can be computed from the partition function zeros using equation (7). Similarly, the energy density $\mathcal{E}^+$ and specific heat $\mathcal{C}^+$ are given by

$$\mathcal{E}^+(a) = \lim_{n\to\infty} \tfrac{1}{n} \sum_{j=1}^{n} \frac{1}{a-a_j}, \quad \text{and} \quad \mathcal{C}^+(a) = \lim_{n\to\infty} \tfrac{-1}{n} \sum_{j=1}^{n} \frac{1}{(a-a_j)^2}. \tag{11}$$

In figure 4 finite size approximations to the excess free energy $\mathcal{A}^+(a) - \log \mu_d$, energy density and specific heat, are plotted for $n \in \{60, 125, 250, 500\}$. Notice the sharp peak in the specific heat curves, and that these curves intersect close to a common point at $\log a_c^+$ in the graph. For values $\log a < \log a_c^+$ the curves decrease with increasing n, and for $\log a > \log a_c^+$ the curves increase with increasing n. This intersection is therefore a good estimage of the critical adsorption activity in the model. By calculating it for $(n, 2n)$ and $n \in \{100, 110, 120, \ldots, 250\}$ a set of estimates of a_c^+ is obtained (see equation (58) in reference [8]). Taking the average to find the best estimate gives

$$a_c^+ = 1.764(16), \text{ in } \mathbb{L}_+^2. \tag{12}$$

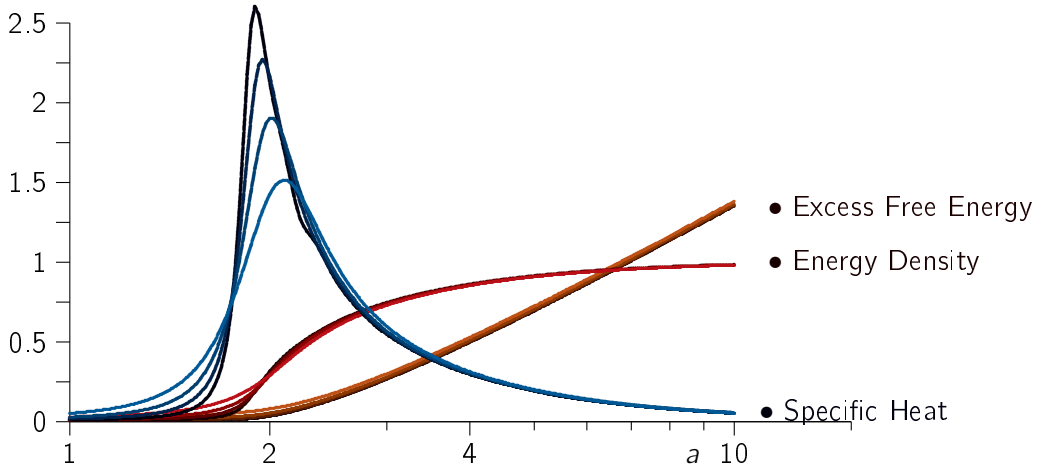

Figure 4: The excess free energy, energy density and specific heat of adsorbing walks as a function of a on a log-linear scale for walks of length $n \in \{60, 125, 250, 500\}$.

This estimate can be compared to the best estimate $a_c^+ = 1.77564$ in the square lattice using exact enumeration methods [1] and $a_c^+ = 1.779$ in reference [8].

3.3. The cumulative angular distribution function

A *cumulative angular distribution function* $\boldsymbol{\alpha}_n(\phi)$ of partition function zeros (of $A_n^+(a)$) around the origin in the complex a-plane is defined by using the function $\alpha_n(\theta, \phi)$ defined in equation (8):

$$\boldsymbol{\alpha}_n(\phi) = \tfrac{1}{n}\alpha_n(-\pi, \phi). \tag{13}$$

$\boldsymbol{\alpha}_n(\phi)$ is a non-decreasing step-function which increments in steps of height $\frac{1}{n}$ each time an increase in ϕ includes new zeros in the interval $(-\pi, \phi]$, and with $\boldsymbol{\alpha}_n(-\pi) = 0$ and $\boldsymbol{\alpha}_n(\pi) = 1$. In other words, $\boldsymbol{\alpha}_n(\phi)$ is the fraction of partition function zeros with principal argument in the interval $(-\pi, \phi]$.

The cumulative angular distribution function $\boldsymbol{\alpha}_n(\phi)$ is plotted in figure 5 for $n \in \{60, 125, 250, 500\}$. It increases with ϕ, except near $\phi = 0$ where it has a slight flattening (this is for zeros close to the positive real axis in the a-plane). This flattening becomes less pronounced as n increases. In the limit the data suggest a straight line increasing from 0 at $\phi = -\pi$ to 1 at $\phi = \pi$. That is, the cumulative distribution function apparently converges such that $\lim_{n\to\infty} \boldsymbol{\alpha}_n(\phi) = \frac{1}{2\pi}\phi + \frac{1}{2}$. This implies that the limiting angular distribution is given by $\lim_{n\to\infty} \frac{1}{n}\alpha_n(\phi, \theta) = \frac{1}{2\pi}(\phi - \theta)$ (this remains unproven).

4. Conclusions

In this paper I report on some aspects of partition function zeros in a self-avoiding walk model of two dimensional adsorbing polymers. The data in figure 5 suggest strongly that the angular distribution of zeros, in the limit as $n \to \infty$, is uniform. Algebraic results in equations (9) and (10) constraining the distribution of partition function zeros were determined, and tested numerically by examining the distribution of partition function zeros. It is found that a positive density of zeros is distributed in an annulus with center at the origin in $\mathbb{C}$ and that the angular distribution is bounded in the sense that $\lim_{n\to\infty} \frac{1}{n}\alpha_n(\theta, \phi)$ approaches zero as $\theta \nearrow \phi$ (and the numerical data in figure 5 suggest that it is uniform).

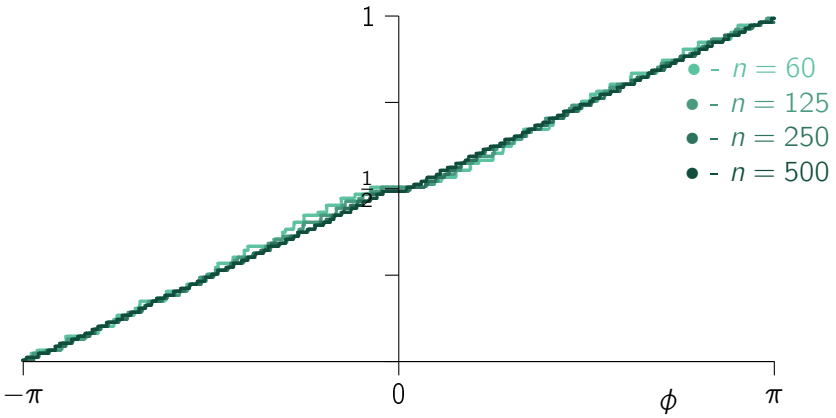

Figure 5: The cumulative distribution function $\frac{1}{n}\alpha_n(-\pi,\phi)$ of the principal arguments of partition function zeros in the complex plane for finite values of n. These data are for $n \in \{60, 125, 250, 500\}$ and appear to converge to the line $\frac{1}{2\pi}\phi + \frac{1}{2}$ as $n \to \infty$.

In section 3.2 the partition function zeros are estimated from numerical data obtained by sampling adsorbing self-avoiding walks in the square lattice using the GAS algorithm [9]. The free energy is approximated in terms of the partition function zeros, and in figure 4 the excess free energy, energy density and specific heat are plotted. The specific heat curves intersect in a point approximating the critical adsorption activity a_c^+, giving the estimate in equation (12).

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