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Location of zeros for the partition function of the Ising model on bounded degree graphs

Han Peters and Guus Regts

Abstract

The seminal Lee–Yang theorem states that for any graph the zeros of the partition function of the ferromagnetic Ising model lie on the unit circle in \mathbb{C} . In fact, the union of the zeros of all graphs is dense on the unit circle. In this paper, we study the location of the zeros for the class of graphs of bounded maximum degree $d \geq 3$, both in the ferromagnetic and the anti-ferromagnetic case. We determine the location exactly as a function of the inverse temperature and the degree d. An important step in our approach is to translate to the setting of complex dynamics and analyze a dynamical system that is naturally associated to the partition function.

1. Introduction and main result

For a graph $G = (V, E), \, \xi, b \in \mathbb{C}$, the partition function of the Ising model $Z_G(\xi, b)$ is defined

$$Z_G(\xi, b) := \sum_{U \subseteq V} \xi^{|U|} \cdot b^{|\delta(U)|}, \tag{1.1}$$

where $\delta(U)$ denotes the collection of edges with one endpoint in U and one endpoint in $V \setminus U$. If ξ and b are clear from the context, we will often just write Z_G instead of $Z_G(\xi, b)$. In this paper, we typically fix b and think of Z_G as a polynomial in ξ . The case 0 < b < 1 is often referred to as the ferromagnetic case, while the case where b > 1 is referred to as the anti-ferromagnetic case.

The Ising model is a simple model to study ferromagnetism in statistical physics. In statistical physics, the partition function of the Ising model is often written as

$$\sum_{\sigma:V\to\{-1,1\}} \exp\left(J/T\cdot \sum_{\{u,v\}\in E} \sigma(u)\sigma(v) + h/T\cdot \sum_{v\in V} \sigma(v)\right),\tag{1.2}$$

where J denotes the coupling constant, h the external magnetic field and T>0 the temperature, normalizing the Boltzmann constant to 1 for convenience. Setting $\xi=e^{-2h/T}$, $b=e^{-2J/T}$ and $U=\{v:\sigma(v)=-1\}$, then up to a factor of $e^{J\cdot|E|/T+h\cdot|V|/T}$, the two partition functions (1.1) and (1.2) are the same.

Lee and Yang [14] proved that for any graph G and any $b \in [-1, 1]$, all zeros of Z_G lie on the unit circle in \mathbb{C} . Their result attracted enormous attention in the literature, and similar statements have been proved in much more general settings, see, for example, [2, 3, 7–9, 16–19, 21, 25, 26, 28].

In both the ferromagnetic and the anti-ferromagnetic case, the union of the roots of Z_G over all graphs G lies dense in the unit circle. Density in the ferromagnetic case in fact follows from our results, as will be pointed out in Remark 16. It is natural to wonder for which classes

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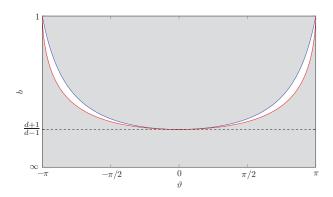


FIGURE 1 (colour online). The values of α_b (upper curve, in blue) and θ_b (lower curve, in red) for d = 2, as b varies from 1 to ∞ .

of graphs and choice of parameters b there are zero-free regions on the circle. For the class of binary Cayley trees (see Section 2 for a definition), this question has been studied by Barata and Marchetti [3] and Barata and Goldbaum [2]. In the present paper, we focus on the collection of graphs of bounded degree, and completely describe the location of the zeros for this class of graphs. For $d \in \mathbb{N}$, we denote by \mathcal{G}_d the collection of graphs with maximum degree at most d. By \mathbb{D} we denote the open unit disk in \mathbb{C} . Moreover, we will occasionally abuse notation and identify $(-\pi, \pi]$ with $\partial \mathbb{D}$, the unit circle. Given $\theta \in (-\pi, \pi)$, we write

$$I(\theta) := \{e^{i\vartheta} \mid \vartheta \in (-\theta, \theta)\}.$$

Our main results are:

THEOREM A (ferromagnetic case). Let $d \in \mathbb{N}_{\geq 2}$ and let $b \in (\frac{d-1}{d+1}, 1)$. Then there exists $\theta_b \in (-\pi, \pi)$ such that the following holds.

- (i) For any ξ ∈ I(θ_b) and any graph G ∈ G_{d+1}, we have Z_G(ξ, b) ≠ 0.
 (ii) The set {ξ = e^{iθ} ∈ ∂D \ I(θ_b) | Z_G(ξ, b) = 0 for some G ∈ G_{d+1}} is dense in ∂D \ I(θ_b).

The dependence of θ_b on b is given explicitly in (the proof of) Lemma 13. For now we remark that as $b \to \frac{d-1}{d+1}$, $\theta_b \to 0$ and as $b \to 1$, $\theta_b \to \pi$.

We remark that part (ii) has recently been independently proved by Chio, He, Ji and Roeder [9]. They focus on the class of Cayley trees and obtain a precise description of the limiting behavior of the zeros of the partition function of the Ising model.

We recall that in the anti-ferromagnetic case the parameters ξ for which $Z_G(\xi, b) = 0$ do not need to lie on the unit circle. For temperatures above the critical temperature, which corresponds to $b \in (1, \frac{d+1}{d-1})$ in our setting, the existence of a zero-free disk normal to the unit circle containing the point $\xi = +1$ was proved by Lieb and Ruelle [15]. Here we describe the maximal disk that can be obtained:

THEOREM B (anti-ferromagnetic case). Let $d \in \mathbb{N}_{\geq 2}$ and let $b \in (1, \frac{d+1}{d-1})$. Then there exists $\alpha_b \in (-\pi, \pi)$ such that the following holds.

- (i) For any $\xi \in I(\alpha_b)$, any $r \geqslant 0$ and any graph $G \in \mathcal{G}_{d+1}$, we have $Z_G(r \cdot \xi, b) \neq 0$; (ii) The set $\{\xi \in \mathbb{C} \mid Z_G(\xi, b) = 0 \text{ for some } G \in \mathcal{G}_{d+1}\}$ accumulates on $e^{i\alpha_b}$ and $e^{-i\alpha_b}$.

The value of α_b can again be explicitly expressed in terms of b, see Figure 1 for an illustration depicting α_b .

Another recent related contribution to the Lee-Yang program is due to Liu, Sinclair and Srivastava [18], who showed that for $\xi = 1$ and $d \ge 2$ there exists an open set $B \subset \mathbb{C}$ containing the interval $(\frac{d-1}{d+1}, \frac{d+1}{d-1})$ such that for any $G \in \mathcal{G}_{d+1}$ and $b \in B$, $Z_G(1, b) \neq 0$.

1.1. Motivation

The motivation for studying the location of zeros of partition functions traditionally comes from statistical physics. Since this is well known and since many excellent expositions exist, see, for example, [4, Section 7.4], we choose not discuss the physical background here. However, recently there has also been interest in understanding the location of zeros from the perspective of theoretical computer science, more precisely from the field of approximate counting.

In theoretical computer science, it is known that the exact computation of partition functions, such as of the Ising model and the hardcore model, or the number of proper k-colorings of a graph G, generally is a #P-hard problem (that is, it is as hard as computing the number of Hamiltonian cycles in a graph, see [1, 29, 30] for detailed information on the class #P). For this reason, much effort has been put in designing efficient approximation algorithms. Traditionally, such algorithms are randomized and are based on Markov chains, see [12]. In particular, Jerrum and Sinclair [13] showed that for all 0 < b < 1 and $\xi > 0$ the partition function of the Ising model can be efficiently approximated on any graph G. Another approach is based on decay of correlations and was initiated by Weitz [31]. This leads to deterministic approximation algorithms. Using decay of correlations, Sinclair, Srivastava and Thurley [27] gave an efficient deterministic approximation algorithm for computing the Ising partition function on graphs of maximum degree at most d+1 ($d \ge 2$) when $\xi=1$ and $b \in (\frac{d-1}{d+1},1]$.

Recently, a new approach for obtaining deterministic approximation algorithms was proposed by Barvinok, see [4], based on truncating the Taylor series of the logarithm of the partition functions in regions where the partition function is nonzero. It was shown by Patel and the second author in [22] that this approach in fact yields polynomial time approximation algorithms when restricted to bounded degree graphs. Combining the approach from [22] (cf. [17]) with Theorem A and the original Lee-Yang result, we immediately obtain the following as a direct corollary:

COROLLARY 1. Let $d \ge 2$, let $b \in (\frac{d-1}{d+1}, 1]$ and let $\xi \in I(\theta_b)$, for θ_b as in Theorem A. Then for any $\varepsilon > 0$, there exists an algorithm that, given an n-vertex graph G of maximum degree at most d+1, computes a relative ε -approximation[†] to $Z_G(\xi, b)$ in time polynomial in n/ε .

An identical statement holds for b > 1, except there it does not follow directly from Theorem B. One also needs that for ξ in a small disk around zero the partition function does not vanish, see Remark 24.

Given the recent progress on understanding the complexity of approximating independence polynomial at nonpositive fugacities based on connections to complex dynamics due to Bezaková, Galanis, Goldberg and Štefankovič [6], a natural question that arises is the following:

QUESTION 2. Let $d \ge 2$. Is it NP-hard (or maybe even #P-hard) to approximate the partition function of the Ising model on graphs of maximum degree at most d+1 when $b \in (\frac{d-1}{d+1},1)$ and $\xi \in \partial \mathbb{D} \setminus I(\theta)$? In fact even the hardness of approximating the partition function of the Ising model for $\xi \in \partial \mathbb{D}$ and $0 \le b \le \frac{d-1}{d+1}$ is not known. See [11] for some related hardness results.

1.2. Approach

Our approach to proving our main theorems is to make use of the theory of complex dynamics and combine this with some ideas from the approximate counting literature. The value of the partition function of a Cayley tree can be expressed in terms of the value of the partition

[†]A relative ϵ -approximation to a nonzero complex number $x=e^a$ is a nonzero complex number $z=e^b$ such that $|a-b|<\varepsilon$.

function for the Cayley tree with one fewer level, inducing the iteration of a univariate rational function. Understanding the dynamical behavior of this function leads to understanding of the location of the zeros of the partition function for Cayley trees. The same approach forms the basis of [2, 3, 9, 18]. To prove our result for general bounded degree graphs, we use the tree of self-avoiding walks, as defined by Weitz [31], to relate the partition function of a graph to the partition function of a tree with additional boundary conditions. This relationship no longer gives rise to the iteration of a univariate rational function, but with some additional effort we can still transfer the results for the univariate case to this setting.

We remark that a similar approach was used by the authors in [23] to answer a question of Sokal concerning the location of zeros of the independence polynomial, a.k.a., the partition function of the hard-core model.

Complex dynamics has also been used to study the location of zeros the chormatic polynomials of certain trees by Royle and Sokal. See the appendix of the arxiv version of [24].

1.2.1. Organization. This paper is organized as follows. In the next section, we will define ratios of partition functions, and prove that for Cayley trees this gives rise to the iteration of a univariate rational function. In Section 3, we employ basic tools from complex dynamics to analyze this iteration. In particular, a proof of part (ii) of our main theorems will be given there. Finally, in Section 4, we collect some additional ideas and provide a proof of part (i) of our main theorems.

2. Ratios

At a later stage, in Section 4, it will be convenient to have a multivariate version of the Ising partition function defined for a graph G = (V, E), complex numbers $(\xi_v)_{v \in V}$ and $b \in \mathbb{C}$ as follows:

$$Z_G((\xi_v), b) := \sum_{U \subseteq V} \prod_{u \in U} \xi_u \cdot b^{|\delta(U)|}.$$

The two-variable version is obtained from this version by setting all ξ_v equal. We will often abuse notation and just write $Z_G(\xi, b)$ for the multivariate version.

Let G = (V, E) be a graph and let $X \subseteq V$. We call any map $\tau : X \to \{0, 1\}$ a boundary condition on X. Let now τ be a boundary condition on $X \subseteq V$. We say that $U \subseteq V$ is compatible with τ if for each vertex $u \in X$ with $\tau(u) = 1$ we have $u \in U$ and for each vertex $u \in X$ with $\tau(u) = 0$ we have $u \notin U$. We shall write $U \sim \tau$ if U is compatible with τ . We define

$$Z_{G,\tau}(\xi,b) = \sum_{\substack{U \subseteq V \\ U}} \prod_{u \in U} \xi_u \cdot b^{|\delta(U)|}.$$

Fix a vertex v of G. We let $\tau_{v,0}$, and $\tau_{v,1}$, respectively, denote the boundary conditions on $X \cup \{v\}$ where v is set to 0, and 1, respectively. In case v is contained in X, we consider $X \cup \{v\}$ as a multiset to make sure $\tau_{v,0}$ and $\tau_{v,1}$ are well defined. For one element $\sigma \in \{\tau_{v,0}, \tau_{v,1}\}$, the vertex v gets two different values, in which case no set $U \subseteq V$ is compatible with σ and consequently we set $Z_{G,\sigma} = 0$.

We denote the extended complex plane, $\mathbb{C} \cup \{\infty\}$, by $\hat{\mathbb{C}}$. We introduce the ratio $R_{G,\tau,v} \in \hat{\mathbb{C}}$, by

$$R_{G,\tau,v} := \begin{cases} \infty & \text{if } Z_{G,\tau_{v,0}}(\xi,b) = 0, \\ \frac{Z_{G,\tau_{v,1}}(\xi,b)}{Z_{G,\tau_{v,0}}(\xi,b)} & \text{otherwise.} \end{cases}$$
 (2.1)

We remark that $R_{G,\tau,v}$ equals a rational function in ξ , except perhaps for values of ξ for which $Z_{G,\tau_{v,0}}$ and $Z_{G,\tau_{v,1}}$ vanish simultaneously. We will however prove in Lemma 27 that this can never happen for the ξ we care about, and therefore it is safe to think of R as a rational function in ξ .

If no boundary condition is present, or if it is clear from the context, we just write $R_{G,v}$ for the ratio. We have the following trivial, but important, observation:

if
$$Z_{G,\tau_{v,0}} \neq 0$$
, or $Z_{G,\tau_{v,1}} \neq 0$, then:
 $R_{G,\tau,v} \neq -1$ if and only if $Z_{G,\tau} \neq 0$. (2.2)

The following lemma shows how to express the ratio for trees in terms of ratios of smaller trees.

LEMMA 3. Let G=(V,E) be a tree with boundary condition τ on $X\subseteq V$. Let u_1,\ldots,u_d be the neighbors of v in G, and let G_1,\ldots,G_d be the components of G-v containing u_1,\ldots,u_d , respectively. We just write τ for the restriction of τ to $X\cap V(G_i)$ for each i. For $i=1,\ldots,d$, let $\tau_{i,0}$ and $\tau_{i,1}$ denote the respective boundary conditions obtained from τ on $(X\cup\{u_i\})\cap V(G_i)$ where u_i is set to 0 and 1, respectively. If for each i, not both $Z_{G_i,\tau_{i,0}}(\xi,b)$ and $Z_{G,\tau_{i,1}}(\xi,b)$ are zero, then

$$R_{G,\tau,v} = \xi_v \prod_{i=1}^d \frac{R_{G_i,\tau,u_i} + b}{bR_{G_i,\tau,u_i} + 1}.$$
 (2.3)

Proof. We can write

$$Z_{G,\tau_{v,1}} = \xi_v \prod_{i=1}^d \left(Z_{G_i,\tau_{i,1}} + b Z_{G_i,\tau_{i,0}} \right), \text{ and } Z_{G,\tau_{v,0}} = \prod_{i=1}^d \left(b Z_{G_i,\tau_{i,1}} + Z_{G_i,\tau_{i,0}} \right).$$

Let us fix $i \in \{1, ..., d\}$. Suppose first that $Z_{G_i, \tau_{i,0}} \neq 0$. Then we can divide the numerator and denominator by $Z_{G_i, \tau_{i,0}}$ to obtain

$$\frac{Z_{G_i,\tau_{i,1}} + bZ_{G_i,\tau_{i,0}}}{bZ_{G_i,\tau_{i,1}} + Z_{G_i,\tau_{i,0}}} = \frac{R_{G_i,\tau,u_i} + b}{bR_{G_i,\tau,u_i} + 1}.$$
(2.4)

If $Z_{G_i,\tau_{i,0}}=0$, then on the left-hand side of (2.4) we obtain 1/b while on the right-hand side, plugging in $R_{G_i,\tau,u_i}=\infty$, we also obtain 1/b. Therefore, this expression is also valid when $Z_{G_i,\tau_{i,0}}=0$. This finishes the proof.

Let us now specialize the previous lemma to a special class of (rooted) trees. Fix $d \in \mathbb{N}_{\geq 2}$. The tree $T_{0,d}$ consists of single vertex, its root. For $k \geq 1$, the tree $T_{k,d}$ consists of a root vertex v of degree d with each edge incident to v connected to the root of a copy of $T_{k-1,d}$. This class of trees is also known as the class of (rooted) Cayley trees. If d is clear from the context, we just write T_k instead of $T_{k,d}$.

Define $f = f_{\xi,b} : \hat{\mathbb{C}} \to \hat{\mathbb{C}}$ for $R \in \hat{\mathbb{C}}$ by

$$f(R) := \xi \cdot \left(\frac{R+b}{bR+1}\right)^d. \tag{2.5}$$

Let us moreover, define $g: \hat{\mathbb{C}} \to \hat{\mathbb{C}}$ by $g: R \mapsto \frac{R+b}{bR+1}$ for $R \in \hat{\mathbb{C}}$ so that $f(R) = \xi g(R)^d$. Since b is real, it follows that the Möbius transformation g preserves $\partial \mathbb{D}$. If $\xi \in \partial \mathbb{D}$, the same holds for f.

COROLLARY 4. Let $d \in \mathbb{N}_{\geq 2}$ and let $\xi \in \partial \mathbb{D}$ and $b \in \mathbb{R}$. Then the orbit of 1 under $f = f_{\xi,b}$ avoids -1 if and only if $Z_{T_k} \neq 0$ for all k.

Proof. We note that $f(1) = \xi$, hence we may just as well consider the orbit of ξ . We observe that, as there is no boundary condition, $R_{T_0,v} = \xi$. Now suppose that $Z_{T_k} \neq 0$ for all $k \in \mathbb{N}$. Then by (2.2), we see that $R_{T_k,v} \neq -1$ for all k. Then since $Z_{T_k,\tau_{v,0}} + Z_{T_k,\tau_{v,1}} = Z_{T_k} \neq 0$, it follows that either $Z_{T_k,\tau_{v,0}} \neq 0$, or $Z_{T_k,\tau_{v,1}} \neq 0$. By Lemma 3, we obtain

$$R_{T_{k,v}} = f(R_{T_{k-1,v}}) = \dots = f^{\circ k}(\xi)$$
 (2.6)

and hence the orbit of 1 avoids -1.

Conversely, suppose that the orbit of 1 avoids -1, while $Z_{T_k}=0$ for some k. Then let k be the smallest integer for which $Z_{T_k}=0$. Then we have $Z_{T_k,\tau_{v,0}}\neq 0$. Indeed, $Z_{T_k,\tau_{v,0}}=(Z_{T_{k-1},\tau_{v,0}}+bZ_{T_{k-1},\tau_{v,1}})^d$ and by assumption, as $Z_{T_{k-1}}\neq 0$ we have that one of $Z_{T_{k-1},\tau_{v,0}}$ and $Z_{T_{k-1},\tau_{v,1}}$ is nonzero. But since

$$\frac{Z_{T_{k-1},\tau_{v,0}}}{Z_{T_{k-1},\tau_{v,1}}} = R_{T_{k-1},v} = f^{\circ k-1}(\xi) \in \partial \mathbb{D} \setminus \{-1\},$$

and therefore $Z_{T_{k-1},\tau_{v,0}} + bZ_{T_{k-1},\tau_{v,1}} \neq 0$, as desired. Now (2.2) implies $R_{T_k} = -1$: a contradiction. This finishes the proof.

This corollary motivates the study of the complex dynamical behavior of the map f at starting point 1 (or ξ). We will do this in the next section, returning to general graphs in Section 4.

3. Complex dynamics of the map $f_{\xi,b}$

Let $d \in \mathbb{N}_{\geq 2}$ and let $b \in \mathbb{R}$. In this section, we study the dynamical behavior of the map $f_{\xi,b}$ for ξ of norm 1. It is our aim to prove the following results.

THEOREM 5 (Ferromagnetic case). Let $d \in \mathbb{N}_{\geq 2}$ and let $b \in (\frac{d-1}{d+1}, 1)$. There exists $\theta_b \in (0, \pi)$ such that

- (i) for each $\xi = e^{i\vartheta}$ with $\vartheta \in (-\theta_b, \theta_b)$, there exists a closed circular interval $I_b \subset \partial \mathbb{D}$, with 1 as boundary point, which is forward invariant under $f_{\xi,b}$ and does not contain -1. In particular, the orbit of $R = \xi$ under $f_{\xi,b}$ avoids the point -1;
- (ii) the interval $(-\theta_b, \theta_b)$ is maximal: The collection $\{\xi\} \subset \partial \mathbb{D}$ for which the orbit of $R = \xi$ under $f_{\xi,b}$ lands on -1 is dense in $\partial \mathbb{D} \setminus (-\theta_b, \theta_b)$.

Remark 6. We can provide an explicit formula for θ_b as a function of b, see Lemma 13 and its proof below.

While a variant of this result was also independently proved in [9] we will provide a proof for it, as certain parts and ideas of our proof will be used to prove the next theorem.

THEOREM 7 (Anti-ferromagnetic case). Let $d \in \mathbb{N}_{\geqslant 2}$ and let $b \in (1, \frac{d+1}{d-1})$. There exists $\alpha = \alpha_b \in (0, \pi)$ such that

- (i) for each $\xi = e^{i\vartheta}$ with $\vartheta \in (-\alpha, \alpha)$ the shortest closed circular interval with boundary points 1 and ξ , I_b , is forward invariant under $f_{\xi,b}$. In particular, the orbit of $R = \xi$ under $f_{\xi,b}$ avoids the point -1;
- (ii) the interval $(-\alpha, \alpha)$ is maximal: The collection $\{\xi\} \subset \mathbb{C}$, for which the orbit of $R = \xi$ under $f_{\xi,b}$ lands on -1 accumulates on $e^{\pm i\alpha}$.

Observe that by Corollary 4, part (ii) of these theorems implies part (ii) of our main theorems. Part (i) of our main theorems, which will be proved in Section 4, will rely upon parts (i) in Theorems 5 and 7.

We moreover note that while both theorems look quite similar, they are not quite the same. In particular, it is not clear whether in the anti-ferromagnetic case roots lie dense on the circular arc containing -1 between α_b and $-\alpha_b$. This question has been studied in recent follow-up work of Bencs, Buys, Guerini and the first author [5].

The difference in nature is also apparent in the proofs of these results. To prove these results, we start with some observations from (complex) analysis and complex dynamics concerning the map $f_{\mathcal{E},b}$, after which we first prove Theorem 5 and then Theorem 7.

3.1. Observations from analysis and complex dynamics

3.1.1. Elementary properties of $f_{\xi,b}$. We start with some basic complex analytic properties of the map $f_{\xi,b}$. Throughout we assume that b is real valued, $\xi \in \partial \mathbb{D}$ and we write $f = f_{\xi,b}$. We first of all note that if b = 1, the map f just equals multiplication by ξ . Therefore, we will restrict to $b \neq 1$.

The behavior of f on the outer disk $\hat{\mathbb{C}} \setminus \overline{\mathbb{D}}$ is conjugate to that on the inner disk \mathbb{D} :

LEMMA 8. The map f is invariant under conjugation by the the anti-holomorphic map

$$R \mapsto \frac{1}{\overline{R}}.$$

Proof. First of all, we have g(1/R) = 1/g(R). Now since $\overline{\xi} = 1/\xi$, it follows that $f(1/\overline{R}) = 1/\overline{f(R)}$, as desired.

Thus, for most purposes, it is sufficient to consider only the behavior on \mathbb{D} and on $\partial \mathbb{D}$.

LEMMA 9. Let $\xi \in \partial \mathbb{D}$. For $b \in \mathbb{R} \setminus \{1\}$, the map $f_{\xi,b}$ induces a d-fold covering on $\partial \mathbb{D}$. For |b| < 1, this covering is orientation preserving, for |b| > 1 it is orientation reversing.

Proof. Since $f = f_{\xi,b}$ has no critical points on $\partial \mathbb{D}$ it follows that the map is a d-fold covering for any real b. If -1 < b < 1, both \mathbb{D} and $\hat{\mathbb{C}} \setminus \mathbb{D}$ are invariant under f, hence conformality of f near $\partial \mathbb{D}$ implies that f is orientation preserving. If |b| > 1, then f maps \mathbb{D} into $\mathbb{C} \setminus \mathbb{D}$ and vice versa, which implies that f is orientation reversing.

From now on, we will only consider b > 0. The derivative of f satisfies:

$$f'(R) = \xi d \left(\frac{R+b}{bR+1}\right)^{d-1} \cdot \frac{1-b^2}{(bR+1)^2} = f(R) \frac{d(1-b^2)}{(R+b)(bR+1)}.$$
 (3.1)

It follows that |f'(R)| is independent of ξ and, since b > 0, is strictly increasing with |Arg(R)|. Let us define

$$b_c := \frac{d-1}{d+1}.$$

Note that

$$|f'_{1,b}(1)| = d \cdot \frac{1-b}{1+b},$$

from which it follows that $|f'_{\xi,b}(1)| > 1$ when $0 < b < b_c$ or $b > \frac{1}{b_c}$, $|f'_{\xi,b}(1)| = 1$ when $b = b_c$ or $b = \frac{1}{b_c}$ and $|f'_{\xi,b}(1)| < 1$ when $b_c < b < 1$ or $1 < b < 1/b_c$.

Recall that a map is said to be expanding if it locally increases distances, and uniformly expanding if distances are locally increased by a multiplicative factor bounded from below by a constant strictly larger than 1. Our above discussion implies the following.

Lemma 10. Let $\xi \in \partial \mathbb{D}$.

- (i) If $0 < b < b_c$ or $b > 1/b_c$, then the covering $f_{\xi,b}|_{\partial \mathbb{D}}$ is uniformly expanding.
- (ii) If $b = b_c$, or if $b = 1/b_c$, then the covering $f_{\xi,b}|_{\partial \mathbb{D}}$ is expanding, but not uniformly expanding: $|f'_{\xi,b}(1)| = 1$.
 - (iii) If $b_c < b < 1/b_c$, then $|f'_{\varepsilon,b}(1)| < 1$.

LEMMA 11. Let $b \in \mathbb{R}$ and $\xi \in \partial \mathbb{D}$. Let $R_0 \in \partial \mathbb{D}$ be a fixed point of $f = f_{\xi,b}$. Then $f'(R_0) \in \mathbb{R}$.

Proof. Let us denote the tangent space at the circle of a point R by T_R ; this is spanned by some vector in $\mathbb{C} = \mathbb{R}^2$. Then since the derivative is a linear map from T_{R_0} to $T_{f(R_0)} = T_{R_0}$, it follows that $f'(R_0)$ has to be a real number.

3.1.2. Observations from complex dynamics. We refer to the book [20] for all necessary background. Throughout we will assume that b > 0, $b \neq 1$, $\xi \in \partial \mathbb{D}$ and we write $f = f_{\xi,b}$.

By Montel's Theorem, the family of iterates $\{f^{\circ n}\}$ is normal on \mathbb{D} and on $\mathbb{C} \setminus \overline{\mathbb{D}}$. Recall that the set where the family of iterates is locally normal is called the *Fatou set*, and its complement is the *Julia set*. Thus, the Julia set of f is contained in $\partial \mathbb{D}$, and there are two possibilities for the connected components of the Fatou set, that is, the Fatou components:

LEMMA 12. Either the Fatou set of f consists of precisely two Fatou components, \mathbb{D} and $\hat{\mathbb{C}} \setminus \overline{\mathbb{D}}$, or there is only a single Fatou component which contains both \mathbb{D} and $\hat{\mathbb{C}} \setminus \overline{\mathbb{D}}$. In the latter case, the component is necessarily invariant. In the former case, the two components are invariant when b < 1, and are periodic of order 2 when b > 1.

Recall that invariant Fatou components are classified: each invariant Fatou component is either the basin of an attracting or parabolic fixed point, or a rotation domain. An invariant attracting or parabolic basin always contains a critical point, while a rotation domain does not. The critical points of f are -b, -1/b, hence it follows that in both of the above cases the Fatou components must be either parabolic or attracting.

If there is only one Fatou component, by Lemma 8 this component must be an attracting or parabolic basin of a fixed point lying in $\partial \mathbb{D}$. If there are two Fatou components, then they are either both attracting basins, or they are both basins of a single parabolic fixed point in $\partial \mathbb{D}$. We emphasize that there can be no other parabolic or attracting cycles.

The parameters for which there exist parabolic fixed points will play a central role in our analysis.

LEMMA 13. Let $b \in (b_c, 1) \cup (1, \frac{1}{b_c})$. Then there exists a unique $\theta = \theta_b \in (0, \pi)$ such that for $\xi = e^{\pm i\theta} \in \partial \mathbb{D}$ the function $f_{\xi,b}$ has a (unique) parabolic fixed point. Moreover, the following holds.

(i) If b < 1, then the parabolic fixed point R of $f = f_{\xi,b}$ satisfies f'(R) = 1 and is a solution of the equation

$$R^{2} + \frac{d(b^{2} - 1) + (1 + b^{2})}{b}R + 1 = 0.$$
(3.2)

(ii) If b > 1, then the parabolic fixed point R of $f = f_{\xi,b}$ satisfies f'(R) = -1 and is a solution of the equation

$$R^{2} + \frac{d(1-b^{2}) + (1+b^{2})}{b}R + 1 = 0.$$
(3.3)

Proof. Recall that for fixed b the value of |f'(R)| is independent of ξ , depends only on $|\operatorname{Arg}(R)|$, is strictly increasing in $|\operatorname{Arg}(R)|$, and satisfies |f'(1)| < 1 and |f'(-1)| > 1. Thus, there exists a unique pair of complex conjugates $R_0, \overline{R_0}$ for which $|f'(R_0)| = |f'(\overline{R_0})| = 1$. Hence, there exists a unique ξ_0 for which $f_{\xi_0,b}(R_0) = R_0$, and by symmetry $f_{\overline{\xi_0},b}(\overline{R_0}) = \overline{R_0}$. Since the action of f on the unit circle is orientation preserving for b < 1, and orientation reversing for b > 1, it follows by Lemma 11 that $f'_{\xi_0,b}(R_0)$ equals 1 for b < 1, and equals -1 for b > 1.

Let us first consider the case that b < 1. We are then searching for solutions to the two equations

$$f(R) = \xi \left(\frac{R+b}{1+bR}\right)^d = R \tag{3.4}$$

$$f'(R) = \xi d \left(\frac{R+b}{1+bR}\right)^{d-1} \frac{1-b^2}{(1+bR)^2} = 1.$$
(3.5)

Rewriting equation (3.4) gives

$$\xi \left(\frac{R+b}{1+bR}\right)^{d-1} = R \cdot \frac{1+bR}{R+b},$$

which can be plugged into (3.5) to give

$$dR \frac{1 - b^2}{(1 + bR)(R + b)} = 1,$$

which is equivalent to

$$R^{2} + \frac{d(b^{2} - 1) + (1 + b^{2})}{b}R + 1 = 0$$

For $b_c < b < 1$, there are two solutions for R, a pair of complex conjugates lying on the unit circle. For each of these solutions, there exists a unique value of $\xi \in \partial \mathbb{D}$ for which equation (3.4) is satisfied. These values of ξ are clearly complex conjugates of each other and, when the two solutions R and \overline{R} are distinct, must be distinct as $f_{\xi,b}$ has at most one parabolic fixed point.

If b > 1, we need to replace 1 by -1 on the right-hand side of (3.5). Similar to the b < 1 case, this then leads to equation (3.3), which, when $b < 1/b_c$, has two solutions for R, a pair of complex conjugates lying on the unit circle. As before, for each of these solutions there exists a unique value of $\xi \in \partial \mathbb{D}$ for which equation (3.4) is satisfied. Again these values of ξ are complex conjugates of each other.

We note that in the lemma above when $b=b_c$ or when $b=1/b_c$ there is a double solution at R=1, and hence the corresponding ξ equals 1. For this map, there are two separate parabolic basins: the inner and outer unit disk. When $b_c < b < 1$, the parabolic fixed point is a double fixed point, and hence has only one parabolic basin. It follows that in this case there is a unique Fatou component, which contains both the inner and outer unit disk, and all orbits approach the parabolic fixed point along a direction tangent to the unit circle. When $1 < b < 1/b_c$, the inner and outer disk are inverted by f, the fact that f' = -1 implies that orbits in these

components converge to the parabolic fixed point along the direction normal to the unit circle, while nearby points on the unit circle move away from the parabolic fixed point.

We have now established some basic properties of the map f and move on to the respective proofs of Theorems 5 and 7.

3.2. Proof of Theorem 5

3.2.1. Proof of part (i). We will consider the behavior for parameters b < 1 and $\xi \in \partial \mathbb{D}$ for which $f = f_{\xi,b}$ has an attracting fixed point on $\partial \mathbb{D}$.

The Julia set J of f, which is nonempty[†], is contained in the unit circle, and the complement is the unique Fatou component, the (immediate) attracting basin. The intersection of $\mathbb{C} \setminus J$ with the unit circle consists of countably many open intervals. We refer to the interval containing the attracting fixed point as the immediate attracting interval. We note that this interval is forward invariant, and the restriction of f to this interval is injective. We emphasize that we may indeed talk about the immediate attracting interval, as there are no other parabolic or attracting cycles.

THEOREM 14. Let $b \in (b_c, 1)$ and let $\theta = \theta_b$ (from Lemma 13). Then for $\xi \in \partial \mathbb{D}$ the map $f_{\xi,b}$ has an attracting or parabolic fixed point on $\partial \mathbb{D}$ if and only if $\xi \in \{e^{i\vartheta} \mid \vartheta \in [-\theta, \theta]\}$. If $\vartheta \in (-\theta, \theta)$, then the point +1 lies in the immediate attracting interval.

Proof. We will consider the changing behavior of the map $f_{\xi,b}$ as $\xi \in \partial \mathbb{D}$ varies, for b fixed. By the implicit function theorem, the fixed points of $f_{\xi,b}$, that is, the solutions of $f_{\xi,b}(R) - R = 0$, depend holomorphically on ξ , except when $f'_{\xi,b}(R) = 1$. By Lemma 13, this occurs exactly at two parameters $\xi = e^{\pm i\theta}$.

Recall that the absolute value of the derivative, $|f'_{\xi,b}(R)|$, is independent of ξ , strictly increasing in $|\operatorname{Arg}(R)|$, and that $|f'_{\xi,b}(+1)| < 1$ while $|f'_{\xi,b}(-1)| > 1$. For each $R \in \partial \mathbb{D}$, there exists a unique $\xi \in \partial \mathbb{D}$ for which R is fixed, inducing a map $R \mapsto \xi(R)$, holomorphic in a neighborhood of $\partial \mathbb{D}$. Since there can be at most one attracting or parabolic fixed point on $\partial \mathbb{D}$, the map $R \mapsto \xi(R)$ is injective on the circular interval $\{R : |f'_{\xi,b}(R)| \leq 1\}$. It follows that the image of this interval under $R \mapsto \xi(R)$ equals $\{e^{i\vartheta} \mid \vartheta \in [-\theta, \theta]\}$, and that for ξ outside of this interval the function $f_{\xi,b}$ cannot have a parabolic or attracting fixed point on $\partial \mathbb{D}$.

When $f_{\xi,b}$ has an attracting fixed point on $\partial \mathbb{D}$, the boundary points of the immediate attracting interval are necessarily fixed points. The fact that there cannot be other attracting or parabolic cycles on $\partial \mathbb{D}$ implies that the two boundary points are repelling. It follows also that R = +1 cannot be a boundary point of the immediate attracting interval, and since these boundary points vary holomorphically (with ξ), and thus in particular continuously, it follows that R = +1 is always contained in the immediate attracting interval.

To complete the proof of Theorem 5(i), we need to define the circular interval I_b . We let I_b be the shortest closed circular interval with boundary points 1 and R_0 , the attracting fixed point of f. Then clearly $-1 \notin I_b$. Since I_b is contained in the immediate attracting interval and since f is orientation preserving it follows that I_b is forward invariant for f.

This finishes the proof of part (i).

3.2.2. Proof of part (ii). We start with analyzing what happens when $b \leq b_c$.

PROPOSITION 15. For $0 < b \le b_c$, the parameters ξ for which the orbit of $R_0 = \xi$ under the map $f_{\xi,b}$ takes on the value -1 is dense in $\partial \mathbb{D}$.

[†]In fact, it can be shown that the Julia set is a Cantor set.

Proof. We consider the orbits for parameters ξ in a small circular interval $[s,t] \subset \partial \mathbb{D}$, with $s \neq t$. The initial values $R_0 = \xi$ lie in this interval. Since the map

$$h: R \mapsto \left(\frac{R+b}{bR+1}\right)^d$$

is expanding, this interval is mapped to an interval [h(s),h(t)] which is strictly larger. Let us write for $\xi \in [s,t]$, $R_1(\xi) = f_{\xi,b}(R_0(\xi))$ and $R_{n+1}(\xi) = f_{\xi,b}(R_n(\xi))$. By Lemma 9, the covering map h is orientation preserving. Noting that $f_{\xi,b}(R) = \xi \cdot h(R)$, it follows that the length $\ell[R_1(s), R_1(t)]$ satisfies

$$\ell[R_1(s), R_1(t)] = \ell[sh(s), th(t)] = \ell[sh(s), sh(t)] + \ell[s, t]$$

Hence, as $n \to \infty$, we have $\ell[R_n(s), R_n(t)] \to \infty$, counting multiplicity. Thus, there must exist $\xi \in [s, t]$ and $n \in \mathbb{N}$ for which $f_{\xi, b}^n(\xi) = -1$.

REMARK 16. We remark that this proposition combined with Corollary 4 implies that for $d \ge 2$ and for $b \in (0, \frac{d-1}{d+1}]$ the roots of the partition function of the Ising model for all graphs of maximum degree d+1 lie dense in the unit circle. In particular, for $b \in (0,1)$, the roots for all graphs lie dense in the unit circle.

We next look at the case $b \in (b_c, 1)$.

PROPOSITION 17. Let $b_c < b < 1$ and let ξ_0 be such that $f_{\xi_0,b}$ has no attracting or parabolic fixed point on $\partial \mathbb{D}$. Then there are parameters ξ arbitrarily close to ξ_0 and $n \in \mathbb{N}$ for which $f_{\xi,b}^n(\xi) = -1$.

Proof. By the assumption that $f_{\xi_0,b}$ has no attracting or parabolic fixed point on $\partial \mathbb{D}$, it follows that both \mathbb{D} and $\overline{\mathbb{D}}^c$ are attracting basins, and hence the orbits of the two critical points stay bounded away from the Julia set $J=\partial \mathbb{D}$. It follows that J is a hyperbolic set, that is, that there exists a metric on J, equivalent to the Euclidean metric, with respect to which f is a strict expansion. We will refer to this metric as the hyperbolic metric on J.

The proof concludes with an argument similar to the one used in Proposition 15. For a circular interval $I \subset \partial \mathbb{D}$, we denote by length I the diameter with respect to the hyperbolic metric on $\partial \mathbb{D}$. Let $[s,t] \subset \partial \mathbb{D}$ be a proper subinterval containing ξ_0 , small enough so that the maps $f_{\xi,b}$ for $\xi \in [s,t]$ are all strict expansions with respect to the hyperbolic metric obtained for the parameter ξ_0 . It follows that

length
$$[f_{s,b}(s), f_{t,b}(t)] = \text{length}[f_{s,b}(s), f_{s,b}(t)] + \text{length}[f_{s,b}(t), f_{t,b}(t)]$$

> $\kappa \cdot \text{length}[s, t],$

where the equality follows from the fact that the maps $f_{\xi,b}$ are all orientation preserving, and the constant $\kappa > 1$ is a uniform lower bound on the expansion of the maps $f_{\xi,b}$ for $\xi \in [s,t]$.

By induction, it follows that length $[f_{s,b}^n(s), f_{t,b}^n(t)] > \kappa^n \cdot \text{length}[s,t]$, counting multiplicity. Thus, for sufficiently large n, the interval $[f_{s,b}^n(s), f_{t,b}^n(t)]$ will contain the unit circle, proving the existence of a parameter $\xi \in [s,t]$ for which $f_{\xi,b}^{n+1}(+1) = -1$.

Together with Lemma 13 and Theorem 14, this result completes the proof of Theorem 5(ii).

3.3. Proof of Theorem 7

3.3.1. Proof of part (i). We start by proving some observations indicating behavior different from the ferromagnetic case.

LEMMA 18. Let $b \in (1, 1/b_c)$, and let ξ be such that $f_{\xi,b}$ has a parabolic fixed point R_0 on $\partial \mathbb{D}$. Then ξ does not lie in the shortest closed circular interval bounded by 1 and R_0 .

Proof. Recall that R_0 is not equal to +1 or -1, and that $|f'_{1,b}|$ is minimal at +1 and increases monotonically with $|\operatorname{Arg}(R)|$, and is therefore strictly smaller than 1 on the open circular interval bounded by 1 and R_0 . By integrating $f'_{1,b}$ over this open interval, it follows from $f_{1,b}(1) = 1$ that $|\operatorname{Arg}(f_{1,b}(R_0))| < |\operatorname{Arg}(R_0)|$. Since $f_{1,b}$ is orientation reversing, it follows that $\operatorname{Arg}(f_{1,b}(R_0))$ and $\operatorname{Arg}(R_0)$ have opposite sign. The statement now follows from

$$\xi = \frac{R_0}{f_{1,b}(R_0)}.$$

LEMMA 19. Let $b \in (1, 1/b_c)$, and let ξ be such that $f = f_{\xi,b}$ has a parabolic fixed point R_0 on $\partial \mathbb{D}$. The shortest closed circular interval I bounded by 1 and ξ cannot be forward invariant.

Proof. First observe that the parabolic fixed point is not equal to 1. By the previous lemma, it also cannot be equal to ξ .

Suppose now that $f(I) \subset I$ for the purpose of contradiction. Then the open interval I° is also forward invariant, and since neither 1 nor ξ is equal to the parabolic fixed point, it follows that I° cannot be contained in the parabolic basin. Hence, I° must intersect the Julia set, say in a point p. Let U be a sufficiently small open disk centered at p so that $U \cap \partial \mathbb{D} \subset I^{\circ}$. Since p lies in the Julia set, it follows that

$$\bigcup_{n\in\mathbb{N}}f^n(U)=\widehat{\mathbb{C}}.$$

Since f is forward invariant on $\mathbb{D} \cup \widehat{\mathbb{C}} \setminus \overline{\mathbb{D}}$, this contradicts the assumption that f is forward invariant on I.

Note that we used here that the exceptional set of the rational function f is empty, which follows immediately from the fact that there are no attracting periodic cycles. We recall that we refer to [20] for background on complex dynamical systems.

It follows from the above lemma that the situation is different from the orientation preserving case: when $f = f_{\xi,b}$ has an attracting fixed point on $\partial \mathbb{D}$, the point +1 does not necessary lie in the immediate attracting interval. If it did, then f would be forward invariant on the shortest interval with boundary points 1 and ξ , which cannot happen for ξ close to the parabolic parameter as follows from the lemma above.

Recall that the boundary points of the immediate attracting interval form a repelling periodic cycle. Since for ξ near +1, the point R=+1 does lie in the immediate attracting interval, while for ξ near the parabolic parameters the point +1 does not, it follows by continuity of the repelling periodic orbit that there must be a parameter for which +1 is one of the boundary points. In fact, it follows quickly from the fact that |f'| strictly increases with $|\operatorname{Arg}(R)|$ that there exists a unique $\alpha=\alpha_b\in(0,\pi)$ (with $\alpha_b<\theta_b$) such that for $\xi=e^{\pm i\alpha}$, +1 is a boundary point of the immediate attracting interval. To see that α is unique, suppose that there is another such $\alpha'\in(0,\pi)$. We may assume that $\alpha'>\alpha$. Set $\xi=e^{i\alpha}$ and $\xi'=e^{i\alpha'}$. Then since $f_{\xi',b}(\xi')=\frac{\xi'}{\xi}f_{\xi}(\xi')$ and since $|f'_{\xi,b}(\xi)|>1$ (as $|(f^{\circ 2})'(1)|>1$), it follows that the distance between $f_{\xi',b}(\xi')$ and $f_{\xi,b}(\xi)$ is strictly larger than the distance between ξ and ξ' , and hence would need to be a positive multiple of 2π larger. But then $f_{\xi',b}$ would map the attracting interval to the entire unit circle, which gives a contradiction.

We note that α_b is the solution in $(0, \pi)$ to

$$e^{i\alpha_b} \cdot \left(\frac{e^{i\alpha_b} + b}{e^{i\alpha_b}b + 1}\right)^d = 1 \tag{3.6}$$

with minimal argument. See Figure 1 for the values of α_b and the parabolic parameter θ_b for varying values of b > 1. For a comparable curve depicting the values of θ_b for b < 1, see [9, Figure 2].

We summarize the above discussion in the following theorem.

THEOREM 20. Let $b \in (1, 1/b_c)$ and let $\alpha = \alpha_b$. If $\vartheta \in (-\alpha, \alpha)$ and $\xi = e^{i\vartheta}$, then the point +1 lies in the immediate attracting interval.

To finish the proof of Theorem 7(i), we need to show that I_b (which was defined as the shortest closed circular interval with boundary points 1 and ξ) is forward invariant for f. This follows since $f:I_b\to\partial\mathbb{D}$ is an orientation reversing injective contraction (with respect to the hyperbolic metric on the attracting basin).

3.3.2. Proof of part (ii). We first note that contrary to the case that b < 1, one cannot expect parameters ξ with $-1 \in \{f_{\xi,b}^n(+1)\}$ arbitrarily close to any point

$$\xi_0 \in \partial \mathbb{D} \setminus \{e^{i\vartheta} : \vartheta \in (-\theta_b, +\theta_b)\},$$

as there will be ξ_0 for which the point +1 lies in the attracting basin, just not in the immediate attracting basin. In this case, the orbit of ξ_0 will still converge to the attracting fixed point, and, except for at most countably many parameters ξ_0 , will avoid -1. This is then still the case for ξ sufficiently close to ξ_0 .

Our goal is to show that there exist parameters $\xi \in \mathbb{C}$ arbitrarily close to $\xi_0 := e^{i\alpha_b}$ for which the orbit of +1 contains -1 (where α_b is defined in (3.6)); the complex conjugate $e^{-i\alpha_b}$ is completely analogues. Recall that $f(\xi_0) = 1$, and that this periodic orbit is repelling. It follows that the point R = +1 cannot be passive, that is, the family of holomorphic maps

$$g_n(\xi) = f_{\varepsilon,b}^n(+1)$$

cannot form a normal family in a neighborhood of ξ_0 . To see this, note that for an open set of parameters ξ (for example, those for which +1 does lie in the immediate attracting interval) accumulating on ξ_0 , the maps $g_n(\xi)$ converge to $R_0(\xi)$, but the points $g_n(\xi_0)$ remain bounded away from $R_0(\xi_0)$. Thus, the sequence of maps g_n cannot have a convergent subsequence in any neighborhood of ξ_0 .

Recall that the strong version of Montel's Theorem says that a family of holomorphic maps into the Riemann sphere avoiding three distinct points is normal. We claim that this implies that the point -1 cannot be avoided for all parameters in a neighborhood of ξ_0 . Of course, if -1is avoided, then so are all its inverse images. Since the map $f_{\xi_0,b}$ induces a d-fold covering on the unit circle, it is clear that there exist points z_{-1}, z_{-2} , distinct from each other as well as from -1, such that $f_{\xi_0,b}(z_{-2})=z_{-1}$ and $f_{\xi_0,b}(z_{-1})=-1$. Since $f_{\xi,b}$ varies holomorphically with ξ , it follows that for all parameters ξ sufficiently close to ξ_0 we can similarly find points $z_{-2}(\xi)$ and $z_{-1}(\xi)$, varying holomorphically with ξ , for which $f_{\xi,b}(z_{-2}(\xi)) = z_{-1}(\xi)$ and $f_{\xi,b}(z_{-1}(\xi)) = -1$. There is a uniquely defined Möbius transformation φ_{ξ} (depending holomorphically) on ξ

that maps -1, $z_{-1}(\xi)$ and $z_{-2}(\xi)$ to -1, z_{-1} and z_{-2} , respectively. Define the holomorphic maps

$$h_n(\xi) = \varphi_{\xi} \circ g_n(\xi).$$

Since the family $\{g_n\}$ cannot be normal near ξ_0 , neither can the family $\{h_n\}$. Hence, the latter cannot avoid the three distinct points $\{-1, z_{-1}, z_{-2}\}$, which implies that there are ξ arbitrarily close to ξ_0 for which there exist $n \in \mathbb{N}$ such that $g_n(\xi)$ lies in $\{-1, z_{-1}(\xi), z_{-2}(\xi)\}$. This completes the proof.

4. Zero-free regions

It is our aim in this section to prove part (i) of Theorems A and B. To this end, let us fix $d \in \mathbb{N}_{\geqslant 2}$ and $b \in (\frac{d-1}{d+1}, 1) \cup (1, \frac{d+1}{d-1})$ and $\vartheta \in (-\theta_b, \theta_b)$ when b < 1 and $\vartheta \in (\alpha_b, \alpha_b)$ when b > 1. Let us fix $\xi = e^{i\vartheta}$, and write $f = f_{\xi,b}$.

Our strategy is as follows. First we give a forward invariant domain for the function f in Subsection 4.1 and then show that this domain is invariant for a multivariate version of the function f. We then use this to prove part (i) for trees with boundary conditions in Subsection 4.2. Finally, we prove the result for all graphs in Subsection 4.3.

4.1. Invariant domain

We let I_b be the forward invariant interval for f from Theorem 5(i) when b < 1 and from Theorem 7(i) when b > 1.

We introduce the $\mathbb{R}_{\geq 0}$ -cone generated by I_b :

$$C = C_b := \{ z = re^{i\phi} \mid 0 \leqslant r \leqslant \infty, \phi \in I_b \}. \tag{4.1}$$

Recall the Möbius transformation

$$g: R \mapsto \frac{R+b}{bR+1}$$
.

LEMMA 21. The cone C is forward invariant under f, that is, for any $z \in C$, $f(z) \in C$.

Proof. We first consider the case b < 1, where f is orientation preserving on the circle. It suffices to show that the half lines H and $\mathbb{R}_{\geqslant 0}$ bounding C are mapped into C by f. Since $\mathbb{R}_{\geqslant 0}$ is mapped to the half line through ξ and $\xi \in I_b$, it remains to show this for H.

We claim that $g(e^{i\phi_0})$ equals the principal value of $(e^{i\phi_0}\xi^{-1})^{1/d}$. To see this, let us denote the preimages of $e^{i\phi_0}$ under f as $R_0 = e^{i\phi_0}, \ldots, R_{d-1}$. They are exactly equal to the d values $g^{-1}((e^{i\phi_0}\xi^{-1})^{1/d})$. Since f is forward invariant on I_b and orientation preserving on $\partial \mathbb{D}$, none of the R_1, \ldots, R_{d-1} lie in the interval I_b . Since g preserves orientation and since g(1) = 1, it follows that $g(e^{i\phi_0})$ is indeed equal to the principal value of $(e^{i\phi_0}\xi^{-1})^{1/d}$. We will write $z = e^{i\phi} := g(e^{i\phi_0})$ from now on.

Now we consider the circle γ through the three points b, 1/b and z. This circle is exactly the image of the line $L := H \cup (-H)$ under the transformation g, as $0 \mapsto b$, $\infty \mapsto 1/b$ and $e^{i\phi_0} \mapsto z$ under g.

We next claim that the half line $z \cdot \mathbb{R}_{\geqslant 0}$ only intersects γ in the point z. Indeed, this follows from the fact that the line H intersects $\partial \mathbb{D}$ normally, and g is conformal. Hence, the circle γ intersects the unit circle $\partial \mathbb{D}$ normally in z, which implies that the line $z \cdot \mathbb{R}$ is the tangent line to γ at z. In other words, the argument of g(z) for $z \in C$ is extremal when $z = R_0$.

This then implies that for any point y on the image of H under g we have that the argument of ξy^d is between 0 and ϕ_0 . In other words, the image of H under f is contained in C, as desired.

Now suppose b>1. Again it suffices to show that the two half lines $H:=\{r\xi\mid r\geqslant 0\}$ and $\mathbb{R}_{\geqslant 0}$ are mapped into C by f, and again we only need to check this for the half line H. Its image under g is contained in the circle through $b,\frac{1}{b}$ and $g(\xi)$, which again intersects $\partial \mathbb{D}$ normally in $g(\xi)$. In this case, the argument of g(z) is therefore extremal when $z=\xi$. It follows that the half line $g(\xi)\cdot \mathbb{R}_{\geqslant 0}$ intersects g(H) only in $g(\xi)$, and the proof is essentially the same as for the b<1 case.

Proof. Let us first consider the case b < 1. We claim that it suffices to prove the statement for $R_1 = R$. Indeed, suppose that there exists $R_1, R \in I_b$ such that $g(R_1)R = -1$. Let

$$m = \min\{|R_1 - R| \mid g(R_1)R = -1, R_1, R \in I_b\}.$$

If $m \neq 0$, then take $R_1, R \in I_b$ such that $g(R_1)R = -1$ and such that $|R_1 - R| = m$. We may assume $\arg(R_1) > \arg(R)$. Then there is $R' \in I_b$ with $\arg(R') > \arg(R)$ and, using that g is orientation preserving, $\arg(R'_1) < \arg(R_1)$ with $g(R'_1)R' = -1$. A contradiction.

The condition that g(R)R = -1 translates to

$$R^2 + 2bR + 1 = 0.$$

It can easily be checked that the coefficient of R, 2b, is strictly larger than the coefficient of R found in equation (3.2), as

$$2b^2 > d(b^2 - 1) + (1 + b^2).$$

Thus, the solutions of g(R)R = -1 lie closer to -1 than R_0 , and there is no such solution in I_b .

When b>1, the maps f and g are orientation reversing. Since f maps I_b into itself, it follows that $g^d=\xi^{-1}\cdot f$ maps I_b into the circular interval between 1 and ξ^{-1} . Since g(1)=1 it follows that g maps the interval I_b into the circular interval bounded by 1 and the principal value of $\xi^{-\frac{1}{d}}$. Hence, $|\operatorname{Arg}(R_1g(R))|$ is maximal when $R_1=\xi$ and R=1, in which case $R_1g(R)=\xi\neq -1$, which completes the proof.

Let us consider for $\mu, b \in \mathbb{C}$ the map $F_{\mu,b} : \hat{\mathbb{C}}^d \to \hat{\mathbb{C}}$ defined by

$$F_{\mu,b}(R_1,\ldots,R_d)\mapsto \mu\cdot\prod_{i=1}^d \frac{R_i+b}{bR_i+1}.$$

PROPOSITION 23. For any $R_1, \ldots, R_{d+1} \in C = C_b$ and any $r \ge 0$:

- (i) $F_{r \cdot \xi, b}(R_1, \dots, R_d) \in C_b;$
- (ii) $|\operatorname{Arg}(g(R_{d+1})F_{r\cdot\xi,b}(R_1,\ldots,R_d))| < \pi.$

Proof. Since C is a cone, it suffices to prove this for r=1. Let us write $F=F_{\xi,b}$. First we prove (i). We note that $\log(C)$ is a rectangle and in particularly it is convex. (We take the branch of the logarithm that is real on the positive real line.) Let us fix $R_1, \ldots, R_d \in C$. Then, since $f(R_i) \in C$ by Lemma 21, we know that $\log(f(R_i)) \in \log(C)$. Then,

$$\log(F(R_1, \dots, R_d)) = \sum_{i=1}^d \frac{\log(\xi)}{d} + \log\left(\frac{R_i + b}{bR_i + 1}\right) = \sum_{i=1}^d \frac{1}{d}\log(f(R_i)),$$

and this is contained in $\log(C)$ by convexity. This implies that $F(R_1, \ldots, R_d)$ is contained in C, as desired.

To prove (ii), by (i) it suffices to show that for any $R_1, R \in C$ we have $|\operatorname{Arg}(g(R_1)R)| < \pi$. Suppose to the contrary that for some $R_1 \in C$ and $R \in C$, we have $g(R_1)R \in \mathbb{R}_{<0}$. The positive half line through R_1 intersects the unit circle normally at some point R'_1 . It follows that $|\operatorname{Arg}(g(R'_1))|$ is not smaller than $|\operatorname{Arg}(g(R_1))|$, cf. Figure 2. Since C is a cone, it then follows that we can find $R''_1, R' \in C$ of norm one such that $g(R''_1)R' = -1$. The previous lemma however gives that $g(R''_1)R' \neq -1$, a contradiction.

REMARK 24. For the purpose of finding an efficient algorithm for approximating $Z_G(\mu, b)$, for any graph G of maximum degree at most d+1, it is important that Z_G does not vanish for μ sufficiently close to zero. By the result of Lee–Yang, this is immediate for 0 < b < 1.

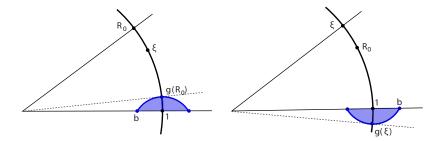


FIGURE 2 (colour online). The image g(C) for b < 1 on the left and for b > 1 on the right.

For b > 1, the statement follows quickly from the formula for $F_{\xi,b}(R_1,\ldots,R_d)$. Indeed, write $D_r = \{z : |z| < r\}$ for some $0 < r < \frac{1}{b}$ and consider $R_1, \ldots, R_d \in D_r \cup \{\infty\}$. Then one observes that the possible values of

$$\prod_{i=1}^{d} \frac{R_i + b}{bR_i + 1}$$

are bounded. Therefore, for $|\mu|$ sufficiently small, one obtains that

$$F_{\mu,b}(R_1,\ldots,R_d)\in D_r.$$

In the analysis that follows, the forward invariant set $D_r \cup \{\infty\}$, which does not contain the point -1, can therefore play the same role as the cone C_b studied in Proposition 23.

We note that the zero-free neighborhood of the origin can also be derived by using a result of Ruelle [25]. In fact, this argument gives a neighborhood that is independent of the maximum degree of the graph.

Trees with boundary conditions

Given a graph G = (V, E). Let $X \subseteq V$ and let $\tau : X \to \{0, 1\}$ be a boundary condition on X. We call vertices $u \in X$ fixed and vertices $v \in V \setminus X$ free.

PROPOSITION 25. Let G = (V, E) be any tree in \mathcal{G}_{d+1} . Let $X \subseteq V$ and let $\tau : X \to \{0, 1\}$ be a boundary condition on X. Set $\xi_v = \xi$ for $v \notin X$ and choose $\xi_v \neq 0$ arbitrarily for $v \in X$. Then for any $v \in V$ the ratio $R_{G,\tau,v}$ does not lie in $\mathbb{R}_{<0}$.

Proof. Let $G = (V, E) \in \mathcal{G}_{d+1}$ and let $v \in V$. We start by proving the following statements assuming that the degree of v is at most d:

- (i) $Z_{G,\tau_{v,0}} \neq 0$, or $Z_{G,\tau_{v,1}} \neq 0$, and (ii) the ratio $R_{G,\tau,v}$ is contained in the cone $C=C_b$.

As $-1 \notin C$, this is clearly sufficient for this case.

The proof is by induction on the number of vertices of G. If this number is equal to 1, then either X = V, or $X = \emptyset$. In the first case, either we have $Z_{G,\tau_{v,0}} \neq 0$, or $Z_{G,\tau_{v,1}} \neq 0$, as desired. Similarly, we have $R_{G,\tau,v}$ is either equal to 0, or to ∞ . In the latter case, we have $Z_{G,\tau_{v,0}}=1$, and $Z_{G,\tau_{v,1}} = \xi$ and hence $R_{G,\tau,v} = \xi \in C$. This verifies the base case.

Let us assume that number of vertices is at least 2. Let v_1, \ldots, v_m be the neighbors of v and let G_1, \ldots, G_m be the components of G-v containing v_1, \ldots, v_m , respectively. We just write τ for the restriction of τ to $X \cap V(G_i)$. For j = 0, 1, we write $\tau_{i,j}$ for the boundary condition

on $(X \cup \{v_i\}) \cap V(G_i)$ obtained from τ where v_i is set to j. Suppose first that $v \notin X$ or that $v \in X$ and $\tau(v) = 0$. Then

$$Z_{G,\tau_{v,0}} = \prod_{i=1}^{m} (bZ_{G_i,\tau_{i,1}} + Z_{G_i,\tau_{i,0}}). \tag{4.2}$$

Now by induction, since the number of vertices in each G_i is less than that in G, we know that for each $i, Z_{G_i,\tau_{i,1}} \neq 0$, or $Z_{G_i,\tau_{i,0}} \neq 0$. Moreover, since for each $i, R_i := R_{G_i,\tau,v_i} \in C$, we have, since b > 0, $bR_i \in C$ and hence $bZ_{G_i,\tau_{i,1}} + Z_{G_i,\tau_{i,0}} \neq 0$, as $-1 \notin C$. This implies $Z_{G,\tau_{v,0}} \neq 0$. One shows with a similar argument (using that $1/b \cdot C = C$) that if $v \in X$ and $\tau(v) = 1$, then $Z_{G,\tau_{v,1}} \neq 0$.

To see (ii), if $v \in X$, we have $R_{G,\tau,v} \in \{0,\infty\}$, otherwise, by Lemma 3 we have

$$R_{G,\tau,v} = \xi_v \prod_{i=1}^d \frac{R_i + b}{bR_i + 1} = F_{\xi,b}(R_1, \dots, R_d),$$

where in case m < d, we set R_{m+1}, \ldots, R_d all equal to 1. By part (i) of Proposition 23, we conclude that $R_{G,\tau,v}$ is contained in C. This concludes the proof of (i) and (ii).

To finish the proof, we must finally consider the case where the degree of v is equal to d+1. We only need to argue that $R_{G,\tau,v} \notin \mathbb{R}_{<0}$, since the argument that $Z_{G,\tau_{v,0}} \neq 0$, or $Z_{G,\tau_{v,1}} \neq 0$ is the same as above. We again let v_1, \ldots, v_{d+1} be the neighbors of v and let G_1, \ldots, G_{d+1} be the components of G-v containing v_1, \ldots, v_{d+1} , respectively. Let us write $R_i := R_{G_i,\tau,v_i}$ for each i. Then, by the first part of the proof, we know that for each u_i we have $R_i \in C$, from which we conclude by Lemma 3 and Proposition 23(ii).

$$R_{G,\tau,v} = g(R_{d+1})F_{\xi,b}(R_1,\ldots,R_d) \notin \mathbb{R}_{<0},$$

This concludes the proof.

4.3. General bounded degree graphs

Here we conclude the proof of part (i) of Theorems A and B by utilizing Proposition 25. To do so, we need the *self-avoiding walk tree* as introduced by Weitz [31].

Let G be a connected graph of maximum degree at most d+1 and fix a vertex v of G, which we call the base vertex. The self-avoiding walk tree of G at v is a tree $T = T_{\text{SAW}}(G, v)$ whose vertices consists of walks in G starting at v that are of the form $w = (v, v_1, \ldots, v_n)$ such that the walk (v, \ldots, v_{n-1}) is self-avoiding (that is, a path in the graph theoretic sense). The walks w that are not self-avoiding, that is, whose last vertex closes a cycle in G, will be leaves of the tree. Note that walks ending in a leaf of G are automatically leaves of the tree as well. Two vertices (walks in G) w_1 and w_2 of T are connected by an edge if one is the one-point extension of the other (as walks in G). Note that the maximum degree of T is at most d+1. See Figure 3 for an example.

We next fix a boundary condition τ_G on some of the leaves of T. To do so, we fix for each vertex u of G an arbitrary ordering of the edges incident with it. We only fix leaves corresponding to walks closing a cycle in G. Such a walk will be set to 0 if the edge closing the cycle is larger than the edge starting the cycle and set to 1 otherwise. If σ is a boundary condition on a subset of the leaves of the graph G, we extend τ_G by assigning the same value to any vertex of T, corresponding to a path ending at such a leaf. Let $(\xi_u)_{u \in V}$ be complex numbers associated with the vertices of G. We associate these variables to the vertices of T as follows. For a vertex w of T, let u be the last vertex in the corresponding walk in G. Then we set $\xi_w := \xi_u$.

PROPOSITION 26. Let G = (V, E) be a connected graph of maximum degree at most d + 1, and with vertex $v \in V$. Let $X \subset V \setminus \{v\}$ be a collection of leaves of G, and let $\sigma : X \to \{0, 1\}$

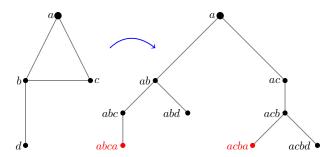


FIGURE 3 (colour online). A graph and its associated tree of self-avoiding walks. The cycles inducing boundary conditions are marked in red.

be a boundary condition on X. Set $\xi_u = \xi$ for all $u \notin X$, and choose $\xi_u \neq 0$ arbitrarily for $u \in X$. Then

$$R_{T,\tau_G,v} = R_{G,\sigma,v},\tag{4.3}$$

where both sides are considered as rational functions in ξ .

We remark that when all ξ_u are positive this lemma is essentially due to Weitz [31] (even though in [31] only the independence polynomial was considered).

Proof. We use induction on the number of free vertices of G. If the number of free vertices is 1, then the free vertex is v, and all other vertices are leaves. Thus, G is a tree and equals its tree of self-avoiding walks, and the statement is immediate.

We may therefore assume that V has at least two free vertices, and that equality (4.3) holds for graphs with fewer free vertices. Let us denote the neighbors of v by u_1, \ldots, u_m . We construct a graph \hat{G} by replacing the vertex v with v_1, \ldots, v_m , each v_j having exactly one neighbor: the vertex u_j . To each of the vertices v_j , we assign the external field parameter $\xi^{\frac{1}{m}}$, using the same holomorphic branch of the mth root for all the vertices v_j . We introduce boundary conditions σ_i , for $i=0,\ldots m$, each extensions of σ , by setting $\sigma_i(v_j)=1$ when $j\leqslant i$ and $\sigma_i(v_j)=0$ when j>i. Thus, σ_0 assigns 0 to all the vertices v_j , and σ_m assigns 1 to all the vertices v_j . It follows from our choice of the external field parameter $\xi^{\frac{1}{m}}$ that

$$Z_{\hat{G},\sigma_0} = Z_{G,\sigma_{v,0}},$$

and

$$Z_{\hat{G},\sigma_m} = Z_{G,\sigma_{v,1}},$$

and therefore

$$R_{G,\sigma,v} = \frac{Z_{\hat{G},\sigma_m}}{Z_{\hat{G},\sigma_0}} = \prod_{i=1}^{m} \frac{Z_{\hat{G},\sigma_i}}{Z_{\hat{G},\sigma_{i-1}}}.$$

Writing $\hat{\sigma}_i$ for the restriction of σ_i obtained by freeing the vertex v_i , it follows that

$$\frac{Z_{\hat{G},\sigma_i}}{Z_{\hat{G},\sigma_{i-1}}} = R_{\hat{G},\hat{\sigma}_i,v_i}.$$

Write \hat{G}_i for the connected component of \hat{G} that contains the vertex v_i , and observe that \hat{G}_i with boundary condition $\hat{\sigma}_i$ has at most as many free vertices as G. Let us stress that G is

not necessarily a tree, hence \hat{G}_i can equal \hat{G}_j for $i \neq j$. It therefore follows from our induction hypothesis that

$$R_{\hat{G}_i-v_i,\hat{\sigma}_i,u_i} = R_{T_{\mathrm{SAW}}(\hat{G}_i-v_i,u_i),\hat{\tau}_i,u_i},$$

where $\hat{\tau}_i$ is the boundary condition on $T_{\text{SAW}}(\hat{G}_i - v_i, u_i)$ induced by $\hat{\sigma}_i$. Observing that the vertex v_i has only one neighbor in \hat{G}_i , namely u_i , it follows from the same argument as used in the proof of Lemma 3 that

$$R_{\hat{G}_{i},\hat{\sigma}_{i},v_{i}} = \xi^{1/d} g(R_{\hat{G}_{i}-v_{i},\hat{\sigma}_{i},u_{i}}) = \xi^{1/d} g(R_{T_{\mathrm{SAW}}(\hat{G}_{i}-v_{i},u_{i}),\hat{\tau}_{i},u_{i}}),$$

where g denotes the Möbius transformation $R \mapsto \frac{R+b}{bR+1}$. By applying Lemma 3 to $T_{\text{SAW}}(G, v)$, we obtain

$$R_{G,\sigma,v} = \prod_{i=1}^{m} R_{\hat{G}_{i},\hat{\sigma}_{i},v_{i}} = \xi \cdot \prod_{i=1}^{m} g(R_{T_{\text{SAW}}(\hat{G}_{i}-v_{i},u_{i}),\hat{\tau}_{i},u_{i}}) = R_{T_{\text{SAW}}(G,v),\tau,v},$$

where the boundary condition τ on $T_{\text{SAW}}(G, v)$ is obtained from the boundary conditions $\hat{\tau}_i$, and therefore satisfies the following.

- Walks ending in a leaf $u \in X$ are assigned the boundary condition $\sigma(u)$.
- Walks ending in a leaf $u \notin X$ are not assigned a boundary condition.
- The boundary condition of a cycle (v, u_i, \ldots, u_j, v) depends on the relative ordering of the neighbors u_i, u_j in the arbitrarily chosen numbering u_1, \ldots, u_m . We stress that this numbering is identical for all the cycles.
- The boundary condition of a walk that is not a cycle but ends with a cycle is determined in the induction process, again depending on the chosen numbering of the edges incident to the vertex at the start and end of the cycle.

Thus, the boundary condition τ satisfies the rules described for τ_G , and the proof is complete.

We will now prove that it was correct to consider the ratios R as rational functions in ξ . We remark that in the previous proposition the choice of ξ was irrelevant, while in what follows it plays an essential role in the proof.

LEMMA 27. Under the hypotheses of the previous proposition, we have that $Z_{G,\sigma_{v,0}} \neq 0$, and $Z_{G,\sigma_{v,1}} \neq 0$.

Proof. Again we prove the statement by induction on the number of free vertices. When the number of free vertices is 1, the free vertex is v. It follows that

$$Z_{G,\sigma_{v,0}} = \prod_{\sigma(u)=1} b\xi_u \neq 0,$$

and similarly $Z_{G,\sigma_{v,1}} \neq 0$.

So let us now assume that $|V \setminus X| > 1$. We again denote by \hat{G} the graph obtained by replacing the vertex v by vertices v_1, \ldots, v_m , each v_i neighboring only the vertex u_i , using again $\xi^{1/m}$ for all the vertices v_i . We denote by $\sigma_0, \ldots, \sigma_m$ the extensions of σ introduced in the proof of the previous proposition, and we write $\hat{\sigma} = \sigma_i$ for some $i \in \{0, \ldots, m\}$. We will prove that $Z_{\hat{G}, \hat{\sigma}} \neq 0$ for all $i = 0, \ldots, m$, which implies the statement of the lemma since $Z_{G, \sigma_{v,0}} = Z_{\hat{G}, \sigma_0}$ and $Z_{G, \sigma_{v,1}} = Z_{\hat{G}, \sigma_m}$.

Denote by H a connected component of \hat{G} . It suffices to show that $Z_{H,\hat{\sigma}} \neq 0$, as the partition function is multiplicative over components. As G was assumed to be connected, H contains a vertex $v_i \in \{v_1, \ldots, v_m\}$. Let $H' := H - v_i$. Then H' contains fewer free vertices than G. Let

us first assume that u_i is not a fixed leaf in G, that is, either a leaf that is not fixed or not a leaf. Then by the induction hypothesis it follows that $Z_{H',\hat{\sigma}_{u_i,0}} \neq 0$ and $Z_{H',\hat{\sigma}_{u_i,1}} \neq 0$, hence by Proposition 26 it follows that

$$R_{H',\hat{\sigma},u_i} = R_{T_{SAW}(H',u_i),\tau_{H'},u_i},$$

where by Proposition 25 the latter ratio does not lie in $\mathbb{R}_{<0}$. Since we have that $Z_{H,\hat{\sigma}}$ equals either $Z_{H',\hat{\sigma}_{u_i,0}} + bZ_{H',\hat{\sigma}_{u_i,1}}$, or $\xi_{v_i}(bZ_{H',\hat{\sigma}_{u_i,0}} + Z_{H',\hat{\sigma}_{u_i,1}})$, it follows that $Z_{H,\hat{\sigma}} \neq 0$. If instead u_i is a fixed leaf in G, then $H' = H - v_i$ just consists of the vertex u_i and therefore

If instead u_i is a fixed leaf in G, then $H' = H - v_i$ just consists of the vertex u_i and therefore $Z_{H',\hat{\sigma}_{u_i,0}} \neq 0$ and $Z_{H',\hat{\sigma}_{u_i,1}} = 0$, or vice versa, from which it again follows that $Z_{H,\hat{\sigma}} \neq 0$. This completes the proof.

Proof of part (i) of Theorems A and B. We may assume that G is connected since the partition function is multiplicative over components. Fix any vertex $v \in V$, and denote by τ the empty boundary condition on G. By the previous lemma, both $Z_{G,\tau_{v,0}}$ and $Z_{G,\tau_{v,1}}$ are nonzero. Moreover, the ratio $R_{G,v}$ is not equal to -1 by Propositions 25 and 26. Therefore, by (2.2), we conclude that $Z_G \neq 0$.

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