Location of zeros of the partition function of the Ising model

Guus Regts

University of Amsterdam

Deterministic Counting, Probability, and Zeros of Partition Functions, Simons Institute Berkeley

20 March, 2019

Based on joint work with Han Peters, UvA
For a graph $G = (V, E)$, and $\lambda, \beta \in \mathbb{C}$, the partition function of the Ising model is defined as

$$Z_G(\lambda, \beta) = \sum_{U \subseteq V} \lambda^{|U|} \cdot \beta^{|\delta(U)|}. $$

Here $|\delta(U)|$ denotes the number of edges between $U$ and $V \setminus U$. 
For a graph $G = (V, E)$, and $\lambda, \beta \in \mathbb{C}$, the partition function of the Ising model is defined as

$$Z_G(\lambda, \beta) = \sum_{U \subseteq V} \lambda^{|U|} \cdot \beta^{|\delta(U)|}.$$ 

- Invented to study ferromagnetism in statistical physics.
- $Z_G(1, \beta)$ is generating functions of edge cuts in $G$.
- $Z_G(1, \beta)$ is the partition function of the 2-state Potts model.
- $Z_G(\lambda, \beta)$ for non-real $\beta, \lambda$ relates to output probabilities for certain quantum circuits (Mann, Brenner 2018+)
Theorem (Lee and Yang, 1952)

Fix $\beta \in [-1, 1]$. Then for any graph $G$, the zeros of the univariate polynomial $Z_G(\lambda, \beta)$, lie on the unit circle in the complex plane.
The Lee-Yang theorem

**Theorem (Lee and Yang, 1952)**

Fix $\beta \in [-1, 1]$. Then for any graph $G$, the zeros of the univariate polynomial, $Z_G(\lambda, \beta)$, lie on the unit circle in the complex plane.

A lot of follow up work by many many people
The Lee-Yang theorem

**Theorem (Lee and Yang, 1952)**

Fix $\beta \in [-1, 1]$. Then for any graph $G$, the zeros of the univariate polynomial, $Z_G(\lambda, \beta)$, lie on the unit circle in the complex plane.

A lot of follow up work by many many people

- Today: where on the circle are these zeros?
The Lee-Yang theorem

Theorem (Lee and Yang, 1952)

Fix $\beta \in [-1, 1]$. Then for any graph $G$, the zeros of the univariate polynomial, $Z_G(\lambda, \beta)$, lie on the unit circle in the complex plane.

A lot of follow up work by many many people

- Today: where on the circle are these zeros?
- If $\beta = 1$, $Z_G = (1 + \lambda)^{|V|}$, which has only one zero: $-1$.
- For any other $\beta$, the roots of all graphs are in fact dense on the circle.
- We will consider the class of bounded degree graphs.
Overview of the rest of the talk

- Results for all bounded degree graphs
- Algorithmic consequences
- Ideas of proof (use of complex dynamics)
- Open problems and questions
\[ G_{d+1} \] is collection of all graphs of maximum degree at most \( d + 1 \).
Denote unit circle by \( \partial \mathbb{D} \); identified with \([-\pi, \pi)\).
\( \mathcal{G}_{d+1} \) is collection of all graphs of maximum degree at most \( d + 1 \).
Denote unit circle by \( \partial \mathbb{D} \); identified with \( [-\pi, \pi) \).

**Theorem (Peters, R. 18+)**

Let \( d \in \mathbb{N}_{\geq 2} \) and let \( \beta \in \left( \frac{d-1}{d+1}, 1 \right) \). Then there exists \( \theta = \theta_\beta \in (-\pi, \pi) \) such that the following holds:

(i) for any \( \lambda = e^{i\theta}, |\theta| < \theta \) and any graph \( G \in \mathcal{G}_{d+1} \) we have \( Z_G(\lambda, \beta) \neq 0 \);
$\mathcal{G}_{d+1}$ is collection of all graphs of maximum degree at most $d + 1$. Denote unit circle by $\partial \mathbb{D}$; identified with $[-\pi, \pi)$.

Theorem (Peters, R. 18+)

Let $d \in \mathbb{N}_{\geq 2}$ and let $\beta \in \left( \frac{d-1}{d+1}, 1 \right)$. Then there exists $\theta = \theta_\beta \in (-\pi, \pi)$ such that the following holds:

(i) for any $\lambda = e^{i\theta}$, $|\theta| < \theta$ and any graph $G \in \mathcal{G}_{d+1}$ we have $Z_G(\lambda, \beta) \neq 0$;

(ii) the set $\{ \lambda \in \mathbb{C} \mid Z_G(\lambda, \beta) = 0 \text{ for some } G \in \mathcal{G}_{d+1} \}$ is dense in $\partial \mathbb{D} \setminus (-\theta, \theta)$.

- Part (ii) independently proved by Chio, He, Ji, and Roeder (2018+).
- Extends some results of Barata and Marchetti and Barata and Goldbaum for $d = 2$ on Cayley trees.
$G_{d+1}$ is collection of all graphs of maximum degree at most $d + 1$.

**Theorem (Peters, R. 18+)**

Let $d \in \mathbb{N}_{\geq 2}$ and let $\beta \in (1, \frac{d+1}{d-1})$. Then there exists $\alpha = \alpha_\beta \in (-\pi, \pi)$ such that the following holds:

(i) for any $\lambda = e^{i\theta}$, $|\theta| < \alpha$, any $r \geq 0$ and any graph $G \in G_{d+1}$ we have $Z_G(r \cdot \lambda, \beta) \neq 0$;

(ii) the set $\{\lambda \in \mathbb{C} \mid Z_G(\lambda, \beta) = 0$ for some $G \in G_{d+1}\}$ accumulates on $e^{i\alpha}$ and $e^{-i\alpha}$.
Algorithmic consequences

**Corollary**

There exists an FPTAS for computing $Z_G(\lambda, \beta)$ for each fixed $\beta$ and $\lambda$ as above and $G \in \mathcal{G}_{d+1}$.
Algorithmic consequences

**Corollary**

There exists an FPTAS for computing $Z_G(\lambda, \beta)$ for each fixed $\beta$ and $\lambda$ as above and $G \in \mathcal{G}_{d+1}$.

(What is known about approximating $Z_G$ when $G \in \mathcal{G}_{d+1}$)

- **FPRAS on all graphs** when $0 < \beta < 1$ and $\lambda > 0$ (Jerrum and Sinclair 1993)
- **FPTAS** when $\lambda = 1$ and $\beta \in (1, \frac{d+1}{d-1})$ (Sinclair, P. Srivastava, and Thurley, 2014)
- **FPTAS** when $\lambda = 1$ and $|\beta - 1| \leq O(1/d)$, (Barvinok and Soberón 2017 combined with Patel, R. 2017)
- **FPTAS** when $\beta \in [-1, 1]$ and $|\lambda| < 1$ (Liu, Sinclair, P. Srivastava, 2017)
High level idea of the proof

- Transform the problem to ratios of partition functions.
- Express the ratio as an iteration of a rational map and apply techniques/ideas from complex dynamics.
- Same structure/idea was used by Peters and R. to solve a conjecture of Sokal concerning the location of zeros for the independence polynomial.
Ratios of partition functions

\[ Z_G(\lambda, \beta) = \sum_{U \subseteq V} \lambda^{|U|} \beta^{|\delta(U)|}. \]

Then ("ignoring" the situation that \( Z_G, v,_{\text{in}} = Z_G, v,_{\text{out}} = 0 \)), \( Z_G \neq 0 \iff R_G, v \neq -1. \)

\[ Z_G = Z_G, v,_{\text{in}} + Z_G, v,_{\text{out}} \]
Ratios of partition functions

\[ Z_G(\lambda, \beta) = \sum_{U \subseteq V} \lambda^{|U|} \cdot \beta^{|\delta(U)|}. \]

\[ Z_G = Z_{G, v, \text{in}} + Z_{G, v, \text{out}} \]

\[ R_{G, v} := \frac{Z_{G, v, \text{in}}}{Z_{G, v, \text{out}}} \]

Then (‘ignoring’ the situation that \( Z_{G, v, \text{in}} = Z_{G, v, \text{out}} = 0 \)),

\[ Z_G \neq 0 \iff R_{G, v} \neq -1. \]
High level idea of proof II

- Step 1: Analyse the ratio on Cayley trees using complex dynamics. (This allows to prove parts (ii))
- Step 2: Extend results to all trees with boundary conditions.
- Step 3: Use Weitz’ self avoiding walk tree to go from trees to all graphs.
Let $T_{k,d}$ be the rooted Cayley tree of down degree $d$ with $k$ layers, i.e. $T_{0,d}$ consists of a single vertex and $T_{k,d}$ consists of $d$ copies of $T_{k-1,d}$ connected to the root.

**Lemma**

$$R_{T_{k,d}} = \lambda \left( \frac{R_{T_{k-1,d}} + \beta}{\beta R_{T_{k-1,d}} + 1} \right)^d.$$
Towards dynamical systems

Define

\[ f : \hat{\mathcal{C}} \to \hat{\mathcal{C}} \, \text{by} \, R \mapsto \lambda \left( \frac{R + \beta}{\beta R + 1} \right)^d. \]

Lemma

For Cayley trees \( T_k = T_{k,d} \):

\[ Z_{T_k}(\beta, \lambda) \neq 0 \, \text{for all} \, k \iff f^{\circ k}(1) \neq -1 \, \text{for all} \, k. \]
Basic observations when $\beta \in (0, 1)$

Let

$$g(R) = \frac{R + \beta}{\beta R + 1}$$

then $f(R) = \lambda \cdot g(R)^d$

Basic observations when $\beta \in (0, 1)$

Let

$$g(R) = \frac{R + \beta}{\beta R + 1}$$

then $f(R) = \lambda \cdot g(R)^d$

- $g$ is a Möbius transformation and preserves the circle, $\partial \mathbb{D}$, its interior and its exterior. (Implies Lee-Yang Thm. for trees.)
Basic observations when $\beta \in (0, 1)$

Let

$$g(R) = \frac{R + \beta}{\beta R + 1} \quad \text{then} \quad f(R) = \lambda \cdot g(R)^d$$

- $g$ is a Möbius transformation and preserves the circle, $\partial \mathbb{D}$, its interior and its exterior. (Implies Lee-Yang Thm. for trees.)
- $f$ is an orientation preserving $d$-fold covering of $\partial \mathbb{D}$
Basic observations when $\beta \in (0, 1)$

Let

$$g(R) = \frac{R + \beta}{\beta R + 1} \quad \text{then} \quad f(R) = \lambda \cdot g(R)^d$$

- $g$ is a Möbius transformation and preserves the circle, $\partial \mathbb{D}$, its interior and its exterior. (Implies Lee-Yang Thm. for trees.)
- $f$ is an orientation preserving $d$-fold covering of $\partial \mathbb{D}$

$$f'(R) = f(R) \frac{d(1 - \beta^2)}{(R + \beta)(\beta R + 1)}.$$

So $|f'(R)|$ is minimal at $R = 1$ and increasing with $|\text{Arg}(R)|$. 
Definition (Informal)

The Fatou set $F$ is the set of points for which nearby points behave similarly under iteration of the map $f$. The Julia set $J$ is the complement of the Fatou set $F$. Montel's theorem implies that the Julia set is contained in the unit circle, $\partial D$. Two options for the Julia set $J$: $J$ is the entire circle (so no attracting fixed points on the circle). $J$ is not the entire circle, in which case the Fatou set is a single component and contains a unique attracting or parabolic fixed point on $\partial D$. 
Observations from complex dynamics

**Definition (Informal)**

The **Fatou set** $F$ is the set of points for which nearby points behave similarly under iteration of the map $f$. The **Julia set** $J$ is the complement of the Fatou set $F$. A fixed point $R$ ($R$ is such that $f(R) = R$) is called **attracting** if $|f'(R)| < 1$, **parabolic** if $f'(R) = 1$ and **repelling** if $|f'(R)| > 1$. Montel's theorem implies that the Julia set is contained in the unit circle, $\partial D$. Two options for the Julia set $J$:

- $J$ is the entire circle (so no attracting fixed points on the circle).
- $J$ is not the entire circle, in which case the Fatou set is a single component and contains a unique attracting or parabolic fixed point on $\partial D$. 
Observations from complex dynamics

**Definition (Informal)**

The Fatou set $F$ is the set of points for which nearby points behave similarly under iteration of the map $f$. The Julia set $J$ is the complement of the Fatou set $F$. A fixed point $R$ ($R$ is such that $f(R) = R$) is called attracting if $|f'(R)| < 1$, parabolic if $f'(R) = 1$ and repelling if $f'(R)| > 1$.

- Montel’s theorem implies that the Julia set is contained in the unit circle, $\partial \mathbb{D}$.
- Two options for the Julia set $J$:
  - $J$ is the entire circle (so no attracting fixed points on the circle).
  - $J$ is not the entire circle, in which case the Fatou set is a single component and contains a unique attracting or parabolic fixed point on $\partial \mathbb{D}$. 
The derivative at 1

\[ f'(R) = f(R) \frac{d(1 - \beta^2)}{(R + \beta)(\beta R + 1)} \]

let \( \beta_c = \frac{d - 1}{d + 1} \).

- if \( \beta \in (0, \beta_c) \), \(|f'(1)| > 1 \) (Julia set is \( \partial \mathbb{D} \))
- if \( \beta = \beta_c \), \(|f'(1)| = 1 \).
- if \( \beta \in (\beta_c, 1) \), \(|f'(1)| < 1 \).
The derivative at 1

\[ f'(R) = f(R) \frac{d(1 - \beta^2)}{(R + \beta)(\beta R + 1)} \]

let \[ \beta_c = \frac{d - 1}{d + 1}. \]

- if \( \beta \in (0, \beta_c) \), \( |f'(1)| > 1 \) (Julia set is \( \partial \mathbb{D} \))
- if \( \beta = \beta_c \), \( |f'(1)| = 1 \).
- if \( \beta \in (\beta_c, 1) \), \( |f'(1)| < 1 \).

**Lemma**

*If \( \beta \in (0, \beta_c) \), then the collection of parameters \( \lambda \) for which \(-1\) is contained in the orbit of the initial value \( R_0 = 1 \) is dense in \( \partial \mathbb{D} \).*
The derivative at 1

\[ f'(R) = f(R) \frac{d(1 - \beta^2)}{(R + \beta)(\beta R + 1)} \quad \text{let } \beta_c = \frac{d - 1}{d + 1}. \]

- if \( \beta \in (0, \beta_c) \), \( |f'(1)| > 1 \) (Julia set is \( \partial \mathbb{D} \))
- if \( \beta = \beta_c \), \( |f'(1)| = 1 \).
- if \( \beta \in (\beta_c, 1) \), \( |f'(1)| < 1 \).

Lemma

If \( \beta \in (0, \beta_c) \), then the collection of parameters \( \lambda \) for which \(-1\) is contained in the orbit of the initial value \( R_0 = 1 \) is dense in \( \partial \mathbb{D} \).

Corollary

If \( \beta \in (0, \beta_c) \), then the zeros of \( Z_{T_k,d}(\lambda, \beta) \) are dense in \( \partial \mathbb{D} \).
Fix $\beta \in (\beta_c, 1)$.

**Lemma**

There exists a unique $\theta \in (0, \pi)$ such that for the two parameters $\lambda = e^{\pm i\theta}$, $f$ has a unique parabolic fixed point $R$. It satisfies the equation:

$$R^2 + \frac{d(\beta^2 - 1) + (1 + \beta^2)}{\beta} R + 1 = 0.$$
Analysis of parabolic fixed points

Fix $\beta \in (\beta_c, 1)$.

**Lemma**

There exists a unique $\theta \in (0, \pi)$ such that for the two parameters $\lambda = e^{\pm i\theta}$, $f$ has a unique parabolic fixed point $R$. It satisfies the equation:

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

**Lemma**

The map $f$ has a parabolic or attracting fixed point on $\partial \mathbb{D}$ if and only if $\lambda = e^{i\vartheta}$ with $|\vartheta| \leq \theta$. 

Guus Regts (University of Amsterdam)  Location of zeros of the partition function of
Fix $\beta \in (\beta_c, 1)$.

**Lemma**

There exists a unique $\theta \in (0, \pi)$ such that for the two parameters $\lambda = e^{\pm i \theta}$, $f$ has a unique parabolic fixed point $R$. It satisfies the equation:

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

**Lemma**

The map $f$ has a parabolic or attracting fixed point on $\partial \mathbb{D}$ if and only if $\lambda = e^{i \vartheta}$ with $|\vartheta| \leq \theta$.

This can be used to prove our theorem for Cayley trees.
High level idea of proof part (i)

- Step 1: Analyse the ratio on Cayley trees using complex dynamics.
- Step 2: Extend results to all trees with boundary conditions.
High level idea of proof part (i)

- **Step 1**: Analyse the ratio on Cayley trees using complex dynamics.
- **Step 2**: Extend results to all trees with boundary conditions.
  - The recurrence for general trees is given as

\[
(R_1, \ldots, R_d) \mapsto F(R_1, \ldots, R_d) := \lambda \prod_{i=1}^{d} \frac{R_i + \beta}{\beta R_i + 1}.
\]

- Let \( I \) be the circular interval \([1, \hat{R}]\) (\( \hat{R} \) is the attracting fixed point.) Then for any \( R \in I, f(R) \in I \).
- Let \( C \) be the cone through \( I \). Then for any \( R_1, \ldots, R_d \in C \), \( F(R_1, \ldots, R_d) \in C \).

- **Step 3**: Use Weitz’ self avoiding walk tree to go from trees to all graphs.
High level idea of proof part (i)

- **Step 1:** Analyse the ratio on Cayley trees using complex dynamics.
- **Step 2:** Extend results to all trees with boundary conditions.
  - The recurrence for general trees is given as
    \[
    (R_1, \ldots, R_d) \mapsto F(R_1, \ldots, R_d) := \lambda \prod_{i=1}^{d} \frac{R_i + \beta}{\beta R_i + 1}.
    \]
  - Let \( I \) be the circular interval \([1, \hat{R}]\) (\( \hat{R} \) is the attracting fixed point.)
  - Then for any \( R \in I \), \( f(R) \in I \).
  - Let \( C \) be the cone through \( I \). Then for any \( R_1, \ldots, R_d \in C \),
    \( F(R_1, \ldots, R_d) \in C \).
- **Step 3:** Use Weitz’ self avoiding walk tree to go from trees to all graphs.
Theorem (Liu, Sinclair, Srivastava, 2018+)
for each \( d \geq 2 \) there exists a region \( B \subset C \) containing the interval \( (d-1, d+1), (d+1, d-1) \) such that for all \( \beta \in B \), and all graphs \( G \in G_{d+1}, \)
\( Z_G(1, \beta) \neq 0. \)

Question
What is the maximal domain \( B \) containing \((d-1, d+1), (d+1, d-1)\) such that the above statement still holds?
Questions/Open Problems I

**Theorem (Liu, Sinclair, Srivastava, 2018+)**

For each \( d \geq 2 \) there exists a region \( B \subset \mathbb{C} \) containing the interval \( \left( \frac{d-1}{d+1}, \frac{d+1}{d-1} \right) \) such that for all \( \beta \in B \), and all graphs \( G \in \mathcal{G}_{d+1} \), \( Z_G(1, \beta) \neq 0 \).

**Question**

What is the maximal domain \( B \) containing \( \left( \frac{d-1}{d+1}, \frac{d+1}{d-1} \right) \) such that the above statement still holds?
Questions/Open Problems II

**Definition**

The **partition function of the Potts model** is defined for \( \beta \in \mathbb{C} \), \( k \in \mathbb{N} \) and a graph \( G \) by

\[
P_G(\beta, k) = \sum_{\phi: V \to [k]} \beta^\# \text{ monochromatic edges}.
\]

Note: \( Z_G(1, \beta) = \beta^{|E|} P_G(1/\beta, 2) \).

**Question**

Let \( k \in \mathbb{N} \). Is it true that there exists a region \( B \) containing the interval \((d + 1 - k/d + 1, 1)\) such that for all \( \beta \in B \) and graphs \( G \in G_{d+1} \), \( P_G(\beta, k) \neq 0 \)?

With Bencs, Davies and Patel: can find a region that contains the interval \( [d + 1 - (k - 1)/e d + 1, 1) \).
Definition

The partition function of the Potts model is defined for $\beta \in \mathbb{C}$, $k \in \mathbb{N}$ and a graph $G$ by

$$P_G(\beta, k) = \sum_{\phi : V \rightarrow [k]} \beta^\# \text{ monochromatic edges}.$$ 

Note $Z_G(1, \beta) = \beta^{|E|} P_G(1/\beta, 2)$.

Question

Let $k \in \mathbb{N}$. Is it true that there exists a region $B$ containing the interval $(\frac{d+1-k}{d+1}, 1)$ such that for all $\beta \in B$ and graphs $G \in \mathcal{G}_{d+1}$, $P_G(\beta, k) \neq 0$?
Definition

The partition function of the Potts model is defined for $\beta \in \mathbb{C}$, $k \in \mathbb{N}$ and a graph $G$ by

$$P_G(\beta, k) = \sum_{\phi : V \to [k]} \beta^{\# \text{ monochromatic edges}}.$$ 

Note $Z_G(1, \beta) = \beta^{|E|} P_G(1/\beta, 2)$.

Question

Let $k \in \mathbb{N}$. Is it true that there exists a region $B$ containing the interval $\left(\frac{d+1-k}{d+1}, 1\right)$ such that for all $\beta \in B$ and graphs $G \in G_{d+1}$, $P_G(\beta, k) \neq 0$?

With Bencs, Davies and Patel: can find a region that contains the interval $\left[\frac{d+1 - (k-1)/e}{d+1}, 1\right)$.
More antiferromagnetic ($\beta > 1$) zeros:

**Theorem (Bencs, Buys, Guerini, Peters, 19+)**

Let $d \in \mathbb{N}_{\geq 2}$ and let $\beta \in (1, \frac{d+1}{d-1})$. Then there exists $\theta = \theta_\beta > \alpha_\beta$ such that the set $\{\lambda \mid Z_G(\lambda, \beta) = 0\}$ for some $G \in \mathcal{G}_{d+1}$ is dense in the circular interval $(-\theta, \theta)$. 
More antiferromagnetic ($\beta > 1$) zeros:

**Theorem (Bencs, Buys, Guerini, Peters, 19+)**

Let $d \in \mathbb{N}_{\geq 2}$ and let $\beta \in (1, \frac{d+1}{d-1})$. Then there exists $\theta = \theta_\beta > \alpha_\beta$ such that the set $\{\lambda \mid Z_G(\lambda, \beta) = 0\}$ for some $G \in \mathcal{G}_{d+1}$ is dense in the circular interval $(-\theta, \theta)$.

**Question**

What happens in between $\theta$ and $\alpha$?

Preliminary work of Bencs, Buys, Guerini and Peters suggests that there is an interval $I \subset (\alpha, \theta)$ on which the roots accumulate.
Let $d \in \mathbb{N}_{\geq 2}$, let $\beta \in \left(\frac{d-1}{d+1}, 1\right)$ and let $\theta = \theta_\beta$.

**Corollary**

For any $\lambda = e^{i\vartheta}$, $|\vartheta| < \theta$ there is an FPTAS for computing $Z_G(\lambda, \beta)$ for all graphs $G \in \mathcal{G}_{d+1}$.

**Question**

How hard is it to approximate $Z_G(\lambda, \beta)$ when $\lambda = e^{i\vartheta}$, $|\vartheta| > \theta_\beta$?
Thank you for your attention!