Lee-Yang zeros and the complexity of the ferromagnetic Ising Model on bounded-degree graphs

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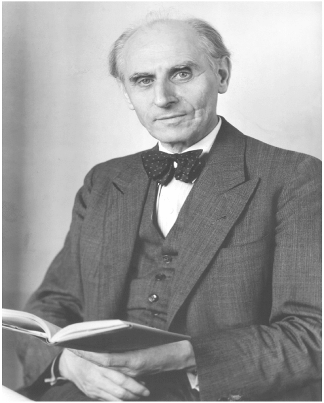
Very short summary

$$\overline{\text{Values for which the Ising partition function is zero.}}$$

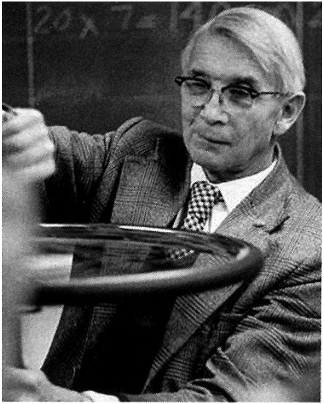
$$=$$

$$\overline{\text{Values for which approximating the Ising partition function is \#P-hard.}}$$

The Ising Model



Wilhelm Lenz (1888 - 1957)



Ernst Ising (1900 - 1998)

The Ising Model

- For a graph $G = (V, E)$ a *configuration* is a map $\sigma : V \to \{+, -\}$.
- Let $b \in (0, 1)$ and $\lambda \geq 1$, we define the *weight* of a configuration to be

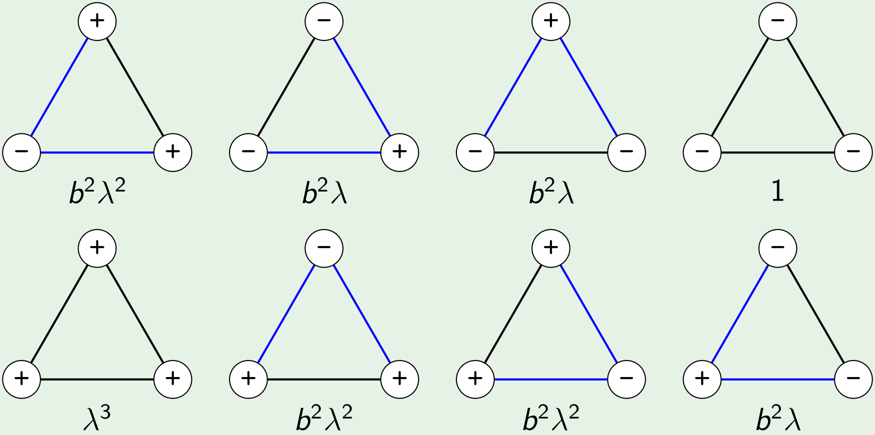
$$W_\sigma(\lambda, b) = \lambda^{n_+(\sigma)} b^{\delta(\sigma)},$$

  where $n_+(\sigma)$ is the number of vertices assigned + and $\delta(\sigma)$ the number of edges with different spins.
- The probability of a certain configuration σ is $W_\sigma(\lambda, b)/Z$, where

$$Z = Z(\lambda, b) = \sum_{\sigma : V \to \{+,-\}} W_\sigma(\lambda, b) = \sum_{\sigma : V \to \{+,-\}} \lambda^{n_+(\sigma)} b^{\delta(\sigma)}.$$

Example

Example



$$Z_G(\lambda, b) = \lambda^3 + 3b^2\lambda^2 + 3b^2\lambda + 1$$

Approximating $Z_G(\lambda, b)$

Let $\mathbb{Q}[i] = \{z \in \mathbb{C} : \mathrm{re}(z), \mathrm{im}(z) \in \mathbb{Q}\}$.
Let $\lambda \in \mathbb{Q}[i]$, $b \in (0,1) \cap \mathbb{Q}$, $K \in \mathbb{Q}_{\geq 1}$ and $\Delta \in \mathbb{Z}_{\geq 3}$.
We consider the following problems.

Name $\#\text{IsingNorm}(\lambda, b, \Delta, K)$.
Instance A graph $G = (V, E)$ with maximum degree $\leq \Delta$.
Output If $Z_G(\lambda, b) = 0$, the algorithm may output any rational. Otherwise, it must return a rational $\widehat{N}$ such that $\widehat{N}/K \leq |Z_G(\lambda, b)| \leq K\widehat{N}$.

and for $\rho \in \mathbb{Q}_{\geq 0}$

Name $\#\text{IsingArg}(\lambda, b, \Delta, \rho)$.
Instance A graph $G = (V, E)$ with maximum degree $\leq \Delta$.
Output If $Z_G(\lambda, b) = 0$, the algorithm may output any rational. Otherwise, it must return a rational $\widehat{A}$ such that $|\widehat{A} - a| \leq \rho$ for some $a \in \arg(Z_G(\lambda, b))$.

Approximating $Z_G(\lambda, b)$

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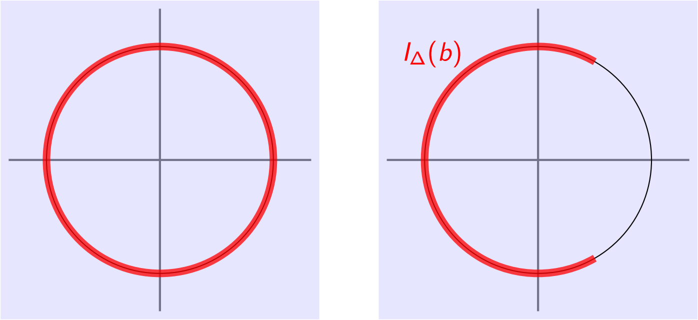
A *fully polynomial time approximation scheme* (FPTAS) for approximating $Z_G(\lambda, b)$ is an algorithm that for any n-vertex graph G of maximum degree at most Δ and any rational $\varepsilon > 0$ solves both problems $\#\text{IsingNorm}(\lambda, b, \Delta, 1 + \varepsilon)$ and $\#\text{IsingArg}(\lambda, b, \Delta, \varepsilon)$ in time polynomial in n/ε.

Approximation schemes and Lee-Yang zeros

The Lee-Yang theorem (1952) states that for fixed $b \in (0,1)$ the complex zeros of $Z_G(\lambda, b)$ for any graph G lie on the unit circle.
Peters and Regts showed in 2018 that the situation for graphs with with maximum degree $\leq \Delta$ is as follows:

$0 < b \leq 1 - 2/\Delta$ $\qquad$ $1 - 2/\Delta < b < 1$



Zeros are dense and contained in the red arcs

Approximation schemes and Lee-Yang zeros

- Liu, Sinclair, and Srivastava (2018) obtained an FPTAS for approximating $Z_G(\lambda, b)$ for $\lambda \notin \mathbb{S}$.
- Using the methods by Barvinok (2017) and Patel and Regts (2017) Peters and Regts obtained an FPTAS for approximating $Z_G(\lambda, b)$ for $1 - 2/\Delta < b < 1$ and $\lambda \in \mathbb{S} \setminus I_\Delta(b)$.

Our main result is the following:

Theorem (B., Galanis, Patel, Regts)

Let $\Delta \geq 3$ be an integer and let $K = 1.001$ and $\rho = \pi/40$.

(a) *Let $b \in \left(0, \frac{\Delta-2}{\Delta}\right]$ be a rational, and $\lambda \in \mathbb{Q}[i] \cap \mathbb{S}$ such that $\lambda \neq \pm 1$. Then the problems $\#\text{IsingNorm}(\lambda, b, \Delta, K)$ and $\#\text{IsingArg}(\lambda, b, \Delta, \rho)$ are #P-hard.*

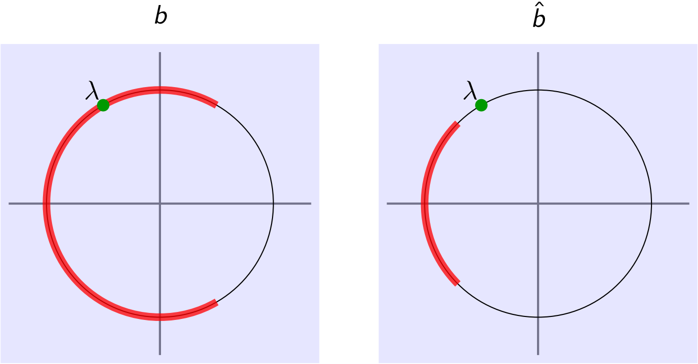
(b) *Let $b \in \left(\frac{\Delta-2}{\Delta}, 1\right)$ be a rational. Then the collection of complex numbers $\lambda \in \mathbb{Q}[i] \cap I_\Delta(b)$ for which $\#\text{IsingNorm}(\lambda, b, \Delta, K)$ and $\#\text{IsingArg}(\lambda, b, \Delta, \rho)$ are #P-hard is dense in the arc $I_\Delta(b)$.*

#P-Hardness

- #P is a complexity class of counting problems.
  - What is the value of the permanent of a given matrix consisting of 1s and 0s?
  - How many perfect matchings are there in a given bipartite graph?
- #IsingNorm(λ, b, Δ, K) being #P-hard implies that if there is a polynomial time algorithm to solve #IsingNorm(λ, b, Δ, K), then any problem in #P can be solved in polynomial time.
- We show that a polynomial time algorithm for #IsingNorm(λ, b, Δ, K) can be used to solve the problem of calculating $Z_G(\lambda, \hat{b})$ **exactly** given a 3-regular graph G in polynomial time.
- This problem is known to be #P-hard [Kowalczyk-Cai '11].

Very rough idea of the reduction

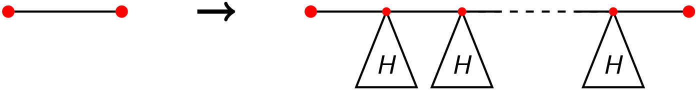
This $\hat{b}$ is chosen to have the property that $Z_G(\lambda, \hat{b})$ cannot be zero.



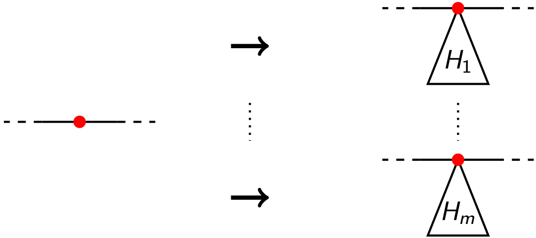
Very rough idea of the reduction

We transform the input graph G in multiple ways. Involving steps like:

- We replace edges of G by paths with gadgets to simulate edge activity $\hat{b}$.

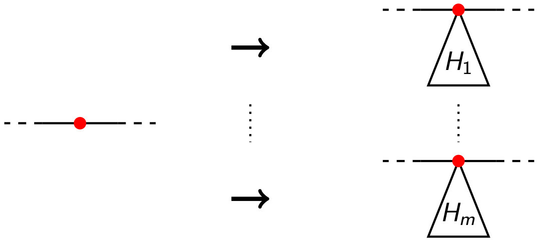


- We *probe* degree 2 vertices with multiple gadgets.



A polynomial amount of applications of $\#\text{IsingNorm}(\lambda, b, \Delta, K)$ to these transformed graphs allow us to calculate $Z_G(\lambda, \hat{b})$ exactly.

Very rough idea of the reduction



- We need our gadgets to exist within the family of rooted trees with bounded degree Δ and root degree 1.
- We need our gadgets to be *small* compared to the size of the input graph G.

Ratios/fields

- Recall that

$$Z_G(\lambda) = \sum_{\sigma : V \to \{+,-\}} \lambda^{|n_+(\sigma)|} b^{|\delta(\sigma)|}.$$

- For a graph G and a vertex $v \in V$ we define

$$Z_{G,v^+}(\lambda) := \sum_{\sigma : V \to \{+,-\};\sigma(v)=+} \lambda^{|n_+(\sigma)|} b^{|\delta(\sigma)|}$$

  and we define $Z_{G,v^-}(\lambda)$ analogously.
- We then define the ratio

$$R_{G,v}(\lambda) = \frac{Z_{G,v^+}(\lambda)}{Z_{G,v^-}(\lambda)}.$$

- **Note:**

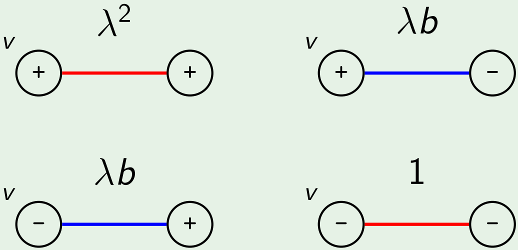
$$Z_G(\lambda) = Z_{G,v^+}(\lambda) + Z_{G,v^-}(\lambda) = 0 \quad \Leftrightarrow \quad R_{G,v}(\lambda) = -1.$$

Ratios/fields: Example

$$R_{G,v}(\lambda) = \frac{Z_{G,v^+}(\lambda)}{Z_{G,v^-}(\lambda)}$$

Example

Let G be an edge and v one of its endpoints.



So

$$R_{G,v}(\lambda) = \frac{\lambda^2 + \lambda b}{\lambda b + 1}.$$

Ratios/fields

These ratios are rational maps $\mathbb{S} \to \mathbb{S}$. Given a particular λ, for our reduction to work we need the following.

- We need the ratios to be dense in the unit circle, i.e. we want

$$\{R_{T,v}(\lambda) : T \text{ tree of bounded degree } \Delta \text{ with } \deg(v) = 1\}$$

  to be dense in $\mathbb{S}$.
- We need exponentially fast implementation, i.e. we need an algorithm that, given a $P \in \mathbb{S}$ and $\epsilon > 0$, yields a rooted tree (T, v) such that
  - T has its degree bounded by Δ and $\deg(v) = 1$;
  - $|R_{T,v}(\lambda) - P| < \epsilon$;
  - the size of T is $\mathcal{O}(\log(1/\epsilon))$.

Ratios/fields

We prove

Lemma

Let $\Delta \geq 3$ be an integer.

(a) *Let $b \in \left(0, \frac{\Delta-2}{\Delta}\right]$ be a rational, and $\lambda \in \mathbb{Q}[i] \cap \mathbb{S}$ such that $\lambda \neq \pm 1$. Then*

$$\{R_{T,v}(\lambda) : T \text{ tree bounded degree } \Delta \text{ with } \deg(v) = 1\}$$

is dense in $\mathbb{S}$.

(b) *Let $b \in \left(\frac{\Delta-2}{\Delta}, 1\right)$ be a rational. Then*

$$\{R_{T,v}(\lambda) : T \text{ tree bounded degree } \Delta \text{ with } \deg(v) = 1\}$$

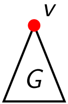
is dense in $\mathbb{S}$ for a dense set of complex numbers in $\lambda \in \mathbb{Q}[i] \cap I_\Delta(b)$.

Lemma

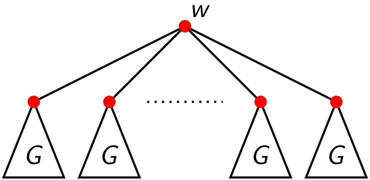
Density implies an algorithm for exponentially fast implementation.

Graph constructions

Suppose we have a rooted graph (G, v) with ratio $R_{G,v}(\lambda)$.



We construct a new graph $\tilde{G}$ by attaching k disjoint copies of G to a new root w.

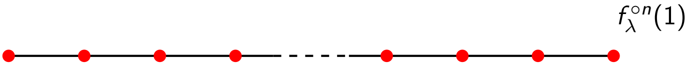


We have $R_{\tilde{G},w}(\lambda) = f_{k,\lambda}(R_{G,v}(\lambda))$, where

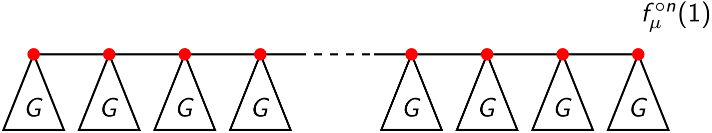
$$f_{k,\lambda}(z) = \lambda \left(\frac{z+b}{bz+1} \right)^k .$$

Graph constructions

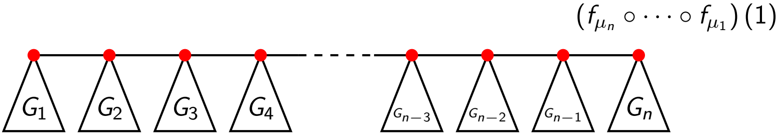
Let $f_\lambda(z) = f_{\lambda,1}(z) = \lambda\left(\frac{z+b}{bz+1}\right)$. Then the ratio of a path on n vertices is



If (G, v) is a rooted graph with ratio $\mu = R_{G,v}(\lambda)$ then the ratio is

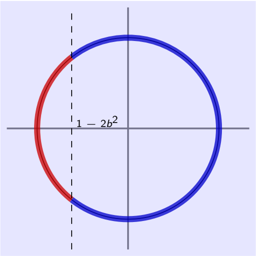


If $(G_1, v_1)\ldots(G_n, v_n)$ are rooted graphs with ratios $\mu_1, \ldots, \mu_n$ then



The Möbius transformation $f_\mu(z) = \mu\left(\frac{z+b}{bz+1}\right)$

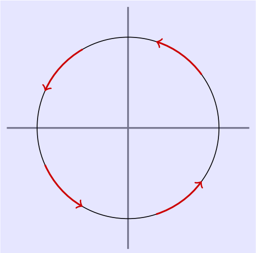
f_μ is elliptic

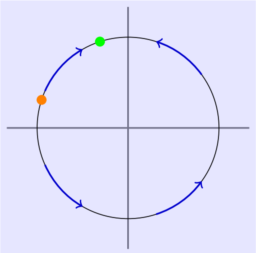


f_μ is hyperbolic

If μ lies in the red arc then f_μ is conjugate to a rotation $z \mapsto e^{i\theta}z$

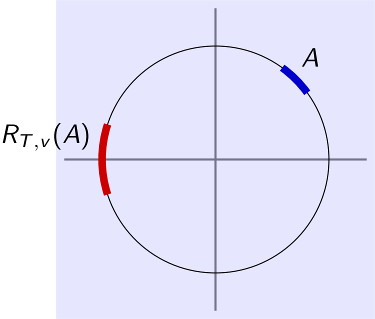
If μ lies in the blue arc then f_μ is conjugate to a map of the form $z \mapsto a \cdot z$ for some $a \in (0,1)$





Zeros imply density (easy version)

- Suppose G is a graph and λ_0 a parameter such that $Z_G(\lambda_0) = 0$.
- Then arbitrarily close to λ_0 there is a parameter λ_1 with a rooted tree (T, v) such that, $\Delta(G) \geq \Delta(T)$, $\deg(v) = 1$ and $R_{T,v}(\lambda_1) = -1$.
- There is an arc A around λ_1 such that for all $\mu \in R_{T,v}(A)$ the map f_μ is elliptic.



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- There is an arc A around λ_1 such that for all $\mu \in R_{T,v}(A)$ the map f_μ is elliptic.

Lemma

If $b \in (0,1) \cap \mathbb{Q}$ and $\mu \in \mathbb{Q}[i] \cap \mathbb{S}$ such that $\mu \neq -1$ and f_μ is elliptic, then f_μ is conjugate to an irrational rotation.

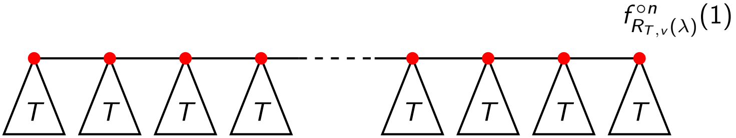
- So (for A small enough) for every $\lambda \in A \cap \mathbb{Q}[i]$ with $\lambda \neq \lambda_1$ the set

$$\{f^{\circ n}_{R_{T,v}(\lambda)}(1) : n \geq 1\}$$

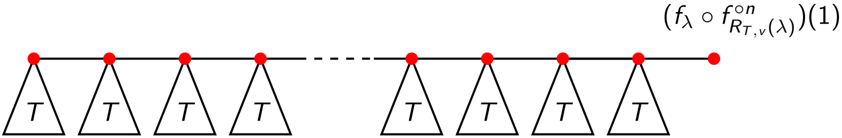
is dense in $\mathbb{S}$.

Zeros imply density (easy version)

Recall that $\{f^{\circ n}_{R_{T,v}(\lambda)}(1) : n \geq 1\}$ are ratios of graphs of the form:

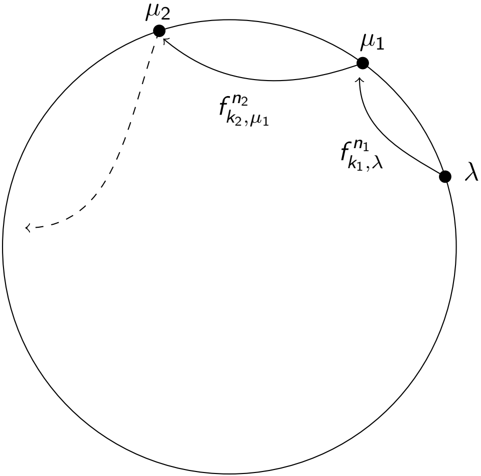


If these are dense in $\mathbb{S}$ then ratios of the following graphs are also dense in $\mathbb{S}$:



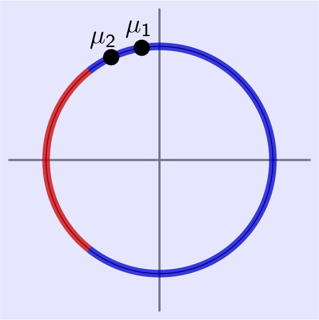
Zeros imply density for all $\lambda \in \mathbb{Q}[i] \cap \mathbb{S} \setminus \{\pm 1\}$

If $b \in \left(0, \frac{\Delta-2}{\Delta}\right]$ and $\lambda \in \mathbb{Q}[i] \cap \mathbb{S} \setminus \{\pm 1\}$ we can find a rooted tree (T, v) with $\Delta(T) \leq \Delta$ and $\deg(v) \leq \Delta - 2$ with its ratio close enough to -1.



Density implies exponentially fast implementation

If ratios are dense in $\mathbb{S}$ we can find two trees (T_1, v_1) and (T_2, v_2) with ratios μ_1 and μ_2 such that f_{μ_1}, f_{μ_2} are hyperbolic but close to parabolic/elliptic.



We choose these parameters such that the attracting fixed points P_1 and P_2 of f_{μ_1} and f_{μ_2} satisfy $1/2 < f'_{\mu_i}(P_i) < 1$.

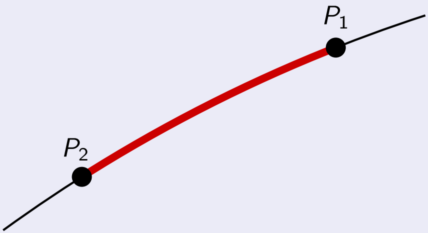
Density implies exponentially fast implementation

Lemma

Let I be the small arc between the fixed points P_1 and P_2. Given any $P \in I$ and $\epsilon > 0$ we can find indices $i_1, \ldots, i_N \in \{1, 2\}$ such that

$$\left|(f_{\mu_{i_N}} \circ \cdots \circ f_{\mu_{i_1}})(1) - P\right| < \epsilon$$

with $N = \mathcal{O}(\log(1/\epsilon))$.



Density implies exponentially fast implementation

Lemma

Let I be the small arc between the fixed points P_1 and P_2. Given any $P \in I$ and $\epsilon > 0$ we can find indices $i_1, \ldots, i_K \in \{1, 2\}$ such that

$$\left|(f_{\mu_{i_N}} \circ \cdots \circ f_{\mu_{i_1}})(1) - P\right| < \epsilon$$

with $N = \mathcal{O}(\log(1/\epsilon))$.

The tree with ratio $(f_{\mu_{i_N}} \circ \cdots \circ f_{\mu_{i_1}})(1)$ has size at most

$$\max\{|V(T_1)|, |V(T_2)|\} \cdot N = \mathcal{O}(\log(1/\epsilon)).$$

When λ is in an arc where zeros are dense, the map $f_{\Delta-1,\lambda}$ is expanding on $\mathbb{S}$. This means that there is a fixed M such that $f_{\Delta-1,\lambda}^M(I) = \mathbb{S}$. With this we can lift the implementation on points on I to arbitrary points in $\mathbb{S}$ with maps of the form

$$(f_{\Delta-1,\lambda}^M \circ f_{\mu_{i_N}} \circ \cdots \circ f_{\mu_{i_1}})(1)$$

belonging to trees of size $(\Delta - 1)^M \cdot \mathcal{O}(\log(1/\epsilon)) = \mathcal{O}(\log(1/\epsilon))$.

Summary

$$\overline{\{\lambda \in \mathbb{C} : Z_G(\lambda) = 0 \text{ for some } G \in \mathcal{G}_\Delta\}}$$

$$=$$

$$\overline{\{\lambda \in \mathbb{S} : \{R_{G,v}(\lambda) : G \in \mathcal{G}_\Delta\} \text{ is dense in } \mathbb{S}\}}$$

$$=$$

$$\overline{\{\lambda \in \mathbb{Q}[i] : \text{approximating } Z_G(\lambda) \text{ for } G \in \mathcal{G}_\Delta \text{ is \#P-hard}\}}$$

$$=$$

$$\{\lambda \in \mathbb{C} : \{R_{G,v} : G \in \mathcal{G}_\Delta\} \text{ is not normal around } \lambda\}.$$

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