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# Regions Without Complex Zeros for Chromatic Polynomials on Graphs with Bounded Degree

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We prove that the chromatic polynomial  $P_{\mathbb{G}}(q)$  of a finite graph  $\mathbb{G}$  of maximal degree  $\Delta$  is free of zeros for  $|q| \geq C^*(\Delta)$  with

$$C^*(\Delta) = \min_{0 < x < 2^{\frac{1}{\Delta}-1}} \frac{(1+x)^{\Delta-1}}{x[2-(1+x)^{\Delta}]}$$

This improves results by Sokal and Borgs. Furthermore, we present a strengthening of this condition for graphs with no triangle-free vertices.

## 1. Introduction

Let  $\mathbb{G} = (\mathbb{V}, \mathbb{E})$  be a finite graph with vertex set  $\mathbb{V}$ , edge set  $\mathbb{E}$ , and maximum degree  $\Delta$ . For any integer  $q$ , let  $P_{\mathbb{G}}(q)$  be equal to the number of proper colourings with  $q$  colours of the graph  $\mathbb{G}$ , that is, colourings such that no two adjacent vertices of the graph have equal colours. The function  $P_{\mathbb{G}}(q)$  is a polynomial known as the *chromatic polynomial*, and it coincides with the partition function of the anti-ferromagnetic Potts model with  $q$  states on  $\mathbb{G}$  at zero temperature. Sokal [12] exploited a well-known representation of the latter which leads to the identity

$$P_{\mathbb{G}}(q) = q^{|\mathbb{V}|} \Xi_{\mathbb{G}}(q). \quad (1.1)$$

Here  $\Xi_{\mathbb{G}}(q)$  is the grand canonical partition function of a ‘gas’ whose ‘particles’ are subsets  $\gamma \subset \mathbb{V}$ , with cardinality  $|\gamma| \geq 2$ , subjected to a non-intersection constraint (hard-core interaction) and endowed with activities  $z_{\gamma}(q)$  that depend on the topological structure of  $\mathbb{G}$  (see (3.7) below). Such a hard-core gas corresponds to an abstract *polymer model* [5] whose analyticity properties are the object of the *cluster expansion* technology [3, 2, 7, 4]. The absolute convergence of the cluster expansion yields the analyticity of  $\log \Xi_{\mathbb{G}}(q)$  as a function of the activities and, thus, the absence of zeros of  $P_{\mathbb{G}}$  for the corresponding *complex disk* in  $q$ .

At this point, one can make use of any of the available convergence conditions for the cluster expansion. Sokal used the Kotecky–Preiss condition [7], which requires the existence of some  $a > 0$  such that

$$\sum_{n \geq 2} e^{an} C_n^q \leq a, \quad (1.2)$$

where

$$C_n^q = \sup_{x \in \mathbb{V}} \sum_{\substack{\gamma \subset \mathbb{V}: x \in \gamma \\ |\gamma| = n}} |z_\gamma(q)|. \quad (1.3)$$

He then combined this condition with the bound [12]

$$C_n^q \leq \left(\frac{1}{q}\right)^{n-1} \sup_{v_0 \in \mathbb{V}_{\mathbb{G}}} t_n(\mathbb{G}, v_0) \quad (1.4)$$

$$\leq \left(\frac{1}{q}\right)^{n-1} t_n(\Delta), \quad (1.5)$$

where  $t_n(\mathbb{G}, v_0)$  is number of subtrees of  $\mathbb{G}$ , with  $n$  vertices, one of which is  $v_0$  and  $t_n(\Delta)$  is the number of  $n$ -vertex subtrees in the  $\Delta$ -regular infinite tree containing a fixed vertex. Using (1.5), Sokal proved that  $P_{\mathbb{G}}(q)$  is free of zeros in the region

$$|q| \geq C(\Delta), \quad (1.6)$$

where  $C(\Delta)$  is defined by

$$C(\Delta) = \min_{a \geq 0} \inf \left\{ \kappa : \sum_{n=1}^{\infty} t_n(\Delta) \left[ \frac{e^a}{\kappa} \right]^{n-1} \leq 1 + a e^{-a} \right\}. \quad (1.7)$$

By numerical methods, Sokal obtained rigorous upper bounds on  $C(\Delta)$  for  $2 \leq \Delta \leq 20$  (see [12, Table 2] for  $\Delta \leq 20$ ). He also showed that for large  $\Delta$  there is a finite limit  $\lim_{\Delta \rightarrow \infty} C(\Delta)/\Delta = K$  with

$$K = \min_{a \geq 0} \inf \left\{ \kappa : \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} \left[ \frac{e^a}{\kappa} \right]^{n-1} \leq 1 + a e^{-a} \right\} \quad (1.8)$$

$$= \min_{a \geq 0} \frac{\exp\{a + \ln(1 + a e^{-a})\}}{\ln(1 + a e^{-a})} \quad (1.9)$$

$$= 7.963906\dots \quad (1.10)$$

The expression (1.8) is the one given originally in [12], where the estimation (1.10) – and the rigorous bound  $K \leq 7.963907$  – were obtained through a computer-assisted calculation. Its identification with (1.9) is due to Borgs [1]. Furthermore, this constant  $K$  is such that  $C(\Delta) \leq K\Delta$  for all  $\Delta$ , thus yielding, for the region free of zeros, the weaker but simpler bound

$$|q| \geq K\Delta, \quad (1.11)$$

which approaches (1.6) in the large- $\Delta$  regime. The bound (1.11)–(1.8) can be obtained in a more direct way simply by combining (1.2) with the previously obtained inequality [10]

$$C_n^q \leq \frac{n^{n-1}}{n!} \left[ \frac{\Delta}{q} \right]^{n-1}. \quad (1.12)$$

In this paper we improve these criteria in two different directions. On the one hand, our bounds improve Sokal's results for graphs for which the maximum degree is the only available information. On the other hand, we are able to exploit relations between vertices with a common neighbour to produce even better bounds if the graph has no triangle-free vertex (a vertex is triangle-free if there is no edge linking two of its neighbours). These improvements have a double source. First, we strengthen the convergence criterion (1.2), replacing  $a$  by  $e^a - 1$  on the right-hand side (Lemma 3.1). Second, we improve the bound (1.5) by considering a restricted family of trees (Lemma 3.2). Both improvements are in fact related, and amount to a more careful consideration of an identity due to Penrose [8]. Our ideas stem from the work reported in [6], even when below we produce independent, self-contained proofs.

## 2. Results

Let us introduce some additional notation. Given  $v_0 \in \mathbb{V}$ , let  $d_{v_0}$  be its degree and let  $\Gamma(v_0) = \{v \in \mathbb{V} : \{v, v_0\} \in \mathbb{E}\}$  be its neighbourhood. For  $k = 1, \dots, \Delta$ , let

$$t_k^{\mathbb{G}} = \sup_{\substack{v_0 \in \mathbb{V} \\ d_{v_0} \geq k}} |\{U \subset \Gamma(v_0) : |U| = k \text{ and } \{v, v'\} \notin \mathbb{E} \forall v, v' \in U\}| \quad (2.1)$$

(maximal number of families of  $k$  vertices that have a common neighbour but are not neighbours between themselves). Consider also

$$\tilde{t}_k^{\mathbb{G}} = \sup_{\substack{v_0 \in \mathbb{V} \\ d_{v_0} \geq k+1}} \max_{v \in \Gamma(v_0)} |\{U \subset \Gamma(v_0) \setminus \{v\} : |U| = k \text{ and } \{v, v'\} \notin \mathbb{E} \forall v, v' \in U\}| \quad (2.2)$$

(the same as above but excluding, in addition, one of the neighbours). We then denote, for  $u > 0$ ,

$$Z_{\mathbb{G}}(u) = 1 + \sum_{k=1}^{\Delta} t_k^{\mathbb{G}} u^k \quad (2.3)$$

and

$$\tilde{Z}_{\mathbb{G}}(u) = 1 + \sum_{k=1}^{\Delta-1} \tilde{t}_k^{\mathbb{G}} u^k. \quad (2.4)$$

Finally, let  $\bar{t}_n(\Delta)$  be the number of subtrees of the  $\Delta$ -regular infinite tree which has  $n$  vertices, containing a fixed vertex, say  $v_0$ , identified as the root, and satisfies the following constraints.

- (i) The maximum number of subsets of descendants of  $v_0$  with fixed cardinality  $k$  (with  $1 \leq k \leq \Delta$ ) is  $t_k^{\mathbb{G}}$ .
- (ii) For any vertex  $v \neq v_0$ , the maximum number of subsets of descendants of  $v$  with fixed cardinality  $k$  (with  $1 \leq k \leq \Delta - 1$ ) is  $\tilde{t}_k^{\mathbb{G}}$ .

**Theorem 2.1.** *The chromatic polynomial of a finite graph  $\mathbb{G}$  of maximal degree  $\Delta$  is free of zeros for*

$$|q| \geq C_{\mathbb{G}}^*, \quad (2.5)$$

with

$$C_{\mathbb{G}}^* = \min_{a \geq 0} \inf \left\{ \kappa : \sum_{n=1}^{\infty} \bar{t}_n(\Delta) \left[ \frac{e^a}{\kappa} \right]^{n-1} \leq 2 - e^{-a} \right\} \quad (2.6)$$

$$= \min_{a > 0} e^a \frac{\tilde{Z}_{\mathbb{G}}(Z_{\mathbb{G}}^{-1}(2 - e^{-a}))}{Z_{\mathbb{G}}^{-1}(2 - e^{-a})} \quad (2.7)$$

$$= \min_{0 < x < Z_{\mathbb{G}}^{-1}(2)} \frac{\tilde{Z}_{\mathbb{G}}(x)}{[2 - Z_{\mathbb{G}}(x)]x}. \quad (2.8)$$

The numbers  $t_k^{\mathbb{G}}$  and  $\tilde{t}_k^{\mathbb{G}}$  depend on the graph structure. They depend on the presence of neighbours of a point that are themselves neighbours, that is, on the existence of triangle diagrams in the graph. In fact, they satisfy the inequalities

$$\Delta \delta_{k1} \leq t_k^{\mathbb{G}} \leq \binom{\Delta}{k}, \quad (\Delta - 1) \delta_{k1} \leq \tilde{t}_k^{\mathbb{G}} \leq \binom{\Delta - 1}{k}. \quad (2.9)$$

The lower bound ( $\delta_{k1} = 1$  if  $k = 1$  and zero otherwise) corresponds to the complete graph with  $\Delta + 1$  vertices. This is the graph with the largest possible number of triangle diagrams per vertex, and hence for which the improvement contained in the previous theorem is maximal. In this case,  $Z_{\mathbb{G}_{\text{cpl}}}(u) = 1 + \Delta u$ ,  $\tilde{Z}_{\mathbb{G}_{\text{cpl}}}(u) = 1 + (\Delta - 1)u$  and a straightforward calculation shows that

$$C_{\mathbb{G}_{\text{cpl}}}^* = \frac{(\Delta - 1)^2}{3\Delta - 1 - 2\sqrt{2\Delta^2 - \Delta}}. \quad (2.10)$$

We check that  $C_{\mathbb{G}_{\text{cpl}}}^*(\Delta)/\Delta$  is an increasing function of  $\Delta$  and

$$\frac{C_{\mathbb{G}_{\text{cpl}}}^*}{\Delta} \nearrow_{\Delta \rightarrow \infty} \frac{1}{3 - 2\sqrt{2}} \Delta \approx 5.83 \Delta. \quad (2.11)$$

The upper bounds in (2.9) corresponds to graphs with a triangle-free vertex of degree  $\Delta$ . It is simple to see, for instance from (2.6), that the use of these upper bounds yields a worst-scenario estimation for any graph. In this case  $Z_{\mathbb{G}}(u) = (1 + u)^{\Delta}$ ,  $\tilde{Z}_{\mathbb{G}}(u) = (1 + u)^{\Delta - 1}$  and  $\bar{t}_n(\Delta) = t_n(\Delta)$ . In this way, Theorem 2.1 yields the following corollary for general graphs with maximum degree  $\Delta$ .

**Corollary 2.2.** *The chromatic polynomial of a finite graph  $\mathbb{G} = (\mathbb{V}, \mathbb{E})$  of maximal degree  $\Delta$  is free of zeros for*

$$|q| \geq C^*(\Delta) \quad (2.12)$$

Table 1. Comparison of the different criteria for graphs of maximum degree  $\Delta$ . Each entry gives the value  $C_{\mathbb{G}}$  such that the chromatic polynomial is free of zeros for  $|q| > C_{\mathbb{G}}$ .

$\Delta$	General graph		Complete graph	
	[12]	(2.12)	(2.5)/(2.10)	exact
	13.23	10.72	9.90	2
3	21.14	17.57	15.75	3
4	29.08	24.44	21.58	4
6	44.98	38.24	33.24	6
any	$7.97\Delta$	$6.91\Delta$	$5.83\Delta$	$\Delta$

with

$$C^*(\Delta) = \min_{a \geq 0} \inf \left\{ \kappa : \sum_{n=1}^{\infty} t_n(\Delta) \left[ \frac{e^a}{\kappa} \right]^{n-1} \leq 2 - e^{-a} \right\} \quad (2.13)$$

$$= \min_{a > 0} \frac{e^a(2 - e^{-a})^{1-\frac{1}{\Delta}}}{(2 - e^{-a})^{\frac{1}{\Delta}} - 1} \quad (2.14)$$

$$= \min_{0 < x < 2^{\frac{1}{\Delta}} - 1} \frac{(1+x)^{\Delta-1}}{x[2 - (1+x)^{\Delta}]} \quad (2.15)$$

The equality of (2.13) and (2.14)/(2.15) is a generalization of Borgs' identity [1] connecting (1.8) with (1.9). In fact, the identity between (2.13) and (2.15) can be equally well applied to (1.7) just replacing the factor  $2 - e^{-a}$  with the factor  $1 + ae^{-a}$ . This yields the following alternative expression for Sokal's constant (1.7):

$$C(\Delta) = \min_{a > 0} \frac{e^a(1 + ae^{-a})^{1-\frac{1}{\Delta}}}{(1 + ae^{-a})^{\frac{1}{\Delta}} - 1}. \quad (2.16)$$

The function  $C^*(\Delta)/\Delta$  increases with  $\Delta$ ; thus, (2.12) implies the following rougher bound.

**Corollary 2.3.** *The chromatic polynomial of a finite graph  $\mathbb{G} = (\mathbb{V}, \mathbb{E})$  of maximal degree  $\Delta$  is free of zeros for*

$$|q| \geq K^* \Delta \quad (2.17)$$

with

$$K^* = \lim_{\Delta \rightarrow \infty} \frac{C^*(\Delta)}{\Delta} = \min_{a > 0} \frac{\exp\{a + \ln[2 - e^{-a}]\}}{\ln[2 - e^{-a}]} = \min_{1 < y < 2} \frac{y}{(2 - y) \ln y}. \quad (2.18)$$

The bound (2.17)–(2.18) is a strengthening of (1.11)–(1.8)/(1.9). For example, for  $y = 1.3702$  (that is,  $a \approx 0,46235$ ), we get  $K^* \leq 6.907\dots$

Table 1 presents some examples of the different estimations discussed in this paper.

### 3. Proofs

#### 3.1. The basic lemmas

Theorem 2.2 is an immediate consequence of the following three lemmas.

**Lemma 3.1.** *Consider the lattice gas with activities  $\{z_\gamma(q) : \gamma \subset \mathbb{V}\}$  described above. Then its cluster expansion converges if  $q > e\Delta$  and there exists  $a > 0$  such that*

$$\sum_{n \geq 2} e^{an} C_n^q \leq e^a - 1. \quad (3.1)$$

**Lemma 3.2.** *Consider the lattice gas with activities  $\{z_\gamma(q) : \gamma \subset V\}$  described above. The activities satisfy the bounds*

$$C_n^q \leq \left(\frac{1}{q}\right)^{n-1} \bar{t}_n(\Delta). \quad (3.2)$$

**Lemma 3.3.** *The formal power series*

$$\bar{T}(x) = \sum_{n=1}^{\infty} \bar{t}_n(\Delta) x^n \quad (3.3)$$

converges for all  $x \in [0, R)$ , where

$$R = \sup_{u \geq 0} \frac{u}{\tilde{Z}_G(u)}$$

and

$$\sup \left\{ 0 < x < R : \frac{1}{x} \bar{T}(x) \leq b \right\} = \frac{Z_G^{-1}(b)}{\tilde{Z}_G(Z_G^{-1}(b))}. \quad (3.4)$$

Condition (3.1) follows from general results on cluster expansions fully developed in [6]. For completeness, we present a simple direct proof in the sequel, which, like the work in [6], crucially depends on an identity due to Penrose [8]. The bound (3.2) is an improvement with respect to the bound (1.5) only for graphs with no triangle-free vertices. Finally, Lemma 3.3 is also a simplified version of the argument in [6].

Before turning to the proof of these lemmas we discuss some required notions of the theory of cluster expansions.

#### 3.2. Activities and polymer expansion

We start by summarizing the fundamental expressions. The reader can consult [12] for its derivation. The activities  $z_\gamma$  of the hard-core partition function  $\Xi_{\mathbb{G}}(q)$  depend on the graphs  $\mathbb{G}_\gamma = (\gamma, \mathbb{E}_\gamma)$ , obtained by restricting the original graph  $\mathbb{G}$  to the vertex set  $\gamma$  (that is,  $\mathbb{E}_\gamma = \{\{x, y\} \in \mathbb{E} : x \in \gamma \text{ and } y \in \gamma\}$ ). Hereafter, given graphs  $G' = (V_{G'}, E_{G'})$  and  $G = (V_G, E_G)$ , we say that  $G'$  is a subgraph of  $G$ , and we write  $G' \subset G$ , if  $V_{G'} \subset V_G$  and  $E_{G'} \subset E_G$ .

Let us denote

$$\mathcal{M}_{\mathbb{G}} = \{\gamma \subset \mathbb{V} : |\gamma| \geq 2, \mathbb{G}_\gamma \text{ connected}\} \quad (3.5)$$

(the set of *monomers*). Then,

$$\Xi_{\mathbb{G}}(q) = \sum_{n \geq 1} \sum_{\substack{\{\gamma_1, \dots, \gamma_n\} : \gamma_i \in \mathcal{M}_{\mathbb{G}} \\ \gamma_i \cap \gamma_j = \emptyset}} z_{\gamma_1}(q) \cdots z_{\gamma_n}(q) \quad (3.6)$$

with

$$z_{\gamma} = \frac{1}{q^{|\gamma|-1}} \sum_{\substack{G' \subset \mathbb{G}_{\gamma} : V_{G'} = \gamma \\ G' \text{ connected}}} (-1)^{|E_{G'}|}. \quad (3.7)$$

Note that the sums above run over all spanning subgraphs of  $\mathbb{G}_{\gamma}$ . The logarithm of this partition function leads to the cluster or polymer expansion for this model. For each ordered family  $(\gamma_1, \dots, \gamma_n)$  of monomers, let  $g(\gamma_1, \dots, \gamma_n)$  be the graph with vertex set  $V_{g(\gamma_1, \dots, \gamma_n)} = \{1, 2, \dots, n\}$  and edge set  $E_{g(\gamma_1, \dots, \gamma_n)} = \{\{i, j\} \subset V_{g(\gamma_1, \dots, \gamma_n)} : \gamma_i \cap \gamma_j \neq \emptyset\}$ . Further, we shall use the abbreviation  $I_n \doteq \{1, 2, \dots, n\}$ .

The hard-core lattice gas cluster expansion, or *Mayer series* (see, e.g., [11] or [3] and references therein), is the *formal series*

$$\Sigma_{\mathbb{G}}(q) = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1, \dots, \gamma_n) \in (\mathcal{M}_{\mathbb{G}})^n} \phi^T [g(\gamma_1, \dots, \gamma_n)] z_{\gamma_1}(q) \cdots z_{\gamma_n}(q), \quad (3.8)$$

with

$$\phi^T [g(\gamma_1, \dots, \gamma_n)] = \begin{cases} \sum_{\substack{G' \subset g(\gamma_1, \dots, \gamma_n) \\ G' \text{ connected}, V_{G'} = I_n}} (-1)^{|E_{G'}|} & \text{if } n \geq 2 \text{ and } g(\gamma_1, \dots, \gamma_n) \text{ connected,} \\ 1 & \text{if } n = 1, \\ 0 & \text{otherwise.} \end{cases} \quad (3.9)$$

We shall prove that under condition (3.1) this formal series converges absolutely. Then  $\Sigma_{\mathbb{G}}(q) = \ln \Xi_{\mathbb{G}}(q)$  is finite and the chromatic polynomial has no zeros.

### 3.3. Labelled trees and the Penrose identity

Expressions (3.7) and (3.9) suggest the study of

$$S_{\mathcal{G}} = \sum_{\substack{G' \subset \mathcal{G}, V_{G'} = I_n \\ G' \text{ connected}}} (-1)^{|E_{G'}|} \quad (3.10)$$

for a connected graph  $\mathcal{G}$  with vertex set  $V_{\mathcal{G}} = I_n$  and edge set  $E_{\mathcal{G}}$ . Penrose [8] produced a crucial identity relating  $S_{\mathcal{G}}$  to the cardinality of a certain subset of the set of all spanning trees of  $\mathcal{G}$ .

Let  $\mathcal{T}_{\mathcal{G}}$  be the family of all possible trees with vertex set  $I_n$  which are subgraphs of  $\mathcal{G}$ . In other words  $\mathcal{T}_{\mathcal{G}}$  is the set of spanning trees of  $\mathcal{G}$ . For any  $\tau \in \mathcal{T}_{\mathcal{G}}$  let us identify the vertex 1 as the *root* of  $\tau$ . So we regard the trees of  $\mathcal{T}_{\mathcal{G}}$  as always rooted in the vertex 1.

Let  $\tau \in \mathcal{T}_{\mathcal{G}}$  with edge set  $E_{\tau}$  and, of course, vertex set  $V_{\tau} = V_{\mathcal{G}} = \{1, \dots, n\}$ . For each vertex  $i \in V_{\tau}$ , let  $d_{\tau}(i)$  be the tree distance of the vertex  $i$  to the root 1, and let  $i'_{\tau} \in V_{\tau}$  be the unique vertex such that  $\{i'_{\tau}, i\} \in E_{\tau}$  and  $d(i'_{\tau}) = d(i) - 1$ . The vertex  $i'_{\tau}$  is called the predecessor of  $i$  and

conversely  $i$  is called the descendant of  $i'_\tau$ . The number  $d_\tau(i)$  is called the *generation number* of the vertex  $i$ .

Now let  $p$  be the map that associates to each tree  $\tau \in \mathcal{T}_\mathcal{G}$  the graph  $p(\tau) \subset \mathcal{G}$  with vertex set  $I_n$  formed by adding (only once) to  $\tau$  all edges  $\{i, j\} \in E_\mathcal{G} \setminus E_\tau$ , such that either

(p1)  $d_\tau(i) = d_\tau(j)$  (edges between vertices of the same generation), or

(p2)  $d_\tau(j) = d_\tau(i) - 1$  and  $j > i'_\tau$  (edges between vertices with generations differing by one).

Then the set  $\mathcal{P}_\mathcal{G} \subset \mathcal{T}_\mathcal{G}$  of *Penrose trees* is defined by

$$\mathcal{P}_\mathcal{G} = \{\tau \in \mathcal{T}_\mathcal{G} : p(\tau) = \tau\}. \quad (3.11)$$

Thus, a tree  $\tau \in \mathcal{T}_\mathcal{G}$  is a Penrose tree, *i.e.*,  $\tau \in \mathcal{P}_\mathcal{G}$ , if and only if the following two conditions are both satisfied.

(t1) If two vertices  $i$  and  $j$  of  $\tau$  have the same generation number (*i.e.*,  $d_\tau(i) = d_\tau(j)$ ), then  $\{i, j\} \notin E_\mathcal{G}$ .

(t2) If two vertices  $i$  and  $j$  of  $\tau$  are such that  $d_\tau(j) = d_\tau(i) - 1$  and  $j > i'_\tau$ , then  $\{i, j\} \notin E_\mathcal{G}$ .

The Penrose identity simply says that

$$\mathcal{S}_\mathcal{G} = (-1)^{|V_\mathcal{G}|-1} |\mathcal{P}_\mathcal{G}|. \quad (3.12)$$

So, by (3.12),  $|\mathcal{S}_\mathcal{G}|$  is just the cardinality of the set of Penrose trees of  $\mathcal{G}$ , and, since  $\mathcal{P}_\mathcal{G} \subset \mathcal{T}_\mathcal{G}$ , we obtain immediately the well-known bound

$$|\mathcal{S}_\mathcal{G}| \leq |\overline{\mathcal{T}}_\mathcal{G}|. \quad (3.13)$$

Inequality (3.13) is the so-called tree-graph bound which, *e.g.*, easily implies the bound (1.5).

To obtain our new estimates in Lemmas 3.1–3.4, it is crucial to derive a new and improved bound on the factor  $|\mathcal{S}_\mathcal{G}|$  (inequality (3.14) below). For that, we consider another family of spanning trees  $\tau$  of  $\mathcal{G}$ , which is larger than  $\mathcal{P}_\mathcal{G}$  but smaller than  $\mathcal{T}_\mathcal{G}$ . The definition of such an intermediate family is obtained from the definition of  $\mathcal{P}_\mathcal{G}$  above by ignoring condition (t2) and keeping only the part of condition (t1) referring to descendants of the same predecessor. That is, let us define the subset  $\overline{\mathcal{P}}_\mathcal{G}$  of  $\mathcal{T}_\mathcal{G}$  formed by all *weakly Penrose trees* of  $\mathcal{G}$  as follows. A tree  $\tau \in \mathcal{T}_\mathcal{G}$  is a weakly Penrose tree, *i.e.*,  $\tau \in \overline{\mathcal{P}}_\mathcal{G}$  if and only if the following condition is satisfied.

( $\bar{t}1$ ) If two vertices  $i$  and  $j$  of  $\tau$  are descendants of the same predecessor (*i.e.*,  $i'_\tau = j'_\tau$ ), then  $\{i, j\} \notin E_\mathcal{G}$ .

Note that (t1) implies ( $\bar{t}1$ ), since any two vertices  $i$  and  $j$  in a tree  $\tau$  which are descendants of the same predecessor have the same generation number. In conclusion, given these definitions we have  $\mathcal{P}_\mathcal{G} \subset \overline{\mathcal{P}}_\mathcal{G} \subset \mathcal{T}_\mathcal{G}$ , and thus

$$\begin{aligned} |\mathcal{S}_\mathcal{G}| &\leq |\overline{\mathcal{P}}_\mathcal{G}| \\ &\leq |\mathcal{T}_\mathcal{G}|. \end{aligned} \quad (3.14)$$

### 3.4. Proof of Lemma 3.1

Let us denote  $\rho_\gamma = |z_\gamma|$ . We shall prove that if (3.1) is satisfied, the series of absolute values

$$\Sigma_{\mathbb{G}}^*(q) = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1, \dots, \gamma_n) \in (\mathcal{M}_{\mathbb{G}})^n} |\phi^T[g_{\{\gamma_1, \dots, \gamma_n\}}]| \rho_{\gamma_1} \cdots \rho_{\gamma_n} \quad (3.15)$$



is finite. Let us denote the  $n$ th term of the sum by  $B_n$ . We see that

$$B_1 = \sum_{\gamma \in \mathcal{M}_{\mathbb{G}}} \rho_{\gamma} \leq |\mathbb{V}| \sup_{x \in \mathbb{V}} \sum_{\substack{\gamma \in \mathcal{M}_{\mathbb{G}} \\ \gamma \ni x}} \rho_{\gamma} = |\mathbb{V}| \sum_{s \geq 2} C_s^q. \quad (3.16)$$

Let us bound  $B_n$ ,  $n \geq 2$ . Given (3.9) and the Penrose identity (3.12),

$$B_n = \frac{1}{n!} \sum_{\tau \in \mathcal{T}_n} w(\tau) \quad (3.17)$$

with

$$w(\tau) = \sum_{\substack{(\gamma_1, \dots, \gamma_n) \in (\mathcal{M}_{\mathbb{G}})^n \\ \tau \in \overline{\mathcal{P}}_{g(\gamma_1, \dots, \gamma_n)}}} \rho_{\gamma_1} \cdots \rho_{\gamma_n}. \quad (3.18)$$

Using in the sum the weaker condition  $\tau \in \overline{\mathcal{P}}_{g(\gamma_1, \dots, \gamma_n)}$ , we obtain the bound

$$w(\tau) \leq \overline{w}(\tau) := \sum_{\substack{(\gamma_1, \dots, \gamma_n) \in (\mathcal{M}_{\mathbb{G}})^n \\ \tau \in \overline{\mathcal{P}}_{g(\gamma_1, \dots, \gamma_n)}}} \rho_{\gamma_1} \cdots \rho_{\gamma_n}. \quad (3.19)$$

It is clear that, in the sum on the last right-hand side, no two monomers labelling descendants of the same vertex can intersect. We now estimate  $\overline{w}(\tau)$ . For each  $\tau \in \mathcal{T}_n$ , let us denote the coordination numbers (degree, incidence number) of its vertices by  $d_1, \dots, d_n$ . Each  $d_i$  is the number of links having vertex  $i$  at one endpoint (thus  $d_i - 1$  is the number of descendants of  $i$ );  $1 \leq d_i \leq n - 1$  and  $\sum_{i=1}^n d_i = 2n - 2$ . Then we have the following result.

**Lemma 3.4.** *For each  $\tau \in \mathcal{T}_n$ ,*

$$\overline{w}(\tau) \leq \sum_{\substack{\gamma_1 \in \mathcal{M}_{\mathbb{V}} \\ |\gamma_1| \geq d_1}} \binom{|\gamma_1|}{d_1} d_1! \rho_{\gamma_1} \prod_{i=2}^n \left[ \sup_x \sum_{\substack{\gamma_i \in \mathcal{M}_{\mathbb{V}}, \gamma_i \ni x \\ |\gamma_i| \geq d_i - 1}} \binom{|\gamma_i|}{d_i - 1} (d_i - 1)! \rho_{\gamma_i} \right]. \quad (3.20)$$

**Proof.** The proof follows the strategy introduced in [3]. The tree is successively ‘defoliated’ by summing over the labels of the leaves; this produces some of the factors on the right-hand side of (3.20) times the weight of a smaller tree. While the idea is simple, its inductive formalization requires some notation. Let us partition  $\{1, \dots, n\} = I_0 \cup I_1 \cup \dots \cup I_r$ , where  $I_i$  is the family of vertices of the  $i$ th generation and  $r$  is the maximal generation number in  $\tau$ . Recall that the unique vertex of  $\tau$  of the zero generation is by definition the root, so we have  $I_0 = \{1\}$ .

We also introduce the ‘inflated’ activities

$$\tilde{\rho}_{\gamma_i} = \rho_{\gamma_i} \binom{|\gamma_i|}{\ell_i} \ell_i! \mathbf{1}_{\{|\gamma_i| \geq \ell_i\}}, \quad (3.21)$$

where  $\ell_i$  is the number of descendants of the vertex  $i$ , namely  $\ell_1 = d_1$  and  $\ell_i = d_i - 1$  if  $i > 1$ . The inductive argument applies to the following expression, which is obtained by reordering the

sum in (3.19):

$$\begin{aligned} \bar{w}(\tau) = & \sum_{\gamma_{I_0} \in (\mathcal{M}_{\mathbb{G}})^{|I_0|}} \rho_{\gamma_{I_0}} \sum_{\gamma_{I_1} \in (\mathcal{M}_{\mathbb{G}})^{|I_1|}} C(\gamma_{I_0}, \gamma_{I_1}) \rho_{\gamma_{I_2}} \\ & \cdots \sum_{\gamma_{I_{r-1}} \in (\mathcal{M}_{\mathbb{G}})^{|I_{r-1}|}} C(\gamma_{I_{r-2}}, \gamma_{I_{r-1}}) \rho_{\gamma_{I_{r-1}}} \sum_{\gamma_{I_r} \in (\mathcal{M}_{\mathbb{G}})^{|I_r|}} C(\gamma_{I_{r-1}}, \gamma_{I_r}) \tilde{\rho}_{\gamma_{I_r}}. \end{aligned} \quad (3.22)$$

We let  $\gamma_{I_k} = (\gamma_j)_{j \in I_k}$  and  $\rho_{\gamma_{I_k}} = \prod_{j \in I_k} \rho_{\gamma_j}$ . At this initial step of the argument, the tilde in the activities of the last generation is for free because it involves leaves, *i.e.*, vertices with  $\ell_i = 0$ . The factors  $C(\gamma_{I_{k-1}}, \gamma_{I_k})$  embody condition (i1), which relates only consecutive generations. To write them in detail we further partition each  $I_k$  according to predecessors. If we decompose  $I_r = \cup_{i \in I_{r-1}} I_r^{(i)}$ , with  $I_r^{(i)}$  being the family of  $\ell_i$  descendants of  $i$ , we have

$$C(\gamma_{I_{r-1}}, \gamma_{I_r}) = \prod_{i \in I_{r-1}} \left[ \prod_{1 \leq j \leq \ell_i} \mathbb{1}_{\{\gamma_i \cap \gamma_{i_j} \neq \emptyset\}} \right] \left[ \prod_{1 \leq j < k \leq \ell_i} \mathbb{1}_{\{\gamma_{i_j} \cap \gamma_{i_k} = \emptyset\}} \right], \quad (3.23)$$

where  $i_1, \dots, i_{\ell_i}$  denotes the descendants of  $i$ .

To trigger the induction, we perform the last sum in (3.22):

$$\sum_{\gamma_{I_r} \in (\mathcal{M}_{\mathbb{G}})^{|I_r|}} C(\gamma_{I_{r-1}}, \gamma_{I_r}) \tilde{\rho}_{\gamma_{I_r}} = \prod_{i \in I_{r-1}} \left[ \sum_{\substack{(\gamma_{i_1}, \dots, \gamma_{i_{\ell_i}}) \in (\mathcal{M}_{\mathbb{G}})^{\ell_i} \\ \gamma_{i_j} \cap \gamma_{i_k} \neq \emptyset, \gamma_{i_j} \cap \gamma_{i_k} = \emptyset}} \tilde{\rho}_{\gamma_{i_1}} \cdots \tilde{\rho}_{\gamma_{i_{\ell_i}}} \right]. \quad (3.24)$$

As the sets  $\gamma_{i_j}$  are disjoint, they must intersect  $\gamma_i$  at  $\ell_i$  *different* points. These points can be chosen in  $|\gamma_i|(|\gamma_i| - 1) \cdots (|\gamma_i| - \ell_i + 1)$  ways. Therefore

$$\sum_{\gamma_{I_r} \in (\mathcal{M}_{\mathbb{G}})^{|I_r|}} C(\gamma_{I_{r-1}}, \gamma_{I_r}) \tilde{\rho}_{\gamma_{I_r}} \leq \prod_{i \in I_{r-1}} \left[ \binom{|\gamma_i|}{\ell_i} \ell_i! \mathbb{1}_{\{|\gamma_i| \geq \ell_i\}} \prod_{1 \leq j \leq \ell_i} \left[ \sup_{x \in \mathbb{V}} \sum_{\substack{\gamma_{i_j} \in \mathcal{M}_{\mathbb{G}} \\ \gamma_{i_j} \ni x}} \tilde{\rho}_{\gamma_{i_j}} \right] \right] \quad (3.25)$$

and

$$\rho_{\gamma_{I_{r-1}}} \sum_{\gamma_{I_r} \in (\mathcal{M}_{\mathbb{G}})^{|I_r|}} C(\gamma_{I_{r-1}}, \gamma_{I_r}) \tilde{\rho}_{\gamma_{I_r}} \leq \left[ \prod_{i \in I_{r-1}} \tilde{\rho}_i \right] \prod_{j \in I_r} \left[ \sup_{x \in \mathbb{V}} \sum_{\substack{\gamma_{i_j} \in \mathcal{M}_{\mathbb{G}} \\ \gamma_{i_j} \ni x}} \tilde{\rho}_{\gamma_{i_j}} \right]. \quad (3.26)$$

Applying this inequality to (3.22), we obtain

$$\bar{w}(\tau) \leq \left[ \sum_{\gamma_{I_0} \in (\mathcal{M}_{\mathbb{G}})^{|I_0|}} \rho_{\gamma_{I_0}} \cdots \sum_{\gamma_{I_{r-1}} \in (\mathcal{M}_{\mathbb{G}})^{|I_{r-1}|}} C(\gamma_{I_{r-2}}, \gamma_{I_{r-1}}) \tilde{\rho}_{\gamma_{I_{r-1}}} \right] \prod_{j \in I_r} \left[ \sup_{x \in \mathbb{V}} \sum_{\substack{\gamma_j \in \mathcal{M}_{\mathbb{G}} \\ \gamma_j \ni x}} \tilde{\rho}_{\gamma_j} \right]. \quad (3.27)$$

The first square bracket has exactly the form of the right-hand side of (3.22) but involving one less generation. Inductively we therefore obtain

$$\bar{w}(\tau) \leq \sum_{\gamma_{l_0} \in (\mathcal{M}_{\mathbb{G}})^{l_0}} \tilde{\rho}_{\gamma_{l_0}} \prod_{1 \leq k \leq r} \prod_{j_k \in I_k} \left[ \sup_{x \in \mathbb{V}} \sum_{\substack{\gamma_{j_k} \in \mathcal{M}_{\mathbb{G}} \\ \gamma_{j_k} \ni x}} \tilde{\rho}_{\gamma_{j_k}} \right]. \quad (3.28)$$

This is precisely the bound (3.20).  $\square$

The bound provided by the preceding lemma is only a function of the coordination numbers  $d_1, \dots, d_n$  of  $\tau$ . Thus, in (3.17) we can combine it with Cayley's formula, which states that the number of trees with such coordination numbers is  $\binom{n-2}{d_1-1 \dots d_n-1}$ , to obtain

$$B_n \leq \frac{|\mathbb{V}|}{n(n-1)} \sum_{\substack{d_1, \dots, d_n \geq 1 \\ \sum d_i = 2n-2}} d_1 F(d_1) \prod_{i=2}^n F(d_i - 1), \quad (3.29)$$

with

$$F(\ell) = \sup_x \sum_{\substack{\gamma \in \mathcal{M}_{\mathbb{G}}, \gamma \ni x \\ |\gamma| \geq \ell}} \binom{|\gamma|}{\ell} \ell! \rho_\gamma. \quad (3.30)$$

To benefit somehow from the restriction  $\sum d_i = 2n - 2$ , we resort to a trick used in [9], which consists in multiplying and dividing by  $\alpha^{n-1} = \alpha^{d_1+(d_2-1)+\dots+(d_n-1)}$ , where  $\alpha > 0$  is left arbitrary:

$$B_n \leq \frac{|\mathbb{V}|}{n(n-1)\alpha^{n-1}} \sum_{d_i \geq 1} d_1 F(d_1) \alpha^{d_1} \prod_{i=2}^n \left[ \sum_{d_i \geq 1} F(d_i - 1) \alpha^{d_i-1} \right]. \quad (3.31)$$

We compute the sums in terms of  $C_n^q$  (recall that  $|\gamma| \geq 2$  if  $\gamma \in \mathcal{M}_{\mathbb{G}}$ ):

$$\begin{aligned} \sum_{d_i \geq 1} F(d_i - 1) \alpha^{d_i-1} &= \sum_{s_i \geq 2} C_{s_i}^q \sum_{0 \leq d_i-1 \leq s_i} \binom{s_i}{d_i-1} \alpha^{d_i-1} \\ &= \sum_{s_i \geq 2} C_{s_i}^q (1 + \alpha)^{s_i}. \end{aligned} \quad (3.32)$$

Likewise

$$\begin{aligned} \sum_{d_1 \geq 1} d_1 F(d_1) \alpha^{d_1} &= \sum_{s_1 \geq 2} C_{s_1}^q \sum_{0 \leq d_1 \leq s_1} \binom{s_1}{d_1} \alpha^{d_1} \\ &= \sum_{s_1 \geq 2} C_{s_1}^q \alpha s_1 (1 + \alpha)^{s_1-1}. \end{aligned} \quad (3.33)$$

Finally,

$$B_n \leq \frac{|\mathbb{V}| \alpha}{n(n-1)} \left[ \sum_{s \geq 2} s (1 + \alpha)^{s-1} C_s^q \right] \left[ \frac{1}{\alpha} \sum_{s \geq 2} (1 + \alpha)^s C_s^q \right]^{n-1}. \quad (3.34)$$

Thus, if

$$\frac{1}{\alpha} \sum_{s \geq 2} (1 + \alpha)^s C_s^q \leq 1, \quad (3.35)$$

we have, from (3.16) and (3.34),

$$\Sigma_{\mathbb{G}}^*(q) = \sum_{n \geq 1} B_n \leq |\mathbb{V}| \sum_{s \geq 2} C_s^q \left[ 1 + \alpha s (1 + \alpha)^{s-1} \sum_{n \geq 2} \frac{1}{n(n-1)} \right], \quad (3.36)$$

which is finite, if  $q > e\Delta$ , because of the bound (1.12). Condition (3.35) is, in fact, identical to (3.1) under the relabelling  $1 + \alpha = e^a$ .

### 3.5. Proof of Lemma 3.2

We combine (3.7) with the bound (3.14) to obtain

$$\sup_{v_0 \in \mathbb{V}} \sum_{\substack{\gamma \in \mathcal{M}_{\mathbb{G}}: v_0 \in \gamma \\ |\gamma| = n}} |z_{\gamma}(q)| \leq \frac{1}{q^{n-1}} \sup_{v_0 \in \mathbb{V}} \sum_{\substack{\gamma \in \mathcal{M}_{\mathbb{G}}: v_0 \in \gamma \\ \mathbb{G}_{\gamma} \text{ connected}}} |\overline{\mathcal{P}}_{\mathbb{G}_{\gamma}}| \leq \frac{1}{q^{n-1}} \bar{t}_n(\Delta). \quad (3.37)$$

### 3.6. Proof of Lemma 3.3

Let  $U_{v_0}(\Delta)$  be the infinite tree in which all vertices have degree  $\Delta$  except for the vertex  $v_0$ , identified as the root, which has degree  $\Delta - 1$  (so that each vertex  $v \in U_{v_0}(\Delta)$ , including the root, has  $\Delta - 1$  descendants). Let  $\bar{u}_n(\Delta)$  be the number of subtrees in  $U_{v_0}(\Delta)$  which have  $n$  vertices, contain the root  $v_0$ , and such that, for any vertex  $v$  of  $U_{v_0}(\Delta)$  and any  $k \leq \Delta - 1$ , the number  $\bar{t}_k^G$  defined in (2.2) is the maximum number of subsets of  $k$  descendants of  $v$  with fixed cardinality  $k$ . Define the formal power series

$$\bar{U}(x) = \sum_{n=1}^{\infty} \bar{u}_n(\Delta) x^n. \quad (3.38)$$

From the recursive structure of  $(\Delta - 1)$ -regular rooted trees, we deduce that  $\bar{U}(x)$  obeys the equations

$$\bar{U} = x \tilde{Z}_{\mathbb{G}}(\bar{U}) = \psi_x(\bar{U}) \quad (3.39)$$

and, recalling the definitions (2.3), (2.4), we also have that the formal series  $\bar{T}(x)$  defined in (3.3) is related to  $\bar{U}$  by

$$\bar{T} = x Z_{\mathbb{G}}(\bar{U}). \quad (3.40)$$

The function

$$f(u) = \frac{u}{\tilde{Z}_{\mathbb{G}}(u)} \quad (3.41)$$

is zero for  $u = 0$ , increases until a point  $u_0 \in [0, \infty]$ , where it attains its maximum, and then decreases monotonically to zero in the interval  $(u_0, \infty)$ . So  $f$  is a bijection from  $[0, u_0]$  to  $[0, R = f(u_0)]$ , with

$$R = \sup_{u \geq 0} \frac{u}{\tilde{Z}_{\mathbb{G}}(u)}. \quad (3.42)$$

The function  $\psi_x(\bar{U})$  defined in (3.39), on the other hand, can be visualized as a sum over single-generation trees where the root, labelled by  $x$ , is followed by up to  $\Delta - 1$  descendants labelled by  $\bar{U}$ . Hence, its  $M$ th iteration,  $\psi_x^M(\bar{U})$ , corresponds to a sum over a set of  $M$ -generation trees where all vertices are labelled by  $x$  except those of the  $M$ th generation, which are labelled by  $\bar{U}$ . Applying this argument to  $\bar{U} = u \in [0, u_0]$  and  $x = f(u) \in [0, R]$ , we have that

$$\sum_{n=1}^M \bar{u}_n(\Delta) x^n \leq \psi_x^{M+1}(u) = u. \tag{3.43}$$

We conclude that the positive series  $\bar{U}(x) = \sum_{n=1}^{\infty} \bar{u}_n(\Delta) x^n$  converges for all  $x \in (0, R)$ , and furthermore

$$\bar{U}^{-1}(u) = f(u) \quad \text{for } u \in [0, u_0].$$

It follows that the positive series  $\bar{T}(x) = \sum_{n=1}^{\infty} \bar{t}_n(\Delta) x^n$  converges in the same interval, since  $xZ_G(u) \leq x(1+u)\tilde{Z}_G(u) = u + u^2$  for all  $u \in [0, u_0]$ .

Finally, we argue:

$$\sup \left\{ 0 < x < R : \frac{1}{x} \bar{T}(x) \leq b \right\} = \sup \{ 0 < x < R : Z_G(\bar{U}(x)) \leq b \} \tag{3.44}$$

$$= \sup \{ 0 < x < R : x \leq f(Z_G^{-1}(b)) \} \tag{3.45}$$

$$= \sup \left\{ 0 < x < R : x \leq \frac{Z_G^{-1}(b)}{\tilde{Z}_G(Z_G^{-1}(b))} \right\} \tag{3.46}$$

$$= \frac{Z_G^{-1}(b)}{\tilde{Z}_G(Z_G^{-1}(b))}. \tag{3.47}$$

□

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