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The Institute of Mathematics, Physics and Mechanics
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The Petra Šparl Award 2022

The Petra Šparl Award was established in 2017 to recognise in each even-numbered year the best paper published in the previous five years by a young woman mathematician in one of the two journals *Ars Mathematica Contemporanea* (AMC) and *The Art of Discrete and Applied Mathematics* (ADAM). It was named after Dr Petra Šparl, a talented woman mathematician who died mid-career in 2016 after a battle with cancer.

The first award was made in 2018 to Dr Monika Pilśniak (AGH University, Poland), for a paper she published in *AMC* **13** (2017) on the distinguishing index of graphs, and then in 2020 two awards were made: one to Dr Simona Bonvicini (Università di Modena e Reggio Emilia, Italy), for her contributions to a paper in *AMC* **14** (2018) on solutions of some Hamilton-Waterloo problems, and one to Dr Klavdija Kutnar (University of Primorska, Slovenia) for her contributions to a paper in *AMC* **10** (2016) on odd automorphisms in vertex-transitive graphs.

Nominations for the 2022 award were invited in 2021, and all cases were considered by a committee (consisting of the three of us, listed below). There were just five nominations, and as in previous rounds we considered the nomination statements, comments by co-authors, reports from referees, and the papers themselves, before making a decision.

This time one nomination stood out from the others, and led to our selection of the winner of the Petra Šparl Award for 2022 as Dr **Jelena Sedlar** (of the University of Split, Croatia), for her single-author paper 'On Wiener inverse interval problem of trees', published in *Ars Mathematica Contemporanea* **15** (2018) 19–37.

In this paper the candidate resolved two open conjectures posed in the literature regarding the Wiener index of trees, which are of considerable interest in mathematical chemistry. It was already known that for connected graphs on n vertices, this index could take at least $\frac{n^3}{6} + O(n^2)$ consecutive integer values, and the conjectures concerned the values of the Wiener index for trees on n vertices, essentially stating that the Wiener index could take almost all values between the minimum and maximum. Dr Sedlar verified and improved both of these conjectures for the case where n is even, and also proved a corrected version of them for the case when n is odd, using a clever construction that recursively increases the value of the Wiener index by 4.

As judges we agreed with the nominator and referee that the candidate's work in this paper was mathematically both very elegant and very intricate, reflecting her mathematical prowess.

We heartily congratulate Dr Sedlar, who will be awarded a certificate and invited to give a lecture in the Mathematics Colloquium at the University of Primorska, and to give lectures at the University of Maribor and the University of Ljubljana.

Finally, we encourage nominations for the next Petra Šparl Award in 2024, as well as submissions of high quality new papers that will be worthy of consideration for future awards.

Marston Conder, Asia Ivić Weiss and Aleksander Malnič
Members of the *2022 Petra Šparl Award Committee*

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The Sierpiński product of graphs*

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Dedicated to Professor Wilfried Imrich on the occasion of his 80th birthday.

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Abstract

In this paper we introduce a product-like operation that generalizes the construction of the generalized Sierpiński graphs. Let G, H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then the *Sierpiński product of graphs* G *and* H *with respect to* f, denoted by $G \otimes_f H$, is defined as the graph on the vertex set $V(G) \times V(H)$, consisting of $|V(G)|$

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copies of H; for every edge $\{g, g'\}$ of G there is an edge between copies gH and $g'H$ of form $\{(g, f(g'), (g', f(g))\}$.

Some basic properties of the Sierpiński product are presented. In particular, we show that the graph $G \otimes_f H$ is connected if and only if both graphs G and H are connected and we present some conditions that G, H must fulfill for $G \otimes_f H$ to be planar. As for symmetry properties, we show which automorphisms of G and H extend to automorphisms of $G \otimes_f H$. In several cases we can also describe the whole automorphism group of the graph $G \otimes_f H$.

Finally, we show how to extend the Sierpiński product to multiple factors in a natural way. By applying this operation n times to the same graph we obtain an alternative approach to the well-known n-th generalized Sierpiński graph.

Keywords: Sierpiński graphs, graph products, connectivity, planarity, symmetry.

Math. Subj. Class. (2020): 05C76, 05C10, 05C40, 20B25

1 Introduction

The motivation for this paper is the study of Sierpiński graphs and their generalizations. Although the body of this work is essentially self contained, a few remarks about the role of Sierpiński graphs seem to be appropriate. The family of *Sierpiński graphs* S_p^n was first introduced by Klavžar and Milutinović in [16] as a variant of the Tower of Hanoi problem. The Sierpiński graphs can be defined recursively as follows: S_p^1 is isomorphic to the complete graph K_p and S_p^{n+1} is constructed from p copies of S_p^n by adding exactly one edge between every pair of copies of S_p^{n+1} in a well-defined manner. The Sierpiński graphs S_3^1, S_3^2, and S_3^3 are depicted in Figure 1. In the "classical" case, when $p = 3$, the Sierpiński graphs are isomorphic to the Hanoi graphs. More about Sierpiński graphs and their connections to the Hanoi graphs can be found in the recent second edition of the book about the Tower of Hanoi puzzle by Hinz et al. [10].

Sierpiński graphs have been extensively studied in most graph-theoretical aspects as well as in other areas of mathematics and even psychology. Some notable papers are [11, 13, 15, 17, 18, 22, 26, 27]. An extensive summary of topics studied on and around Sierpiński graphs is available in the survey paper by Hinz, Klavžar and Zemljič [12]. In that paper the authors introduced *Sierpiński-type graphs* as graphs that are derived from or lead to the Sierpiński triangle fractal.

These families of graphs have been generalized by Gravier, Kovše and Parreau to a family called *generalized Sierpiński graphs* [8]. Instead of the complete graph, an arbitrary graph G is used as a base graph to form a self-similar graph in the same way as the Sierpiński graphs are derived from the complete graph: the generalized Sierpiński graph S_G^1 is isomorphic to the graph G. To construct the n-th iteration generalized Sierpiński graph S_G^n for $n > 1$, take $|V(G)|$ copies of S_G^{n-1} and add to the labels of vertices in copy x of S_G^{n-1} the letter x at the beginning. Then, for any edge $\{x, y\}$ of G, add an edge between the vertex $xy \dots y$ and the vertex $yx \dots x$. See Figure 2 for an example of the second iteration generalized Sierpiński graph, where the base graph is the house graph, i.e. the cycle on five vertices with a chord.

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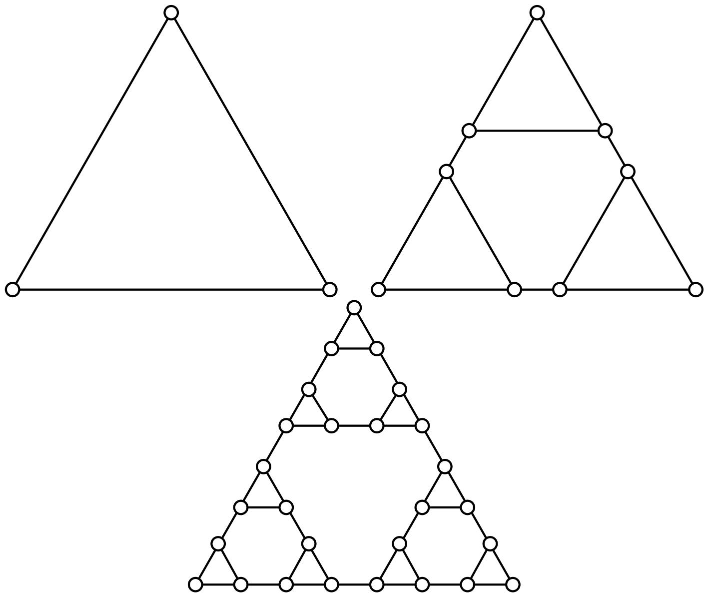

Figure 1: The Sierpiński graphs S_3^1, S_3^2, and S_3^3.

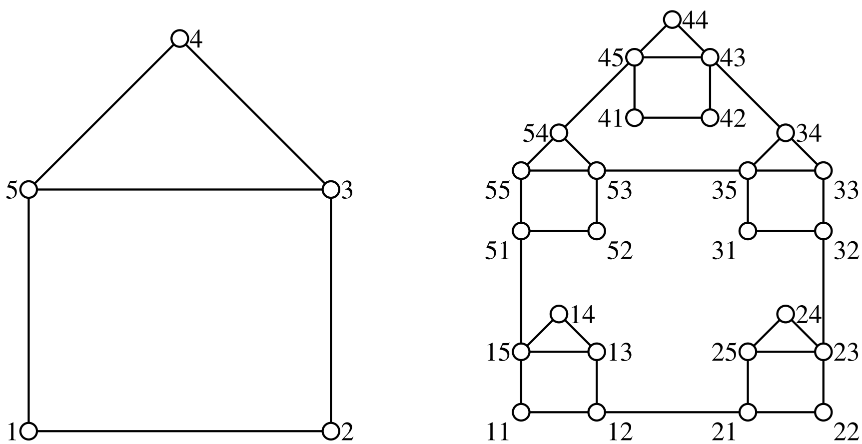

Figure 2: The generalized Sierpiński graphs S_G^1 and S_G^2 when G is the house graph.

The generalized Sierpiński graphs have been extensively studied in the past few years on topics including chromatic number, Randić index, vertex cover number, clique number, domination number and metric properties; see, for example, [5, 7, 24, 25].

At this point we would like to mention another approach towards the Sierpiński graphs. The graphs S_3^n appear naturally as subgraphs of repeated truncations of cubic graphs. More generally, by applying truncation to a p-valent vertex of a graph n times, i.e. by replacing each p-valent vertex of the graph by the complete graph K_p repeatedly, the corresponding part of the obtained graph looks like S_p^n; see Pisanski and Tucker [23] and Alspach and Dobson [1]. The truncation operation on graphs has been generalized in several ways; see Boben, Jajcay and Pisanski [2] and Exoo and Jajcay [6]. In [4], Eiben, Jajcay and Šparl study automorphisms of generalized truncations. These constructions show significant similarities to our construction, although they are distinct in general. A related construction, called the *clone cover*, is considered by Malnič, Pisanski and Žitnik in [20].

In this paper we generalize the generalized Sierpiński graphs even further. Notice that S_G^n can be viewed as an operation of S_G^{n-1} and G. This was a motivation for our introduction of the *Sierpiński product* of graphs. If we take any two graphs G and H, the resulting product locally has the structure of H, but globally it is similar to G. The formal definition of the Sierpiński product is given in Section 2.

The Sierpiński product shows some features of classical graph products, for instance the vertex set of the Sierpiński product of two graphs G and H is $V(G) \times V(H)$. However, to define the Sierpiński product of two graphs G and H, one needs some extra information besides G and H. This information can be encoded as a function $f\colon V(G) \to V(H)$. Furthermore, the product is defined so that we can extend it to multiple factors. We will see that by definition the Sierpiński product of two graphs is always a subgraph of their lexicographic product. Such layer-like structure also plays an important role in studying symmetries of the Sierpiński product. For extensive information about graph products, see the monograph by Hammack, Imrich and Klavžar [9].

The paper is organized as follows. In Section 2 we give a formal definition of the Sierpiński product of two graphs G and H with respect to $f\colon V(G) \to V(H)$; this product is denoted by $G \otimes_f H$. We explore some graph-theoretical properties such as connectedness and planarity of a Sierpiński product. In particular, we show that $G \otimes_f H$ is connected if and only if both G and H are connected and we present some necessary and sufficient conditions that G and H must fulfill in order for $G \otimes_f H$ to be planar. In Section 3 we study symmetries of the Sierpiński product of two graphs. We focus on the automorphisms of $G \otimes_f H$ that arise from the automorphisms of its factors and study the group generated by these automorphisms. In several cases we can also describe the whole automorphism group of $G \otimes_f H$. Finally, in Section 4 we consider the Sierpiński product of more than two graphs. A special case of n equal factors is considered.

2 Definition of the Sierpiński product and basic properties

Let us first review some necessary notions. All the graphs we consider are undirected, simple and finite. Let G be a graph and x be a vertex of G. By $N(x)$ we denote the set of vertices of G that are adjacent to x, i.e. the neighbourhood of x. Vertices in this paper will usually be tuples, but instead of writing them in vector form $(x_m, \dots, x_1)$, we will sometimes write them as words $x_m \dots x_1$ (especially in figures). More precisely, vertices $(0, 0, 0)$ or $(0, (0, 0))$ will simply be denoted by 000, except in the case when we will want to emphasize their origins. The number of vertices of a graph G, i.e. the order of G, will be denoted by $|G|$, and the number of edges of G, i.e. the size of G, will be denoted by $||G||$. For other graph theory concepts not defined here we refer the reader to [21].

Definition 2.1. Let G, H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then the *Sierpiński product of the graphs G and H with respect to f*, denoted by $G \otimes_f H$, is defined as the graph on the vertex set $V(G) \times V(H)$ with two types of edges:

- $\{(g, h), (g, h')\}$ is an edge of $G \otimes_f H$ for every vertex $g \in V(G)$ and every edge $\{h, h'\} \in E(H)$,
- $\{(g, f(g')), (g', f(g))\}$ is an edge of $G \otimes_f H$ for every edge $\{g, g'\} \in E(G)$.

If $V(G) \subseteq V(H)$ and f is the identity function on its domain, we will skip the index f and denote the corresponding Sierpiński product of G and H simply by $G \otimes H$. Note that there are no restrictions on the function $f\colon V(G) \to V(H)$. However, sometimes it is convenient to assume that for every $g, g_1, g_2 \in V(G)$, $g_1 \neq g_2$, the following property holds: if $g_1, g_2 \in N(g)$, then $f(g_1) \neq f(g_2)$. In this case we say that f is *locally injective*.

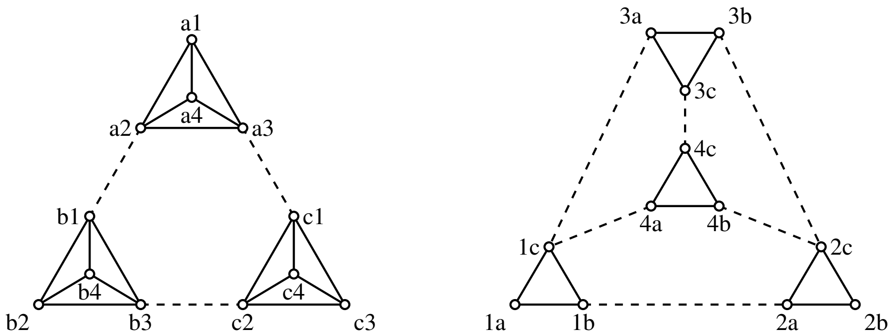

Figure 3: The graph $K_3 \otimes_{f_1} K_4$, where $V(K_3) = \{a, b, c\}, V(K_4) = \{1, 2, 3, 4\}, f_1(a) = 1, f_1(b) = 2, f_1(c) = 3$, and the graph $K_4 \otimes_{f_2} K_3$, where $f_2(1) = a, f_2(2) = b, f_2(3) = c, f_2(4) = c$. The inner edges are solid while the connecting edges are dashed. The solid subgraphs are aH, bH, cH for $H = K_4$ and $1H, 2H, 3H, 4H$ for $H = K_3$.

For any vertex g of G, the subgraph of $G \otimes_f H$ induced by the set of vertices $\{(g, h) \mid h \in V(H)\}$ is called the *subgraph associated with* g and is denoted by gH. We may view the graph $G \otimes_f H$ as partitioned into graphs gH, one for every vertex g of G, and connecting for every edge $\{g, g'\} \in E(G)$ the corresponding vertex $f(g)$ in $g'H$ to the vertex $f(g')$ in gH. The edges of $G \otimes_f H$ naturally fall into two classes. The edges connecting different subgraphs gH are called *connecting edges*, while the edges inside some subgraph gH are called *inner edges*. Given gH, we may add its neighbourhood, i.e. all connecting edges and their endvertices, to obtain a graph denoted by gH^N. If we identify all newly added vertices to a single vertex, denoted by g_H, we obtain a graph, denoted by $H + g$.

Example 2.2. Figure 3 (left) shows the Sierpiński product of K_3 and K_4 with respect to the following function f_1. The vertices of K_3 are labelled with letters a, b, c, the vertices of K_4 are labelled with numbers $1, 2, 3, 4$ and $f_1\colon V(K_3) \to V(K_4)$ is given by

$f_1(a) = 1, f_1(b) = 2, f_1(c) = 3$. Figure 3, right, shows the Sierpiński product of K_4 and K_3 with respect to $f_2\colon V(K_4) \to V(K_3)$ defined by $f_2(1) = a, f_2(2) = b, f_2(3) = c, f_2(4) = c$. This shows that the Sierpiński product is not commutative. Figure 4 depicts examples of the graphs gH^N and $H + g$ in $K_3 \otimes_{f_1} K_4$ and $K_4 \otimes_{f_2} K_3$.

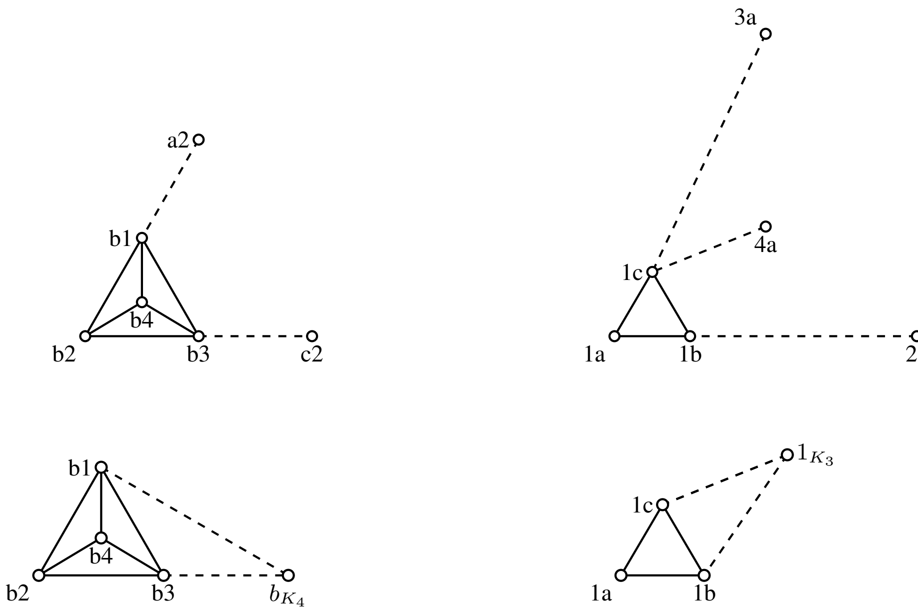

Figure 4: Top: the graphs bH^N for $H = K_4$ and $1H^N$ for $H = K_3$. Bottom: the graphs $H + b$ for $H = K_4$ and $H + 1$ for $H = K_3$.

2.1 Basic properties of the Sierpiński product of graphs

We now state some observations regarding the structure of the Sierpiński product of two graphs. We omit most of the proofs, since they follow straight from the definition.

Proposition 2.3. *Let G, H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then the following statements hold.*

(i) *If $|G| = 1$, then $G \otimes_f H$ is isomorphic to H.*

(ii) *If $|H| = 1$, then $G \otimes_f H$ is isomorphic to G.*

Lemma 2.4. *Let G, H be graphs and let $f\colon V(G) \to V(H)$ be a function. Let G', H' be subgraphs of G, H, respectively, and let f' be the restriction of f to $V(G')$ such that $\mathrm{Im}(f') \subseteq V(H')$. Then the graph $G' \otimes_{f'} H'$ is a subgraph of the graph $G \otimes_f H$.*

The following result explains the role of the graphs G and gH in $G \otimes_f H$.

Lemma 2.5. *Let G, H be graphs, and let $f\colon V(G) \to V(H)$ be a function. Then the following statements hold.*

(i) *For every vertex g of G, the subgraph gH of $G \otimes_f H$ is isomorphic to H.*

(ii) *If, in addition, the graph H is connected, then the graph G is a minor of $G \otimes_f H$.*

(iii) *In particular, if the graph H is connected and the graph $G \otimes_f H$ is planar, then the graphs G and H are planar.*

Notice that planarity of both factors G and H in (iii) easily follows from the fact that H is a connected subgraph, and G is a minor of $G \otimes_f H$. However, if H is not connected, the conclusion in (ii) that G is a minor of $G \otimes_f H$ does not necessarily follow, since we cannot simply contract every subgraph gH of $G \otimes_f H$ to a single vertex. This is shown by the following example.

Example 2.6. Take G to be K_5 with vertices from 1 to 5 and H to be two isolated vertices, denoted by a and b, and then let f map 1 and 2 from K_5 to a of H and the remaining three vertices of K_5 to b of H. The resulting graph $G \otimes_f H$ is isomorphic to the disjoint union of K_2, K_3 and $K_{2,3}$ and is therefore planar. Hence, it cannot have K_5 as a minor.

Proposition 2.7. *Let G, H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then the graph $G \otimes_f H$ has $|G| \cdot |H|$ vertices and $||H|| \cdot |G| + ||G||$ edges. In particular, $G \otimes_f H$ has $||H|| \cdot |G|$ inner edges and $||G||$ connecting edges.*

Lemma 2.8. *Let G and H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then the following holds.*

(i) *For every $g, g' \in V(G)$ there exists at most one edge connecting graphs gH and $g'H$. In addition, graphs gH and $g'H$ are joined by an edge if and only if vertices g and g' are adjacent in graph G.*

(ii) *If a vertex $g \in V(G)$ has d neighbours in G, then there are d vertices and d edges belonging to gH^N that are not a part of gH. These d edges are connecting edges.*

(iii) *The function f is locally injective if and only if the connecting edges form a matching in $G \otimes_f H$ or, equivalently, if and only if every vertex of $G \otimes_f H$ is an endvertex of at most one connecting edge.*

Proof. (i) Only an edge of form $\{(g, f(g')), (g', f(g))\}$ can connect graphs gH and $g'H$ and this happens if and only if there exists an edge between g and g'. Hence, there exists a bijective correspondence between the connecting edges of $G \otimes_f H$ and the edges of G.
(ii) This follows from (i) and the fact that the connecting edges with an endvertex in gH are in bijective correspondence with the edges connecting g to its neighbours in G.
(iii) For every $g \in V(G)$, the connecting edges leading from gH to the rest of the graph $G \otimes_f H$ have distinct endvertices outside gH. If f is locally injective, they have distinct endvertices within gH. It follows that no two connecting edges share a common endvertex, so the connecting edges form a matching in $G \otimes_f H$. Conversely, if f fails to be locally injective, then at least two connecting edges share a common endvertex. □

The lexicographic product of two graphs G and H is the graph $G \circ H$ with vertex set $V(G) \times V(H)$ and two vertices (g, h) and (g', h') are adjacent in $G \circ H$ if and only if either g is adjacent with g' in G or $g = g'$ and h is adjacent with h' in H. For $g \in V(G)$, we denote by gH the subgraph of $G \circ H$ induced by the set $\{(g, h) |\, h \in V(H)\}$. Then the graph $G \circ H$ consists of $|G|$ copies of H, and for every edge $\{g, g'\}$ in G, every vertex of gH is connected to every vertex in $g'H$. Therefore, the next result follows straight from Definition 2.1.

Proposition 2.9. *Let G and H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then the graph $G \otimes_f H$ is a spanning subgraph of the lexicographic product $G \circ H$.*

Note that for different functions f, f', the graphs $G \otimes_f H$ and $G \otimes_{f'} H$ may be isomorphic or nonisomorphic.

Proposition 2.10. *Let G, H be graphs and let $f\colon V(G) \to V(H)$ be a function. Let $\alpha \in \mathrm{Aut}(G)$, $\beta \in \mathrm{Aut}(H)$ and $f' = \beta \circ f \circ \alpha$. Then $G \otimes_f H$ is isomorphic to $G \otimes_{f'} H$.*

Proof. Define the function $\gamma\colon V(G \otimes_f H) \to V(G \otimes_{f'} H)$ by $\gamma(g, h) = (\alpha^{-1}(g), \beta(h))$ for $g \in V(G)$ and $h \in V(H)$. Since α, β are bijections, γ is also a bijection. Since β is an automorphism, γ maps inner edges to inner edges.

Take a connecting edge in $G \otimes_f H$, say $\{(g, f(g')), (g', f(g))\}$, where $\{g, g'\} \in E(G)$. Then $\gamma(g, f(g')) = (\alpha^{-1}(g), \beta(f(g'))$ and $\gamma(g', f(g)) = (\alpha^{-1}(g'), \beta(f(g))$. Since $f'(\alpha^{-1}(g)) = \beta(f(\alpha(\alpha^{-1}(g)))) = \beta(f(g))$ and $f'(\alpha^{-1}(g')) = \beta(f(\alpha(\alpha^{-1}(g')))) = \beta(f(g'))$, we see that γ also maps a connecting edge to a connecting edge. Therefore γ is an isomorphism. □

Corollary 2.11. *Let G be a graph and let $f \in \mathrm{Aut}(G)$. Then $G \otimes G$ is isomorphic to $G \otimes_f G$.*

In the remainder of this section we consider when the Sierpiński product of two graphs is connected.

Proposition 2.12. *Let G and H be graphs and let $f\colon V(G) \to V(H)$ be a function. Then $G \otimes_f H$ is connected if and only if G and H are connected.*

Proof. Suppose G and H are connected. Then $G \otimes_f H$ is connected by Definition 2.1 and Lemma 2.5.

Conversely, suppose $G \otimes_f H$ is connected. Pick two vertices g and g' from G. Then a path from gH to $g'H$ in $G \otimes_f H$ corresponds to a path in G from g to g'. Therefore, G is also connected. Suppose now that H is not connected. Denote by H_1 a connected component of H such that $V_1 = \{g \in G |\ f(g) \in V(H_1)\}$ is nonempty. Take any vertices $g \in V_1$ and $h \in V(H_1)$. If there exists an edge of form $\{(g, h), (g', f(g))\}$, then $h = f(g')$, so $g' \in V_1$. Note that $f(g) \in V(H_1)$. Therefore, all the neighbours of (g, h) belong either to gH_1 or to $g'H_1$ for some $g' \in V_1$. It follows that there are no edges between the set of vertices $\{(g, h) \in V(G \otimes_f H) |\ g \in V_1 \text{ and } h \in V(H_1)\}$ and the rest of the vertices of $G \otimes_f H$. So $G \otimes_f H$ is not connected. This is a contradiction, so H must be connected. □

In [19], Klavžar and Zemljič have characterized which generalized Sierpiński graphs are k-connected and k-edge connected. Unfortunately, their results do not carry over directly to the Sierpiński product of distinct graphs since the factors may have different connectivity properties. Moreover, the result does not depend only on the connectivity of its factors, but also on the choice of the function f. For instance, $C_5 \otimes C_5$ is 2-connected. However, for a constant function f, the product $C_5 \otimes_f C_5$ is only 1-connected.

2.2 Planarity

In this section we study planarity of the Sierpiński product $G \otimes_f H$ of graphs G and H with respect to a function $f\colon V(G) \to V(H)$. We have already mentioned in Lemma 2.5 that for a connected graph H, planarity of the graph $V(G \otimes_f H)$ implies planarity of both factors. The next theorem characterizes when a Sierpiński product $G \otimes_f H$ is planar when f is a locally injective function. Recall that the construction of a graph $H + g$ was introduced in the beginning of Section 2.

Theorem 2.13. *Let G be a 2-connected graph or $G = K_2$, let H be a connected graph and let $f\colon V(G) \to V(H)$ be a locally injective function. Then the graph $G \otimes_f H$ is planar if and only if the following three conditions are fulfilled:*

(i) *the graphs G and H are planar,*

(ii) *for every $g \in V(G)$ the graph $H + g$ is planar,*

(iii) *there exists an embedding of the graph G in the plane with a chosen orientation which has the following property: for every $g \in V(G)$, with $g_1, g_2, \ldots, g_k$ being the cyclic order of vertices around the vertex g, there exists an embedding of the graph $H + g$ in the plane such that the cyclic order of vertices around the vertex g_H in graph $H + g$ is $f(g_k), f(g_{k-1}), \ldots, f(g_1)$.*

Proof. The fact that f is a locally injective function simplifies the arguments. Namely, all the vertices in $N(g)$ are distinct for every $g \in V(G)$.

($\Rightarrow$) First, assume that the graph $G \otimes_f H$ is planar. Then, the graphs G, H are planar by Lemma 2.5 and (i) is established.

Suppose $G \otimes_f H$ is embedded in the plane. Note that for every $g \in V(G)$, the embedding of $G \otimes_f H$ induces a planar embedding of gH. For every $g \in V(G)$, let $N(gH) = \{g'H | g' \in N(g)\}$ denote the collection of graphs $g'H$ that are adjacent to gH. Since the graph G is 2-connected, or $G = K_2$, and the graph H is connected, all the graphs from $N(gH)$ are inside the same face F_g of the graph gH (otherwise the vertex g would be a cut vertex in G). For a fixed g_0 we may assume that F_{g_0} is the outer face of g_0H. If not, we take a different stereographic projection of $G \otimes_f H$. But then, for every $g \in V(G)$, the corresponding face F_g is the outer face of gH. Hence, we may contract every graph gH to a single vertex. From now on we assume that the graph $G \otimes_f H$ is embedded in the plane as we just explained and choose an orientation of the plane. If we contract every subgraph gH of $G \otimes_f H$ to a single vertex, we obtain a minor of $G \otimes_f H$ which is isomorphic to G. Its planar embedding is determined from the planar embedding of $G \otimes_f H$. Hence, for every vertex of G the cyclic order of its neighbours is defined.

Now again take the embedding of $G \otimes_f H$ as described above. Take an arbitrary $g \in V(G)$ and consider the subgraph gH^N that inherits the planar embedding and has all of its pending edges attached to the vertices in the outer face of gH. This establishes a planar embedding of $H + g$, which, in turn, is obtained from gH^N by a suitable vertex identification. This proves (ii).

Now it is easy to see that the embedding of G, obtained from $G \otimes_f H$ by contracting every copy of H to a single vertex, fulfills (iii). Namely, the cyclic order $g_1, g_2, \ldots, g_k$ of vertices around a vertex g of G in this embedding corresponds to the ordering of the vertices $(g, f(g_1)), (g, f(g_2)), \ldots, (g, f(g_k))$ around the outer face of gH in the planar embedding of $G \otimes_f H$. The cyclic order of vertices around g_H in the planar embedding of $gH + g$

described above is then $(g, f(g_k)), (g, f(g_{k-1})), \dots, (g, f(g_1))$. Therefore, an appropriate embedding of $H + g$ exists for every $g \in V(g)$.

($\Leftarrow$) The converse is proved by construction. By (i), the graphs G and H are planar. Moreover, by (ii), for every $g \in V(G)$, the graph $H + g$ is planar. Using (iii), we embed the graph G in the plane. Then for each vertex g of G, we replace the vertex g by the planar embedding of the graph gH, induced by the embedding of $H + g$ from (iii). Again by (iii), it is possible to connect the copies of H among themselves in such a way that a planar embedding of the resulting graph, isomorphic to $G \otimes_f H$, is obtained. □

We believe that Theorem 2.13 holds also if the function f is not locally injective. However, the arguments in the proof become much more involved in this case.

Remark 2.14. Note that the condition in Theorem 2.13 that the graph G is 2-connected is essential. For example, take G to be the graph obtained from K_4 (whose vertices are denoted by $1, 2, 3, 4$) by adding a new vertex (named 5) to it and joining it to the vertex 4 only. The graph $G \otimes G$ is then planar, but $G + 4$ is not and the condition (ii) in Theorem 2.13 does not hold. See Figure 5.

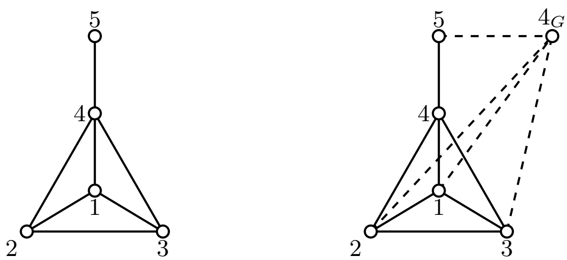

Figure 5: The graph G is planar but not 2-connected. The graph $G + 4$ contains a subdivision of K_5 and is not planar.

The next result is evident from the proof of Theorem 2.13.

Corollary 2.15. *Let G be a 2-connected graph or $G = K_2$, let H be a connected graph and let $f : V(G) \to V(H)$ be a locally injective function. If the graph $G \otimes_f H$ is planar, then for every $g \in V(G)$ there exists an embedding of the graph H in the plane such that the vertices $\{f(g');\ g' \in N(g)\}$ lie on the boundary of the same face.*

Using Theorem 2.13 we can now determine when the graph $G \otimes G$ is planar for a connected graph G. We also give a sufficient condition for the graph $G \otimes_f H$ to be planar when $G \neq H$. By a *block* we mean a maximal connected subgraph of a given graph that has no cut-vertices. Note that a block with more than two vertices is 2-connected.

Theorem 2.16. *Let G be a connected graph. Then the graph $G \otimes G$ is planar if and only if every block of G is outerplanar or equal to K_4.*

Proof. Note that for every block B of G, the identity function $V(B) \to V(B)$ is locally injective. So we may use Theorem 2.13 and Corollary 2.15 for every block of G.

First assume that the graph $G \otimes G$ is planar. Let B be a block of G. Suppose that B is planar but it is not outerplanar or equal to K_4. Then it contains a subdivision of $K_{2,3}$ or a subdivision of K_4 (with at least one additional vertex) as a subgraph, see [3]. Such a graph B always contains a vertex such that in every planar embedding of B, not all of its neighbours will be on the boundary of the same face. Therefore $B \otimes B$ is not planar by Corollary 2.15. On the other hand, $B \otimes B$ is a subgraph of $G \otimes G$ by Lemma 2.4, so it is planar. A contradiction. Therefore, the graph B must be outerplanar or equal to K_4.

We prove the converse by induction on the number of blocks of the graph G. If G has just one block that is outerplanar or equal to K_4, then the conditions (i), (ii), (iii) from Theorem 2.13 are fulfilled, so $G \otimes G$ is planar.

Suppose now that G has more than one block and that every block of G is outerplanar or equal to K_4. Let B be a block that corresponds to a leaf in the block-cut tree of G and let v be the only cut vertex of G contained in B. Let G' be the graph obtained from G by deleting all the vertices of B with the exception of v. Then the graph G' has one block less than G and, by the induction hypothesis, the graph $G' \otimes G'$ is planar. Take a planar embedding of $G' \otimes G'$. We obtain a planar embedding of $G \otimes G$ in the following way. We take a planar embedding of B in which v appears on the boundary of the outer face; moreover if B is outerplanar, we take an embedding of B such that every vertex of B lies on the boundary of the outer face. For every $g \in V(G')$, we insert a copy of B in a face of gG' that contains the vertex (g, v) and then identify the vertex (g, v) with the vertex v of B. We denote the graph obtained so far by K. Observe that K is embedded in the plane. To the graph K we still need to add a copy of G for every vertex of B except v. These copies of G are connected only to the copies of G in $G \otimes G$ corresponding to the vertices of B. Choose an orientation of the plane. Now we consider two cases.

First, let $B = K_4$, with vertices v, v_1, v_2, v_3. Any three vertices of B are on the boundary of a same face in every embedding of B in the plane. Therefore, in the subgraph vG of K there exists a face such that the vertices $(v, v_1), (v, v_2), (v, v_3)$ all lie on its boundary; without loss of generality we may assume that they are arranged in this order (with respect to the chosen orientation of the plane). We may embed the graph v_1G in the plane such that the vertices $(v_1, v), (v_1, v_3), (v_1, v_2)$ lie on the outer face in this order, likewise, we may embed the graph v_2G in the plane such that the vertices $(v_2, v), (v_2, v_1), (v_2, v_3)$ lie on the outer face in this order, and we may embed the graph v_3G in the plane such that the vertices $(v_3, v), (v_3, v_2), (v_3, v_1)$ lie on the outer face in this order. Now place v_iG in the face of the subgraph vG of K that contains the vertices $(v, v_1), (v, v_2), (v, v_3)$ close to vertex (v, v_i) and connect vertices (v, v_i) and (v_i, v), for $i = 1, 2, 3$. The graphs v_iG are embedded in the plane such that it is possible to also connect the pairs of vertices $(v_1, v_2), (v_2, v_1)$, $(v_1, v_3), (v_3, v_1)$ and $(v_2, v_3), (v_3, v_2)$ without crossings. This gives us a planar embedding of the graph $G \otimes G$.

Next, let B be outerplanar. The subgraph vG of K is embedded in the plane and it contains a copy of B such that all the vertices of B are on the boundary of the same face of K, say F. We consider a planar embedding of the graph G in which all the vertices of the block B are on the boundary of the outer face and in the reverse order as the corresponding vertices in vG. For every vertex u of B except v, we place such a copy of G with vertex set $\{u\} \times V(G)$ into face F close to the vertex (v, u). Then we connect vertices (v, u) and (u, v) with an edge if u is a neighbour of v in G. The graphs uG, $u \in V(B)\backslash\{v\}$ are now all in the same face of K. Moreover, the subgraphs uB, $u \in V(B)\backslash\{v\}$, are all in the same face of K with all their vertices on the boundary of the outer face (of the embedding of uG in the plane) and the order of these vertices is reversed compared to the order of the corresponding vertices in vB. Note that the cyclic order of the graphs uB, $u \in V(B)\backslash\{v\}$ is the same as the order of the corresponding vertices in vB. Therefore, it is possible to connect the vertices (u, u') and (u', u) for every edge $\{u, u'\}$ of B without crossings. Again we obtain a planar embedding of the graph $G \otimes G$. This completes the proof. □

Theorem 2.17. *Let G, H be connected graphs and let $f \colon V(G) \to V(H)$ be a function. Assume that G is planar, $\Delta(G) \leq 3$ and H is outerplanar. Then $G \otimes_f H$ is planar.*

Proof. Denote $K = G \otimes_f H$ for convenience. Suppose K is not planar. Then it contains a subdivision of $K_{3,3}$ or K_5 as a subgraph. First assume that K contains a subdivision of $K_{3,3}$. Denote the set vertices of degree 3 of the subdivision of $K_{3,3}$ in K by X. There are four cases to consider, depending on how many vertices from X are in the same copy of H in K.

1. Every vertex from X is in a separate copy of H. If no path connecting two vertices from X passes through any other copies of H containing vertices from X, and at most one such path passes through every copy of H not containing vertices from X, then by contracting gH to a single vertex, for every $g \in V(G)$, we see that $K_{3,3}$ is a minor in G, so G is not planar. Otherwise we need at least four edges connecting some copy of H to the other copies of H in K. This is not possible, since the maximal degree in G is at most three.

2. There are between two and four vertices from X in some gH. Then we need at least four edges connecting gH to the other copies of H in K. This is again not possible, since the maximal degree of G is at most 3.

3. There are five vertices from X in some gH and one vertex from X in some $g'H$ for $g \neq g'$. Since H is outerplanar, gH cannot contain a subdivision of $K_{2,3}$. Therefore, we need at least two edges going out of gH to obtain a subdivision of $K_{2,3}$ from the five vertices in gH. We also need three edges going out of gH to connect gH to the vertex of $K_{3,3}$ in $g'H$. This is again not possible, since the maximal degree of G is at most 3.

4. The only remaining possibility is that all six vertices from X are in the same copy gH of H. Since H is outerplanar, there can be at most seven edges (or paths) between pairs of vertices of $K_{3,3}$ in gH. The remaining two paths must go through the other copies of H, which means that we again need at least four edges connecting gH to the other copies of H in K. A contradiction.

Therefore, K does not contain a subdivision of $K_{3,3}$. Next assume that K contains a subdivision of K_5. Denote the set vertices of degree 4 of the subdivision of K_5 in K by Y. There are two cases to consider, depending on how many vertices from Y are in the same copy of H.

1. There are between one and four vertices from Y in some gH. Then we need at least four edges connecting gH to the other copies of H in K. This is not possible, since the maximal degree in G is at most three.

2. All five vertices from Y are in the same copy of H. Since H is outerplanar, it does not contain a subdivision of K_4 or $K_{2,3}$. Therefore, there can be at most eight edges (or paths) between pairs of these vertices in gH (in fact, there can be at most six such paths). The remaining two paths must go through other copies of H, which means that we need at least four edges connecting gH to other copies of H in K. A contradiction.

It follows that K does not contain a subdivision of $K_{3,3}$ or K_5, so it is planar. □

If a connected graph is not planar, it is natural to consider its genus. The genus of a graph G is denoted by $\gamma(G)$. Recall that by Lemma 2.5, if the graph H is connected, the graph G is a minor of $G \otimes_f H$ for any function $f\colon V(G) \to V(H)$, and the graph $G \otimes_f H$ contains $|G|$ copies of the graph H as induced subgraphs. Suppose G, H are connected and f is arbitrary. Then it is easy to see, cf. [21, Theorem 4.4.2], that

$$\gamma(G \otimes_f H) \geq \gamma(G) + |G| \cdot \gamma(H). \tag{2.1}$$

Note that the bound is not sharp even if the factors are planar. In the case of a planar Sierpiński product, we were able to settle the case in Theorem 2.13. It would be interesting to find some sufficient condition for the equality in (2.1) to hold also for non-planar Sierpiński products.

3 Symmetries of the Sierpiński product of graphs

Throughout this section let G, H be connected graphs and let $f\colon V(G) \to V(H)$ be a function. Recall that the edge set of $G \otimes_f H$ can be naturally partitioned into two subsets:

- *inner edges* $\{(g,h),(g,h')\}$ for every vertex $g \in V(G)$ and every edge $\{h,h'\} \in E(H)$, and
- *connecting edges* $\{(g,f(g'),(g',f(g))\}$ for every edge $\{g,g'\} \in E(G)$.

We call this partition of the edge set the *fundamental edge partition*. We will say that an automorphism of $G \otimes_f H$ *respects the fundamental edge partition* if it takes inner edges to inner edges and connecting edges to connecting edges. We denote the set of all automorphisms of $G \otimes_f H$ that respect the fundamental edge partition by $\tilde{A}(G,H,f)$. This set is a subgroup of the whole automorphism group of $G \otimes_f H$. For connected graphs G and H, the automorphisms that respect the fundamental edge partition have the following useful property.

Proposition 3.1. *Let G and H be connected graphs. Then every automorphism $\tilde{\gamma} \in \tilde{A}(G,H,f)$ permutes the subgraphs gH, $g \in G$. Moreover, the restriction $\tilde{\gamma}|_{V(gH)} : V(gH) \to V(g'H)$, where $g' \in V(G)$, is a graph isomorphism.*

In this section we first show that every automorphism of $G \otimes_f H$ that respects the fundamental edge partition induces automorphisms of G and H. And conversely, we define two families of automorphisms of $G \otimes_f H$ that respect the fundamental edge partition using automorphisms of G and H. As it turns out, one of them is a subfamily of the other one. Then we show that in several cases all the automorphisms of $G \otimes_f H$ respect the fundamental edge partition. Finally, we focus on the case when $G = H$ and f is an automorphism. In this case we can completely describe the group of automorphisms that respect the fundamental edge partition.

3.1 Automorphisms that respect the fundamental edge partition

Let $\tilde{\gamma}$ be an automorphism of $G \otimes_f H$ that respects the fundamental edge partition. Then, it permutes the subgraphs gH, $g \in G$. Define the function $\gamma\colon V(G) \to V(G)$ such that $\gamma(g) = g'$ if $\tilde{\gamma}$ maps gH to $g'H$. Obviously, γ is a bijection. Let $\{g, g_1\}$ be an edge of G. Then $\{(g, f(g_1)), (g_1, f(g))\}$ is a connecting edge of $G \otimes_f H$. Since $\tilde{\gamma}$ respects the fundamental edge partition, it maps this edge to another connecting edge, say $\{(g', f(g'_1)), (g'_1, f(g'))\}$, where g' and g'_1 are adjacent in G. But then γ maps the edge $\{g, g_1\}$ to an edge (i.e. to $\{g', g'_1\}$) and γ is an automorphism. We will say that γ is the *projection* of $\tilde{\gamma}$ on G. Conversely, $\tilde{\gamma}$ is a *lift* of γ. Note that the projection of $\tilde{\gamma} \in \mathrm{Aut}(G \otimes_f H)$ on G is uniquely defined. However, given an automorphism of G, it can have a unique lift, more than one lift or none at all.

On the other hand, the application of $\tilde{\gamma}$ on every copy of gH in $G \otimes_f H$ induces an automorphism γ_g of H, defined by $\gamma_g(h) = h'$ if $\tilde{\gamma}$ sends (g, h) to (g_1, h') for some $g_1 \in V(G)$ and $h' \in V(H)$.

We will now introduce the first family of automorphisms of $G \otimes_f H$ that can be obtained from automorphisms of G and H. All such automorphisms respect the fundamental edge partition.

Definition 3.2. Let G, H be connected graphs and let $f\colon V(G) \to V(H)$ be a function. Let $\alpha \in \mathrm{Aut}(G)$ and let $\mathcal{B} : V(G) \to \mathrm{Aut}(H)$ be a function. For simplicity we will write β_g instead of $\mathcal{B}(g)$ for $g \in V(G)$. Define the function $\Psi(\alpha, \mathcal{B})\colon V(G \otimes_f H) \to V(G \otimes_f H)$ by

$$\Psi(\alpha, \mathcal{B})\colon (g, h) \mapsto (\alpha(g), \beta_g(h)).$$

If $\mathcal{B}$ is a constant function, say $\beta_g = \beta$ for all $g \in V(G)$, we denote $\Psi(\alpha, \mathcal{B})$ by $\Psi(\alpha, \beta)$.

By the discussion at the beginning of this section, we may conclude that the following holds.

Theorem 3.3. *Let G, H be connected graphs and let $f\colon V(G) \to V(H)$ be a function. Then, every automorphism of $G \otimes_f H$ that respects the fundamental edge partition is of form $\Psi(\alpha, \mathcal{B})$ for some $\alpha \in \mathrm{Aut}(G)$ and some function $\mathcal{B}\colon V(G) \to \mathrm{Aut}(H)$.*

We now determine when the function $\Psi(\alpha, \mathcal{B})$ from Definition 3.2 is an automorphism. In Propositions 3.4, 3.5, 3.6 and Corollaries 3.7, 3.8, and 3.9, the assumptions from Definition 3.2 hold.

Proposition 3.4. *The function $\Psi(\alpha, \mathcal{B})$ is a bijection.*

Proof. It is enough to prove that $\Psi(\alpha, \mathcal{B})$ is injective. This is straightforward since α and β_g, $g \in V(G)$, are all injective. □

Proposition 3.5. *The function $\Psi(\alpha, \mathcal{B})$ is an automorphism if and only if for every $g \in V(G)$ we have $f \circ \alpha = \beta_g \circ f$ on $N(g)$. Moreover, in this case $\Psi(\alpha, \mathcal{B})$ respects the fundamental edge partition.*

Proof. We first show that $\Psi(\alpha, \mathcal{B})$ always maps an inner edge to an inner edge. To see this, let $e = \{(g, h_1), (g, h_2)\}$ be an inner edge. Then $\Psi(\alpha, \mathcal{B})$ maps the edge e to $\{(\alpha(g), \beta_g(h_1)),(\alpha(g), \beta_g(h_2))\}$, which is an inner edge since β_g is an automorphism of H.

Suppose now that $\Psi(\alpha, \mathcal{B})$ is an automorphism. Since $\Psi(\alpha, \mathcal{B})$ maps inner edges to inner edges, it must map connecting edges to connecting edges. Let $e = \{(g, f(g_1)), (g_1, f(g))\}$ be a connecting edge. Then $\Psi(\alpha, \mathcal{B})(e) = \{(\alpha(g), \beta_g(f(g_1))), (\alpha(g_1), \beta_{g_1}(f(g)))\}$ is also a connecting edge. Therefore $f(\alpha(g_1)) = \beta_g(f(g_1))$. Since g_1 can be any neighbour of g in G, we have $f \circ \alpha = \beta_g \circ f$ on $N(g)$.

Conversely, let $f \circ \alpha = \beta_g \circ f$ on $N(g)$ for every $g \in V(G)$. Let $e = \{(g, f(g_1)), (g_1, f(g))\}$ be a connecting edge in $G \otimes_f H$. Then $\Psi(\alpha, \mathcal{B})(e) = \{(\alpha(g), \beta_g(f(g_1))), (\alpha(g_1), \beta_{g_1}(f(g)))\}$. Since $f(\alpha(g)) = \beta_{g_1}(f(g))$ and $f(\alpha(g_1)) = \beta_g(f(g_1))$, $\Psi(\alpha, \mathcal{B})(e)$ is a connecting edge. Therefore, $\Psi(\alpha, \mathcal{B})$ is an automorphism. □

Proposition 3.6. *The function $\Psi(\alpha, \beta)$ is an automorphism if and only if $f \circ \alpha = \beta \circ f$.*

Proof. Let $f \circ \alpha = \beta \circ f$ on $N(G)$ for every $g \in V(G)$. Since G is connected, it has no isolated vertices, and so $f \circ \alpha = \beta \circ f$ on $V(G)$. The claim then follows from Proposition 3.5. □

A few special cases now follow as simple corollaries. Recall that $\alpha, \beta, \Psi(\alpha, \beta)$ are defined in Definition 3.2.

Corollary 3.7. *Suppose $G = H$ and f is a bijective function. Then the function $\Psi(\alpha, \beta)$ is an automorphism if and only if $\beta = f \circ \alpha \circ f^{-1}$.*

Corollary 3.8. *Suppose $G = H$ and f is the identity function. Then the function $\Psi(\alpha, \beta)$ is an automorphism if and only if $\alpha = \beta$.*

Corollary 3.9. *Suppose $V(G) \subseteq V(H)$, f is the identity function on its domain and $\beta|_{V(G)} = \alpha$. Then the function $\Psi(\alpha, \beta)$ is an automorphism.*

Remark 3.10. If f is injective and $G \neq H$, we can always relabel the vertices of G, H such that f is the identity on its domain.

We now give some examples showing that f need not be injective or surjective and we can still have automorphisms of type $\Psi(\alpha, \mathcal{B})$.

Example 3.11. Let $G = K_3$ and $H = K_{3,3}$ with $V(G) = \{1, 2, 3\}$ and $V(H) = \{1, 2, \ldots, 6\}$, with adjacencies as in Figure 6. Let $f\colon V(G) \to V(H)$ map $1 \mapsto 1$, $2 \mapsto 3$, $3 \mapsto 5$. Let $\alpha = (1\ 2\ 3)$, $\beta_1 = (1\ 3\ 5)(2\ 4\ 6)$, $\beta_2 = (1\ 3\ 5)(2\ 6\ 4)$, $\beta_3 = (1\ 3\ 5)$ and let $\mathcal{B}\colon V(G) \to \mathrm{Aut}(G)$ be defined by $B(g) = \beta_g$. Then $f \circ \alpha = \beta_1 \circ f = \beta_2 \circ f = \beta_3 \circ f$ and

$$\Psi(\alpha, \mathcal{B}) = (11\ 23\ 35)(12\ 24\ 32)(13\ 25\ 31)(14\ 26\ 34)(15\ 21\ 33)(16\ 22\ 36)$$

is an automorphism of $G \otimes_f H$ that cyclically permutes the subgraphs gH, see Figure 6.

Example 3.12. Let $G = H = K_{1,3}$ with the edge set $\{\{1, 2\}, \{2, 3\}, \{2, 4\}\}$, and let $f\colon V(G) \to V(G)$ be defined as $f = (1\ 2\ 3\ 4)$. Note that f is a bijection that is not an automorphism of G. If $\alpha = (3\ 4)$ and $\beta = f \circ \alpha \circ f^{-1} = (1\ 4)$, then $f \circ \alpha = \beta \circ f$ and

$$\Psi(\alpha, \beta) = (11\ 14)(21\ 24)(31\ 44)(32\ 42)(33\ 43)(34\ 41)$$

is an automorphism of $G \otimes_f G$, that swaps the copies $3G$ and $4G$, see Figure 7.

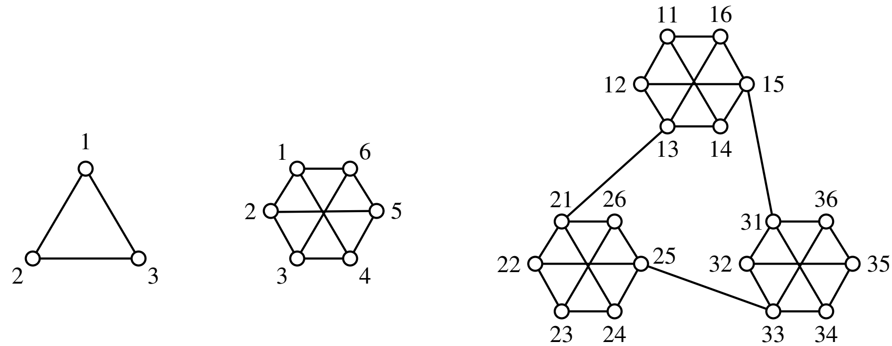

Figure 6: The graphs K_3, $K_{3,3}$ and their Sierpiński product with respect to $f : V(K_3) \to V(K_{3,3})$, $f : 1 \mapsto 1, 2 \mapsto 3, 3 \mapsto 5$.

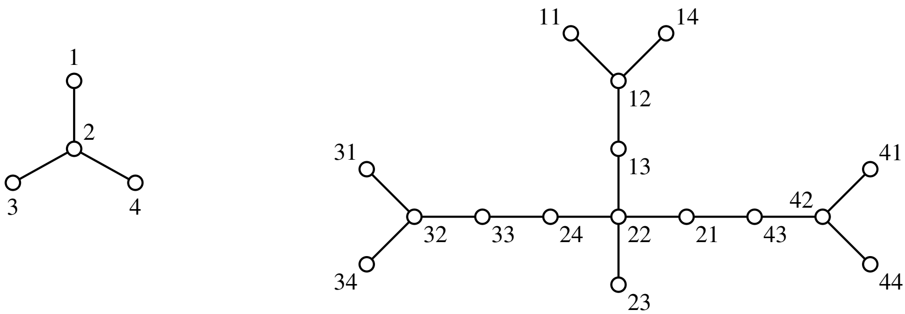

Figure 7: The graph $G = K_{1,3}$ and the Sierpiński product $G \otimes_f G$ with respect to $f = (1\ 2\ 3\ 4)$.

Example 3.13. Let $G = C_4$ with $V(G) = \{1, 2, 3, 4\}$ and adjacencies as in Figure 8, and let H be a star $K_{1,3}$, with the edge set $\{\{1, 2\}, \{2, 3\}, \{2, 4\}\}$. Let $f\colon V(G) \to V(H)$ map $1 \mapsto 2$, $2 \mapsto 2$, $3 \mapsto 4$ and $4 \mapsto 3$. Note that the function f is neither injective nor surjective. If $\alpha = (1\ 2)(3\ 4)$ and $\beta = (3\ 4)$, then $f \circ \alpha = \beta \circ f$ and

$$\Psi(\alpha, \beta) = (11\ 21)(12\ 22)(13\ 24)(14\ 23)(31\ 41)(32\ 42)(33\ 44)(34\ 43)$$

is a reflection automorphism of $G \otimes_f H$, swapping the copies $1H, 2H$ and $3H, 4H$, see Figure 8.

Now let us introduce the second family of automorphisms of $G \otimes_f H$. Let $g \in V(G)$ and $\beta \in \mathrm{Aut}(H)$. Define the function $\Phi(g, \beta) : V(G \otimes_f H) \to V(G \otimes_f H)$ by

$$\Phi(g, \beta)\colon (g_1, h_1) \mapsto \begin{cases} (g_1, h_1) & \text{if } g_1 \neq g, \\ (g_1, \beta(h_1)) & \text{if } g_1 = g. \end{cases}$$

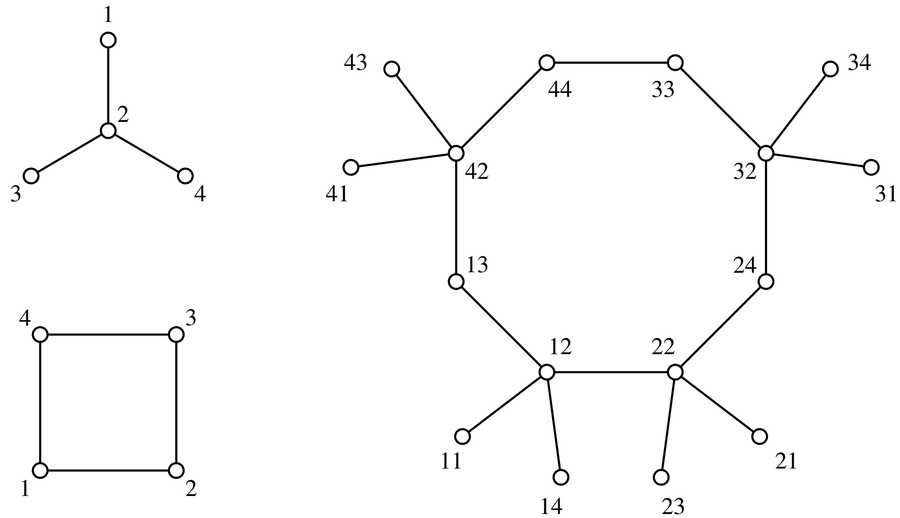

Figure 8: The graphs C_4, $K_{1,3}$ and their Sierpiński product with respect to $f\colon V(C_4) \to V(K_{1,3})$, $f\colon 1 \mapsto 2, 2 \mapsto 2, 3 \mapsto 4, 4 \mapsto 3$.

Proposition 3.14. *Let $g \in V(G)$ and let $\beta \in \mathrm{Aut}(H)$. The function $\Phi(g,\beta)$ is an automorphism of $G \otimes_f H$ if and only if β is in the pointwise stabilizer of $f(N(g))$. Moreover, in this case $\Phi(g,\beta)$ respects the fundamental edge partition.*

Proof. The function $\Phi(g,\beta)$ is obviously a bijection since it fixes all the vertices of $G \otimes_f H$ not in gH and it permutes the vertices in gH. It also fixes the inner edges and connecting edges that do not have any endvertices in gH and it permutes the inner edges in gH.

Take a vertex $g' \in N(g)$. Then $\{(g, f(g')), (g', f(g))\}$ is a connecting edge. The function $\Phi(g,\beta)$ maps $\{(g, f(g')), (g', f(g))\}$ to the set $\{(g, \beta(f(g')), (g', f(g))\}$, which is an edge if and only if $\beta(f(g')) = f(g')$. So $\Phi(g,\beta)$ is an automorphism if and only if β is in the stabilizer of $f(g')$ for every $g' \in N(G)$. □

Remark 3.15. Note that by Theorem 3.3, the function $\Phi(g,\beta)$ is the same as $\Psi(\alpha,\mathcal{B})$ for some $\alpha \in \mathrm{Aut}(G)$ and $\mathcal{B}\colon V(G) \to \mathrm{Aut}(H)$. Indeed, it is easy to verify that for $\alpha = \mathrm{id}$ and $\mathcal{B}$ defined by the rules $\mathcal{B}\colon g_1 \to \mathrm{id}$ if $g_1 \neq g$ and $\mathcal{B}\colon g \to \beta$, we have $\Phi(g,\beta) = \Psi(\alpha,\mathcal{B})$.

Given a group X acting on a set Y, we denote by $X_{(Y)}$ the pointwise stabilizer of Y, i.e. the subgroup of X that fixes every element of Y. For $g \in G$ denote by $\hat{B}_g(G,H,f)$ the group generated by $\{\Phi(g,\beta_g) |\, \beta_g \in \mathrm{Aut}(H)_{(f(N(g)))}\}$. Denote by $\hat{B}(G,H,f)$ the group generated by $\{\hat{B}_g(G,H,f) |\ g \in V(G)\}$. We will now study the structure of the group $\hat{B}(G,H,f)$.

Proposition 3.16. *Let g, g' be distinct vertices of G and let $\beta_g \in \mathrm{Aut}(H)_{(f(N(g)))}$, $\beta_{g'} \in \mathrm{Aut}(H)_{(f(N(g')))}$. Then $\Phi(g,\beta_g)$ and $\Phi(g',\beta_{g'})$ commute.*

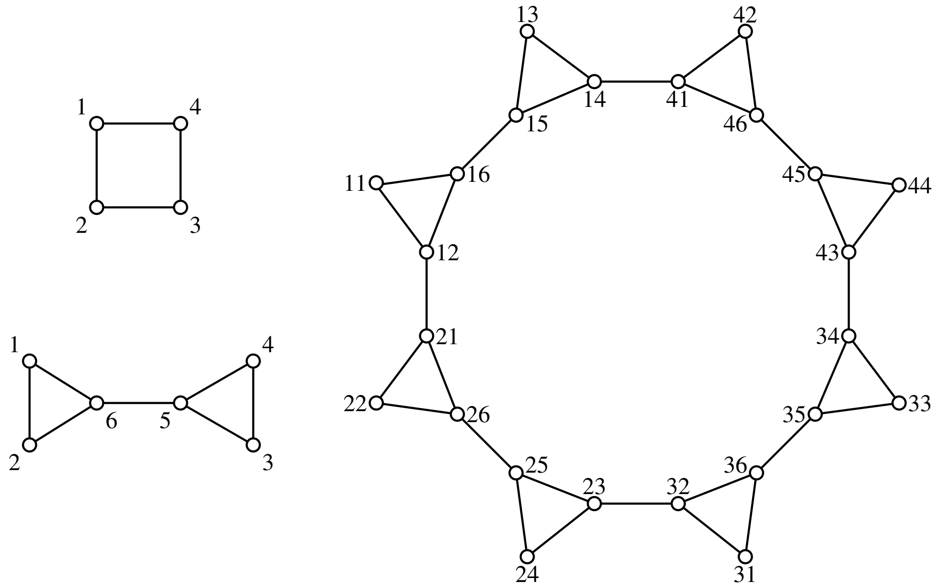

Figure 9: The graphs C_4, $2K_3 + e$ and their Sierpiński product with respect to $f = \mathrm{id}$.

Proof. The functions $\Phi(g, \beta_g)$ and $\Phi(g', \beta_{g'})$ commute since as permutations they have disjoint supports. $\square$

Theorem 3.17. *The group $\hat{B}(G, H, f)$ is a subgroup of the group $\tilde{A}(G, H, f)$ and is a direct product*

$$\hat{B}(G, H, f) = \prod_{g \in V(G)} \hat{B}_g(G, H, f). \tag{3.1}$$

Moreover, the group $\hat{B}(G, H, f)$ is isomorphic to the group $\prod_{g \in V(G)} \mathrm{Aut}(H)_{(f(N(g)))}$.

Proof. The group $\hat{B}(G, H, f)$ is a subgroup of the group $\tilde{A}(G, H, f)$ by definition and Propositon 3.14. The groups $\hat{B}_g(G, H, f)$, $g \in V(G)$, have pairwise only the identity in common, they generate the group $\hat{B}(G, H, f)$, and the elements of two distinct groups $\hat{B}_g(G, H, f)$ commute, therefore equation (3.1) holds. The last claim is true since for every $g \in G$, the groups $\hat{B}_g(G, H, f)$ and $\mathrm{Aut}(H)_{(f(N(g)))}$ are isomorphic in the obvious way. $\square$

3.2 When do all the automorphisms respect the fundamental edge partition

Given connected graphs G, H and a function $f\colon V(G) \to V(H)$, in general there can exist automorphisms of $G \otimes_f H$ that do not respect the fundamental edge partition. Figure 9 shows such an example. There, $G = C_4$, $H = 2K_3 + e$ and $f\colon V(G) \to V(H)$ is the identity function on its domain. One can easily observe that by rotating the graph $G \otimes_f H$, the inner edge $\{16, 15\}$ can be mapped to the connecting edge $\{14, 41\}$.

Note that in the example above, the graph H is not 2-connected. When two graphs G and H are both 2-connected, we have so far not been able to find an automorphism of

$G \otimes_f H$ that does not respect the fundamental edge partition. Therefore, we propose the following conjecture.

Conjecture 3.18. *Let G, H be 2-connected graphs and let $f\colon V(G) \to V(H)$ be a function. Then*

$$\tilde{A}(G, H, f) = \mathrm{Aut}(G \otimes_f H).$$

In this section we prove this conjecture for two special cases. In the first case $G = H, f \in \mathrm{Aut}(G)$ and G is a regular triangle-free graph. In the second case every edge of H is contained in a short cycle. Note that in these two cases the assumption that G, H are 2-connected is not needed.

Theorem 3.19. *Let G be a connected regular triangle-free graph and let $f\colon V(G) \to V(G)$ be an automorphism of G. Then every automorphism of $G \otimes_f G$ respects the fundamental edge partition. In other words,*

$$\tilde{A}(G, G, f) = \mathrm{Aut}(G \otimes_f G).$$

Proof. Let k denote the valency of G. Then the endvertices of every connecting edge in $G \otimes_f G$ have valency $k + 1$ by Lemma 2.8. An endvertex of an inner edge may have valency k or $k + 1$. Clearly, if at least one endvertex of an inner edge has valency k, this edge cannot be mapped to a connecting edge by any automorphism.

Suppose now that both endvertices of an inner edge $\{(g, g_1), (g, g_2)\}$ have degree $k+1$. This is only possible if (g, g_1) and (g, g_2) are the endvertices of some connecting edges, say $\{(g, g_1), (g'_1, f(g))\}$ and $\{(g, g_2), (g'_2, f(g))\}$ where $g_1 = f(g'_1)$ and $g_2 = f(g'_2)$. But then g'_1 and g'_2 are adjacent to g in G. Since g_1 and g_2 are adjacent in G and f is an automorphism, g'_1 and g'_2 are also adjacent. But then g, g'_1, g'_2 form a triangle in G, a contradiction. Therefore no inner edge can be mapped to a connecting edge, so every automorphism of $G \otimes_f G$ respects the fundamental edge partition. □

Lemma 3.20. *Let G and H be graphs and let $f\colon V(G) \to V(H)$ be a function. Let $\{g, g'\}$ be an edge of G.*

(i) *If $\{g, g'\}$ is not contained in any cycle of G, then the edge $\{(g, f(g')), (g', f(g))\}$ is not contained in any cycle of $G \otimes_f H$.*

(ii) *Let c be the length of the shortest cycle that contains $\{g, g'\}$. Then the shortest cycle that contains the edge $\{(g, f(g')), (g', f(g))\}$ in $G \otimes_f H$ has length at least c.*

(iii) *Suppose that f is locally injective and let c be the length of the shortest cycle that contains $\{g, g'\}$. Then the shortest cycle that contains the edge $\{(g, f(g')), (g', f(g))\}$ in $G \otimes_f H$ has length at least $2c$.*

Proof. Let C be a cycle in $G \otimes_f H$ that contains $\{(g, f(g')), (g', f(g))\}$. Suppose that $\{(g, f(g')), (g', f(g))\}, \{(g', f(g_1)), (g_1, f(g'))\}, \ldots, \{(g_k, f(g)), (g, f(g_k))\}$ are the connecting edges in C in that order. Then $gg'g_1g_2 \ldots g_kg$ is a cycle of length k in G that contains the edge $\{g, g'\}$, so $k \geq c$. Furthermore, if $\{g, g'\}$ is not contained in any cycle of G, then the edge $\{(g, f(g')), (g', f(g))\}$ cannot be contained in any cycle of $G \otimes_f H$. Recall that if f is locally injective, any vertex of $G \otimes_f H$ is an endvertex of at most one connecting edge by Lemma 2.8. Therefore, in this case the shortest cycle that contains $\{(g, f(g')), (g', f(g))\}$ has length at least $2c$. □

Theorem 3.21. *Let G and H be connected graphs, let $f\colon V(G) \to V(H)$ be a function and let the girth of G be equal to c. In any of the following cases, every automorphism of $G \otimes_f H$ respects the fundamental edge partition, i.e.*

$$\tilde{A}(G, G, f) = \mathrm{Aut}(G \otimes_f G).$$

(i) *G is a tree and H is a bridgeless graph;*

(ii) *every edge of H is contained in a cycle of length at most $c-1$;*

(iii) *the function f is locally injective and every edge of H is contained in a cycle of length at most $2c-1$.*

Proof. By Lemma 3.20, the shortest cycle that contains a connecting edge has length at least c in case (ii), length at least $2c$ in case (iii) and is not contained in any cycle in case (i). Since every inner edge is contained in a cycle in case (i), in a cycle of length at most $c-1$ in case (ii), and in a cycle of length at most $2c-1$ in case (iii), a connecting edge cannot be mapped to an inner edge by any automorphism. □

3.3 Group of automorphisms of $G \otimes_f G$

We now consider the group of automorphisms that respect the fundamental edge partition in the special case when $G = H$ and $f\colon V(G) \to V(G)$ is an automorphism. Since in this case $G \otimes_f G$ is isomorphic to $G \otimes G$, we could restrict ourselves to the case where f is the identity. Note that in that case, the structure of the automorphism group was sketched in the paper [8], but the proofs were never published.

Recall that by Corollary 3.7, every automorphism α of G has a lift, $\Psi(\alpha, f \circ \alpha \circ f^{-1})$. We call this automorphism the *diagonal automorphism* of $G \otimes_f G$ corresponding to α, and denote it by $\bar{\alpha}$. Denote by $\bar{A}(G, f)$ the set of all diagonal automorphisms. The following proposition is straightforward to prove.

Proposition 3.22. *The set $\bar{A}(G, f)$ is a subgroup of $\tilde{A}(G, G, f)$, isomorphic to* $\mathrm{Aut}(G)$.

To determine the structure of the group $\tilde{A}(G, G, f)$, we first show that every element of $\tilde{A}(G, G, f)$ can be written as a product of an element from $\hat{B}(G, G, f)$ and an element of $\bar{A}(G, f)$. Furthermore, we show that $\hat{B}(G, G, f)$ is a normal subgroup of $\tilde{A}(G, G, f)$.

Proposition 3.23. *Let G be a connected graph and let $f\colon V(G) \to V(G)$ be an automorphism. Let $\tilde{\gamma}$ be an automorphism of $G \otimes_f G$ that preserves the fundamental edge partition. Then there exist $\alpha \in \mathrm{Aut}(G)$ and $\beta_g \in \mathrm{Aut}(G)_{(f(N(g)))}$ for every $g \in V(G)$ such that $\tilde{\gamma} = \bar{\alpha} \left(\prod_{g \in V(G)} \Phi(g, \beta_g)\right)$.*

Proof. Let α be the projection of $\tilde{\gamma}$ to $\mathrm{Aut}(G)$. Then $\bar{\alpha} = \Psi(\alpha, f \circ \alpha \circ f^{-1})$ permutes the copies gG in the right way, such as $\tilde{\gamma}$ does. Observe that $\bar{\alpha}$ already agrees with $\tilde{\gamma}$ on the endvertices of all the connecting edges. To obtain $\tilde{\gamma}$ from $\bar{\alpha}$, we only need to adjust, for every $g \in V(G)$, the action of $\bar{\alpha}$ on the vertices from $f(N(g))$ that are not endvertices of connecting edges. We can do this on every copy gG separately, by acting with $\Phi(g, \beta_g)$, where $\beta_g \in \mathrm{Aut}(G)$ is induced by $\bar{\alpha}^{-1}\tilde{\gamma}$. Also, $\beta_g \in \mathrm{Aut}(G)_{(f(N(g)))}$ since the vertices from $f(N(g))$ have the right image already and are fixed by β_g. □

Proposition 3.24. *Let G be a connected graph and let $f\colon V(G) \to V(G)$ be an automorphism. Then the group $\hat{B}(G,G,f)$ is a normal subgroup of the group $\tilde{A}(G,G,f)$.*

Proof. Observe that the function $\lambda\colon \tilde{A}(G,G,f) \to \bar{A}(G,f)$ defined by $\lambda\colon \Psi(\alpha,\mathcal{B}) \to \Psi(\alpha, f\circ\alpha\circ f^{-1})$ is a homomorphism of groups, with $\hat{B}(G,G,f)$ being its kernel. Therefore, $\hat{B}(G,G,f)$ is a normal subgroup of $\tilde{A}(G,G,f)$. □

Theorem 3.25. *Let G be a connected graph and let $f\colon V(G) \to V(G)$ be an automorphism. Then the group $\tilde{A}(G,G,f)$ is a semidirect product,*

$$\tilde{A}(G,G,f) = \bar{A}(G,f) \ltimes \hat{B}(G,G,f).$$

Proof. The group $\hat{B}(G,G,f)$ is a normal subgroup of $\tilde{A}(G,G,f)$ by Proposition 3.24. By Proposition 3.23, every element of $\tilde{A}(G,G,f)$ can be written as a product of a diagonal automorphism and an element from $\hat{B}(G,G,f)$. Moreover, only the identity is in both $\bar{A}(G,f)$ and $\hat{B}(G,G,f)$. This proves that $\tilde{A}(G,G,f)$ is a semidirect product of $\bar{A}(G,f)$ and $\hat{B}(G,G,f)$. □

4 Sierpiński product with multiple factors

To form a Sierpiński product $G_3 \otimes_f (G_2 \otimes_{f_1} G_1)$ of graphs G_3, G_2 and G_1, one needs functions $f_1\colon V(G_2) \to V(G_1)$ and $f\colon V(G_3) \to G_2 \otimes_{f_1} G_1$, which is rather impractical. Suppose a function $f_2\colon V(G_3) \to V(G_2)$ is given. Then a function $f\colon V(G_3) \to V(G_2 \otimes_{f_1} G_1)$ can be defined in a natural way as $f(g) = (f_2(g), f_1(f_2(g))$ for $g \in V(G_3)$. In other words, let $\varphi\colon V(G_2) \to V(G_2 \otimes_{f_1} G_1)$ be the function that maps every vertex $g \in V(G_2)$ to the vertex $(g, f_1(g)) \in V(G_2 \otimes_{f_1} G_1)$. Then $f = \varphi \circ f_2$. Now we can define the Sierpiński product of the graphs G_3, G_2 and G_1 with respect to f_2 and f_1 in the following way:

$$G_3 \otimes_{f_2} G_2 \otimes_{f_1} G_1 = G_3 \otimes_{\varphi\circ f_2} (G_2 \otimes_{f_1} G_1).$$

Note that with given functions f_2 and f_1, we cannot form this product in any other way, therefore, the Sierpiński product is not associative.

In Figure 10 it is shown how the product $C_3 \otimes_{f_2} C_4 \otimes_{f_1} C_3$ is formed in two steps (with $f_1\colon V(C_4) \to V(C_3)$, $f_1\colon i \mapsto i \pmod 3$ and $f_2\colon V(C_3) \to V(C_4)$ being the identity function on its domain).

It is now easy to see that Sierpiński products possess a nice recursive structure, similar to Sierpiński graphs and generalized Sierpiński graphs. By the same reasoning as above, the product $G_m \otimes_{f_{m-1}} \cdots \otimes_{f_2} G_2 \otimes_{f_1} G_1$, where $V(G_\ell) = \{0,1,\ldots,|G_\ell|-1\}$, and $f_\ell\colon V(G_{\ell+1}) \to V(G_\ell)$, $\ell = 1,\ldots,m-1$, are arbitrary functions, can be constructed as follows.

- First, take $|G_2|$ copies of the graph G_1 and label them iG_1, $i \in \{0,\ldots,|G_2|-1\}$. Vertices of these graphs have labels of form g_2g_1, where $g_2 \in V(G_2)$ and $g_1 \in V(G_1)$.

- Connect any two copies iG_1 and jG_1 if there is an edge $\{i,j\}$ in G_2. More precisely, if $\{i,j\} \in E(G_2)$, we add an edge $\{if_1(j), jf_1(i)\}$ between iG_1 and jG_1. The resulting graph is then indeed the Sierpiński product $G_2 \otimes_{f_1} G_1$.

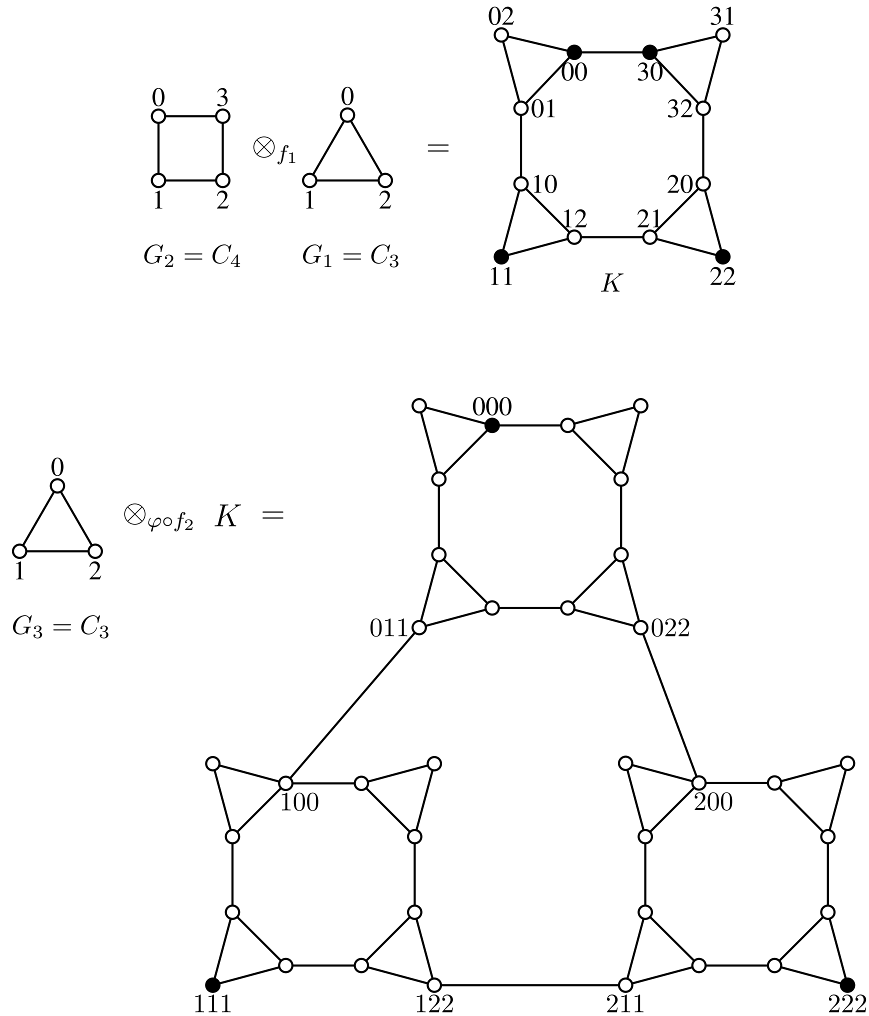

Figure 10: Construction of the graph $C_3 \otimes_{f_2} C_4 \otimes_{f_1} C_3$, where $f_1 \colon i \mapsto i \pmod 3$ and $f_2 = \mathrm{id}$.

- Next, we form the Sierpiński product of the graphs G_3 and $K(2) := G_2 \otimes_{f_1} G_1$. To do so we take $|G_3|$ copies of the graph $K(2)$, label them $iK(2)$, $i \in \{0, \dots, |G_3| - 1\}$, and connect $iK(2)$ and $jK(2)$ whenever $\{i, j\}$ is an edge in G_3. Such an edge then has the form $\{if_2(j)f_1(f_2(j)), jf_2(i)f_1(f_2(i))\}$.

- The final step is to form the Sierpiński product of the graphs G_m and $K(m-1)$ in the same way as we formed all the products so far: make $|G_m|$ copies of $K(m-1)$ and label them $iK(m-1)$; then for every edge $\{i, j\}$ in G_m we add an edge between copies $iK(m-1)$ and $jK(m-1)$. Such an edge has then the following form

$$\{if_{m-1}(j) \dots f_1(f_2 \dots (f_{m-1}(j)) \dots),\ jf_{m-1}(i) \dots f_1(f_2 \dots (f_{m-1}(i)) \dots)\}.$$

The resulting graph is the product $G_m \otimes_{f_{m-1}} \cdots \otimes_{f_2} G_2 \otimes_{f_1} G_1$.

If $G_1 = \cdots = G_m = G$ and functions $f_1, \ldots, f_{m-1}$ are all the identity function, then $G_m \otimes_{f_{m-1}} \cdots \otimes_{f_2} G_2 \otimes_{f_1} G_1$ is the generalized Sierpiński graph S_G^n; see also [8].

We can calculate the order and the size of the Sierpiński product of multiple factors directly from the above construction.

Proposition 4.1. *Let $m \geq 2$, and let $G_1, \ldots, G_m$ be arbitrary graphs. Further, let $f_1 \colon V(G_2) \to V(G_1), \ldots, f_{m-1} \colon V(G_m) \to V(G_{m-1})$ be arbitrary functions. Then the order and the size of the Sierpiński product $G_m \otimes_{f_{m-1}} \cdots \otimes_{f_1} G_1$ are as follows*

$$|G_m \otimes_{f_{m-1}} \cdots \otimes_{f_1} G_1| = \prod_{\ell=1}^{m} |G_\ell| \,,$$

$$||G_m \otimes_{f_{m-1}} \cdots \otimes_{f_1} G_1|| = \sum_{\ell=1}^{m} \left(\prod_{j=\ell+1}^{m} |G_j| \right) ||G_\ell|| \,.$$

Note that neither the order nor the size of the Sierpiński product depends on the functions f_ℓ. It would also be interesting to study some properties of the Sierpiński product with multiple factors, such as diameter and girth.

5 Conclusion

This paper generalizes Sierpiński graphs even further than generalized Sierpiński graphs, where the whole structure is based only on one graph. Here we create a product-like structure of two (or more) factors. Some basic graph theoretical properties are studied in detail, and planar Sierpiński products are completely characterized. Apart from this, the symmetries of Sierpiński products are studied as well. In general, these are not fully understood. In several cases we are able to determine the automorphism group of the Sierpiński product of two graphs exactly.

In [14] an algorithm is given for recognizing generalized Sierpiński graphs. Given a graph it is also natural to ask whether it can be represented as a Sierpiński product of two or more graphs. Moreover, one can ask if such a representation is unique. The latter question has a negative answer. Consider the Sierpiński product of C_4 and $2K_3 + e$ with function f as in Figure 9. It can be easily verified that it is isomorphic to $C_8 \otimes_{f'} K_3$ where $f' \colon V(C_8) \to V(K_3)$ is defined by $f'(1) = f'(2) = f'(5) = f'(6) = 1$ and $f'(3) = f'(4) = f'(7) = f'(8) = 2$. However, in this case not all the factors are prime with respect to the Sierpiński product: C_8 can be represented as a Sierpiński product of C_4 and K_2 while $2K_3 + e$ can be represented as a Sierpiński product of K_2 and K_3. It would be interesting to see whether there exist prime graphs with respect to the Sierpiński product G, H, G', H' and functions $f \colon V(G) \to V(H)$, $f' \colon V(G') \to V(H')$ such that G, H are not isomorphic to G', H' while $G \otimes_f H$ is isomorphic to $G' \otimes_{f'} H'$.

The Sierpiński product can also be defined in a similar way for graphs with loops and multiple edges. In this case, a loop in G, say $\{g, g\}$, would correspond to a loop $\{(g, f(g)), (g, f(g))\}$ in $G \otimes_f H$ and a multiple edge in G would correspond to a multiple edge in $G \otimes_f H$. Finally, as with other products, one could also study the Sierpiński product of infinite graphs.

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Total graph of a signed graph

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Abstract

The total graph is built by joining the graph to its line graph by means of the incidences. We introduce a similar construction for signed graphs. Under two similar definitions of the line signed graph, we define the corresponding total signed graph and we show that it is stable under switching. We consider balance, the frustration index and frustration number, and the largest eigenvalue. In the regular case we compute the spectrum of the adjacency matrix of the total graph and the spectra of certain compositions, and we determine some with exactly two main eigenvalues.

Keywords: Bidirected graph, signed line graph, signed total graph, graph eigenvalues, regular signed graph, Cartesian product graph.

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1 Introduction

We define the total graph of a signed graph in a way that extends to signed graphs the spectral theory of ordinary total graphs of graphs. The usual total graph is built by joining the graph to its line graph by means of its vertex-edge incidences; this construction coordinates well with the adjacency matrix. When we consider signed graphs, there is a similar definition which extends the notion of line graph of a signed graph and which coordinates combinatorial and matrix constructions. Working from two similar definitions of the line signed graph we define the corresponding total graphs, and we show they are stable under switching. We examine fundamental properties of the signed total graph including balance, the degree of imbalance as measured by the frustration index and frustration number, and the largest eigenvalue. In the regular case we compute the spectrum of the adjacency matrix and the spectra of certain compositions and determine some with exactly two main eigenvalues.

A *signed graph* Σ is a pair $(G, \sigma) = G_\sigma$, where $G = (V, E)$ is an ordinary (unsigned) graph, called the *underlying graph*, and $\sigma\colon E \longrightarrow \{-1, +1\}$ is the *sign function* (the signature). The edge set of a signed graph is composed of subsets of positive and negative edges. We interpret an unsigned graph G as the *all-positive* signed graph $(G, +) = +G$, whose signature gives $+1$ to all the edges. Similarly, by $(G, -) = -G$ we denote a graph G with the *all-negative signature*. In general, we have $-\Sigma = (G, -\sigma)$.

Many familiar notions about unsigned graphs extend directly to signed graphs. For example, the degree $d(v)$ of a vertex v in G_σ is simply its degree in G. On the other hand, there also are notions exclusive to signed graphs, most importantly the sign of a cycle, namely the product of its edge signs. A signed graph or its subgraph is called *balanced* if every cycle in it, if any, is positive. Oppositely, Σ is *antibalanced* if $-\Sigma$ is balanced, i.e., every odd (resp., even) cycle of Σ is negative (resp., positive), e.g., if $\Sigma = -G$. Balance is a fundamental concept of signed graphs and measuring how far a signed graph deviates from it is valuable information. The *frustration index* l (resp., the *frustration number* ν) of a signed graph is the minimum number of edges (resp., vertices) whose removal results in a balanced signed graph. These numbers generalize the edge biparticity and vertex biparticity of a graph G, which equal $l(-G)$ and $\nu(-G)$, respectively.

Also important is the operation of switching. If U is a set of vertices of Σ, the switched signed graph Σ^U (in which the vertices in U are switched) is obtained from Σ by reversing the signs of the edges in the cut $[U, V \setminus U]$. The signed graphs Σ and Σ^U are said to be *switching equivalent*, written $\Sigma \sim \Sigma^U$, and the same is said for their signatures. Notably, a signed graph is balanced if and only if it is switching equivalent to the all-positive signature [15] and it is antibalanced if and only if it switches to the all-negative signature. For basic notions and notation on signed graphs not given here we refer the reader to [15, 18].

The *adjacency matrix* A_Σ of $\Sigma = G_\sigma$ is obtained from the standard $(0, 1)$-adjacency matrix of G by reversing the sign of all 1's which correspond to negative edges. The *eigenvalues* of Σ are identified to be the eigenvalues of A_Σ; they form the *spectrum* of Σ. The *Laplacian matrix* of Σ is defined by $L_\Sigma = D_G - A_\Sigma$, where D_G is the diagonal matrix of vertex degrees of G. Analogously, the *Laplacian eigenvalues* of Σ are the eigenvalues of L_Σ.

It is well known that the signed graphs $\Sigma = G_\sigma$ and $\Sigma' = G_{\sigma'}$ are switching equivalent if and only if there exists a diagonal matrix S of ± 1's, called the *switching matrix*, such that $A_{\Sigma'} = S^{-1} A_\Sigma S$, and we say that the corresponding matrices are *switching similar*. More generally, the signed graphs Σ and Σ' are *switching isomorphic* if there exist a permutation matrix P and a switching matrix S such that $A_{\Sigma'} = (PS)^{-1}A_{\Sigma}(PS)$; in fact, PS can be seen as a signed permutation matrix (or a $\{1, 0, -1\}$-monomial matrix).

The frustration index and the frustration number are among the most investigated invariants – for more details one can consult [18]. Similarly, the largest eigenvalue of the adjacency matrix is the most investigated spectral invariant of graphs. Evidently, switching preserves the eigenvalues of A_{Σ} and L_{Σ}, and it also preserves the signs of cycles, so that switching equivalent signed graphs share the same set of positive (and negative) cycles and have the same frustration index and frustration number. For the above reasons, when we consider a signed graph Σ perspective, we are considering its switching isomorphism class $[\Sigma]$, and we focus our attention to the properties of Σ which are invariant under switching isomorphism.

Here is the remainder of the paper. In Section 2 we discuss the concept of line graph of a signed graph. The total graph is presented in Section 3. In Section 4 we consider regular underlying graphs and, similarly to what is known for unsigned graphs [6], we give the eigenvalues of a total graph of a signed graph by means of the eigenvalues of its root signed graph.

We stress that a line (total) graph of a signed graph is always signed, so "line (total) graph" of Σ means the same as "signed line (total) graph" of Σ. For brevity we also call these graphs "line (total) signed graphs" and "signed line (total) graphs" (although literally the latter can mean any signature on an unsigned line or total graph; indeed an entirely different signed total graph has been defined by Sinha and Garg [10]).

2 Line graph(s)

The line graph is a well-known concept in graph theory: given a graph $G = (V(G), E(G))$, the line graph $\mathcal{L}(G)$ has $E(G)$ as vertex set, and two vertices of $\mathcal{L}(G)$ are adjacent if and only if the corresponding edges are adjacent in G. If we consider signed graphs $\Sigma = G_\sigma$, then a (signed) line graph $\mathcal{L}(G_\sigma)$ should have $\mathcal{L}(G)$ as its underlying graph. However, what signature should we associate to it? The answer to this question is a matter of discussion because it is possible to have several very different signatures. In this section we shall consider the two relevant ones defined in the literature.

2.1 Definitions of a line graph

Zaslavsky gave the first definition of incidence matrix of signed graphs [15], which is a necessary step in a spectrally consistent definition of a line graph. For a signed graph $\Sigma = G_\sigma$, we introduce the vertex-edge *orientation* $\eta\colon V(G) \times E(G) \longrightarrow \{1, 0, -1\}$ formed by obeying the following rules:

(O1) $\eta(i, jk) = 0$ if $i \notin \{j, k\}$;

(O2) $\eta(i, ij) = 1$ or $\eta(i, ij) = -1$;

(O3) $\eta(i, ij)\eta(j, ij) = -\sigma(ij)$.

(The minus sign in (O3) is necessary for several purposes, such as with signed-graph orientations [14, 17] and geometry [17].) The *incidence matrix* $B_\eta = (\eta_{ij})$ is a vertex-edge incidence matrix derived from G_σ, such that its (i, e)-entry is equal to $\eta(i, e)$. However, it is not uniquely determined by Σ alone. As in the definition of the oriented incidence matrix for unsigned graphs, one can randomly choose an entry $\eta(i, ij)$ to be either $+1$ or -1, but the entry $\eta(j, ij)$ is then determined by $\sigma(ij)$, so η is called an *orientation of* G_σ (and a *biorientation of* G, the unsigned underlying graph). Zaslavsky later interpreted B_η as the incidence matrix of an oriented signed graph [17] and recognized that the same was an alternate definition of *bidirected graphs* as in [7]. From a signed graph Σ we get many bidirected graphs Σ_η, but each of them leads back to the same signed graph Σ.

Let $A^\intercal$ denote the transpose of the matrix A. The incidence matrix has an important role in spectral theory. The Laplacian matrix can be derived as the row-by-row product of the matrix B_η with itself:

$$B_\eta B_\eta^\intercal = L_\Sigma.$$

Notably, regardless of the orientation η chosen, we get the same L_Σ. It is well known that the column-by-column product of B_η with itself is a matrix sharing the nonzero eigenvalues with the row-by-row product. This was one motive for Zaslavsky [16, 18] to define the line graph of a signed graph as the signed graph $\mathcal{L}_C(\Sigma) = (\mathcal{L}(G), \sigma_C)$ whose signature σ_C is determined by the adjacency matrix is $A_{\mathcal{L}_C(\Sigma)}$ defined here:

$$A_{\mathcal{L}_C(\Sigma)} = 2I - B_\eta^\intercal B_\eta. \tag{2.1}$$

Unlike in the case of the Laplacian matrix of Σ, the matrix $A_{\mathcal{L}_C(\Sigma)}$ does depend on the orientation η. On the other hand, choosing a different orientation η' of Σ leads to a matrix $A_{(\mathcal{L}(G),\sigma')}$ that is switching similar to $A_{(\mathcal{L}_C(G),\sigma)}$ (cf. [18]). Hence, $A_{(\mathcal{L}(G),\sigma)}$ defines a line graph up to switching similarity, so it can be used for spectral purposes. One of the benefits of this definition is that the line graph of a signed graph with an all-negative signature is a line graph with an all-negative signature. In other words, if $-G$ is a graph G whose edges are taken negatively, we get

$$\mathcal{L}_C(-G) = -\mathcal{L}(G).$$

The above fact has two evident consequences. The first one is that the iteration of the (Zaslavsky) line graph operator always gives a signed graph with all-negative signature, namely $\mathcal{L}_C^{(k)}(-G) = -\mathcal{L}^{(k)}(G)$. The second one is that if we map simple unsigned graphs to the theory of signed graphs as signed graphs with the all-negative signature (instead of the all-positive, as stated in the introduction), then Zaslavsky's line graph is a direct generalization of the usual line graph defined for unsigned graphs. We shall call this line graph the *combinatorial line graph* of Σ.

However, from a spectral viewpoint, the fact that the matrix $A_{\mathcal{L}_C(\Sigma)}$ has spectrum in the real interval $(-\infty, 2]$, is in contrast with the usual concept of spectral graph theory for which a line graph has spectrum in the real interval $[-2, +\infty]$. Hence, the authors of [3] decided to modify Zaslavsky's definition to

$$A_{(\mathcal{L}_S(G),\sigma)} = B_\eta^\intercal B_\eta - 2I. \tag{2.2}$$

In fact, the two definitions are virtually equivalent, as $\mathcal{L}_C(\Sigma) = -\mathcal{L}_S(\Sigma)$. Moreover, they can be used for different purposes. The latter definition is tailored for those spectral investigations in which an unsigned graph is considered as a signed one with all-positive signature. Clearly, in this case its adjacency (and Laplacian) matrix remains unchanged and the spectral theory of unsigned graphs can easily be encapsulated into the spectral theory of signed graphs. For example, in this case $\mathcal{L}_S(\Sigma)$ is coherent with the usual Laplacian and signless Laplacian spectral theories of unsigned graphs, and it can be used to investigate their spectra (cf. [2]). For these reasons, we shall call $\mathcal{L}_S(\Sigma)$ the *spectral line graph*. We note that Hoffmann's theory of generalized line graphs [9] fits well with both signatures.

In Figure 1 we illustrate an example of a signed graph Σ, an orientation Σ_η, and the consequent line graph $\mathcal{L}_C(\Sigma)$. Here and later, positive edges are represented by solid lines and negative edges are represented by dotted lines.

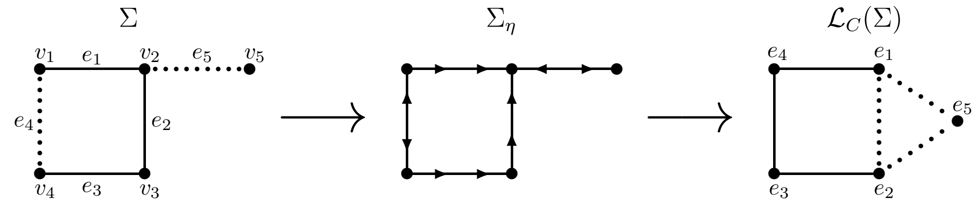

Figure 1: A signed graph, an orientation and the combinatorial line graph.

The matrix definitions of line graphs have combinatorial analogs; in fact, Zaslavsky's original definition of the line graph of a signed graph (even prior to [16]) was combinatorial. For $\Sigma = G_\sigma$ the underlying graph of $\mathcal{L}_*(\Sigma)$ is the line graph $\mathcal{L}(G)$, while the sign of the edge ef (e, f being the edges of Σ with a common vertex v) is

$$\sigma(ef) = \begin{cases} -\eta(ve)\eta(vf) & \text{for } * = C, \\ \eta(ve)\eta(vf) & \text{for } * = S. \end{cases} \tag{2.3}$$

Indeed, we may orient the line graph by defining $\eta_{\mathcal{L}}(e, ef) = \eta(v, e)$ for two edges e, f with common vertex v in Σ [18]. Then the combinatorial definition of line graph signs follows the rule (O3).

Remark 2.1. Which is the best definition of a line graph of a signed graph? Zaslavsky prefers the one defined in (2.1) because it is consistent with the basic relationship between signs and orientation stated in (O3). Belardo and Stanić instead prefer (2.2) because it is the one coherent with existing spectral graph theory and it is more prominent in the literature. This led to a long discussion among the three authors of this manuscript and the late Slobodan Simić. In the end, we recognize the validity of each definition, since either variant can be used and, after all, they are easily equivalent.

Remark 2.2. The identities (2.1) and (2.2) remain valid even if Σ contains multiple edges. A pair of edges located between the same pair of vertices form a *digon*, i.e., a 2-vertex cycle, which is positive if and only if the edges share the same sign. Here the matrix definition diverges from the combinatorial definition. In the combinatorial definition, a digon in Σ with edges e and f gives rise to a digon in the line graph having the same sign as the original digon; aside from signs, this is as in the unsigned line graph. In the matrix definitions of $\mathcal{L}_*(\Sigma)$ it gives rise to a pair of non-adjacent vertices if the corresponding digon is negative and a pair joined by two parallel edges of the same sign if the corresponding digon is positive; this is consistent with the fact that a negative digon in Σ disappears in the adjacency matrix A_Σ. Zaslavsky calls this kind of line graph, where parallel edges of opposite sign cancel each other, *reduced*. Therefore, an unreduced line graph has no multiple edges if and only if Σ has no digons, and a reduced line graph has no multiple edges if and only if Σ has no positive digons.

2.2 Properties of line graphs

Here are some observations that follow directly from (2.1) and (2.2). All triangles that arise from a star of Σ are negative (resp., positive) in $\mathcal{L}_C(\Sigma)$ (resp., $\mathcal{L}_S(\Sigma)$). Every cycle of Σ keeps its signature in $\mathcal{L}_C(\Sigma)$. Every even cycle of Σ keeps its signature in $\mathcal{L}_S(\Sigma)$ and every odd cycle of Σ reverses its signature in $\mathcal{L}_S(\Sigma)$.

Theorem 2.3. *Let G be an unsigned graph. Then $-\mathcal{L}_C(-G)$ and $\mathcal{L}_S(-G)$ are balanced signed graphs, and therefore switching equivalent to $+\mathcal{L}(G)$.*

First Proof. Recall that a balanced graph has no negative cycles. If we consider the line graph $\mathcal{L}(G)$, we distinguish three types of cycle:

(i) those that arise from the cycles of G,

(ii) those that arise from induced stars in G (forming cliques),

(iii) those obtained by combining the types (i) and (ii).

Let us consider $-\mathcal{L}_C(-G)$ and $\mathcal{L}_S(-G)$. We have to prove that $\mathcal{L}_C(-G)$ is antibalanced, or equivalently that $\mathcal{L}_S(-G)$ is balanced. In $\mathcal{L}_S(\Sigma)$ the signed cycles of type (i), originating from cycles C_k of Σ, get the sign $(-1)^k\sigma(C_k)$. Hence, they are all transformed into positive cycles of $\mathcal{L}_S(\Sigma)$ if and only if $\Sigma \sim -G$. Consider next the cycles of type (ii). The cliques (K_t, σ) of $\mathcal{L}_S(\Sigma)$, originating from an induced $K_{1,t}$ of G, are switching equivalent to $+K_t$. To see the latter, without loss of generality one can choose the biorientation of $K_{1,t}$ for which the vertex-edge incidence at the center of the star is positive (the arrows are inward directed), so the obtained clique is indeed $+K_t$. These cycles are always positive, regardless of the signature of Σ. Finally, for the cycles of type (iii), we know from [13] that the signs of a set of cycles that span the cycle space determine all the signs. Hence, the cycles of type (iii) are positive if and only if the cycles of type (i) are positive, that is, $\Sigma = -G$. □

Second Proof. Choose the orientation for $-G$ in which $\eta(v, e) = +1$ for every incident vertex and edge. Then $\mathcal{L}_C(-G)$ is easily seen to be all negative by the combinatorial definition (2.3) of edge signs, thus $\mathcal{L}_C(-G) = -\mathcal{L}(G)$, which is antibalanced. Then, $\mathcal{L}_S(-G) = -\mathcal{L}_C(-G) = +\mathcal{L}(G)$, which is balanced. Choosing a different orientation for $-G$ has the effect of switching both line graphs, so it does not change the state of balance or antibalance. □

We conclude this section by analysing balance and the degree of imbalance of line graphs. Because $\mathcal{L}_S(\Sigma) = -\mathcal{L}_C(\Sigma)$, balance of the combinatorial line graph $\mathcal{L}_C(\Sigma)$ is equivalent to antibalance of the spectral line graph $\mathcal{L}_S(\Sigma)$, and balance of the latter is equivalent to antibalance of the former.

Theorem 2.4. *Let $\Sigma = G_\sigma$ be a signed graph of order n and size m. The following hold true:*

(i) *$\mathcal{L}_C(\Sigma)$ is balanced (and $\mathcal{L}_S(\Sigma)$ is antibalanced) if and only if Σ is a disjoint union of paths and positive cycles.*

(ii) *$\mathcal{L}_S(\Sigma)$ is balanced (and $\mathcal{L}_C(\Sigma)$ is antibalanced) if and only if Σ is antibalanced.*

(iii) $l(\mathcal{L}_S(\Sigma)) \geq \nu(\mathcal{L}_S(\Sigma)) = l(-\Sigma)$.

(iv) $l(\mathcal{L}_C(\Sigma)) \geq \sum_{v\in V(\Sigma)} \lfloor \frac{(d(v)-1)^2}{4} \rfloor$.

Proof. (i): Balance of $\mathcal{L}_C(\Sigma)$ means that Σ does not contain a vertex of degree 3 or greater, as the corresponding edges produce negative triangles. Evidently, Σ cannot contain negative cycles, because this leads to negative cycles in $\mathcal{L}_C(\Sigma)$. If Σ is a disjoint union of paths and positive cycles, then $\mathcal{L}_C(\Sigma)$ is again a disjoint union of paths and positive cycles.

(ii): A line graph $\mathcal{L}(G)$ has three kinds of cycle. A vertex triangle corresponds to three edges incident with a single vertex of G; all vertex triangles are negative in $\mathcal{L}_C(\Sigma)$. A line cycle is derived from a cycle C in G and has the same sign in $\mathcal{L}_C(\Sigma)$. The remaining cycles are obtained by concatenation of cycles of the first two kinds. It follows that $\mathcal{L}_C(\Sigma)$ is antibalanced if and only if every line cycle is antibalanced, thus if and only if Σ is antibalanced.

(iii): An edge set A in $-\Sigma$ is a set A of vertices in $\mathcal{L}_S(\Sigma)$; and $\mathcal{L}_S(\Sigma)\setminus A = \mathcal{L}_S(\Sigma\setminus A)$. By (ii), $\mathcal{L}_S(\Sigma) \setminus A$ is balanced if and only if $-\Sigma \setminus A$ is balanced. Thus, the smallest size of an edge set A such that $-\Sigma \setminus A$ is balanced, which is $l(-\Sigma)$, equals the smallest size of a vertex set A such that $\mathcal{L}_S(\Sigma \setminus A)$ is balanced, which is $\nu(\mathcal{L}_S(\Sigma))$.

The inequality follows from the general observation that $l \geq \nu$ for every signed graph.

(iv): A vertex of degree $d(v)$ in Σ generates in $\mathcal{L}_C(\Sigma)$ an antibalanced vertex clique $-K_{d(v)}$. An edge set B in the line graph such that $\mathcal{L}_C(\Sigma) \setminus B$ is balanced must contain enough edges to make each such clique balanced; this number is $l(-K_{d(v)}) = \lfloor \frac{(d(v)-1)^2}{4} \rfloor$, obtained by dividing the vertices of $K_{d(v)}$ into two nearly equal sets and deleting the edges within each set. Each edge of the line graph is in only one vertex clique, so the minimum number of edges required to balance every vertex clique is the sum of these quantities. That proves the inequality. □

We do not expect equality in part (iv) because deleting the edges as in the proof may not eliminate all negative cycles in $\mathcal{L}_C(\Sigma)$. The problem of finding an exact formula for $l(\mathcal{L}_C(\Sigma))$ or $l(\mathcal{L}_S(\Sigma))$ in terms of Σ, or even a good lower bound that involves the signs of Σ, seems difficult.

3 Total graph(s)

Recall (say, from [6, page 64]) that, for a given graph G, the *total graph* $\mathcal{T}(G)$ is the graph obtained by combining the adjacency matrix of a graph with the adjacency matrix of its line graph and its vertex-edge incidence matrix. Precisely, the adjacency matrix of $\mathcal{T}(G)$ is given by

$$A_{\mathcal{T}(G)} = \begin{pmatrix} A_G & B \\ B^{\intercal} & A_{\mathcal{L}(G)} \end{pmatrix},$$

where $\mathcal{L}(G)$ denotes the line graph of G and B is the (unoriented) incidence matrix. Is it possible to have an analogous concept for signed graphs?

We will give a positive answer to the latter question. However, since we have multiple possibilities for line graphs of signed graphs, we build multiple total graphs.

3.1 Definitions of a total graph

Definition 3.1. The *total graph* of $\Sigma = G_\sigma$ is the signed graph determined by

$$A_{\mathcal{T}_*(\Sigma)} = \begin{pmatrix} A_\Sigma & B_\eta \\ B_\eta^\intercal & A_{\mathcal{L}_*(\Sigma_\eta)} \end{pmatrix}, \tag{3.1}$$

where $* \in \{C, S\}$.

In other words, in the combinatorial view, $\mathcal{T}_*(\Sigma)$ consists of two induced subgraphs, Σ and $\mathcal{L}_*(\Sigma_\eta)$, along with edges joining a vertex v of Σ to all vertices of $\mathcal{L}_*(\Sigma_\eta)$ that arise from the edges which are incident with v in Σ. The signature on these connecting edges is given by η, i.e., for a root-graph vertex v and an incident line-graph vertex e, $\sigma_{\mathcal{T}}(ve) = \eta(v, e)$. Note that this does not specify an orientation of the edge ve. One may adopt the convention that $\eta_{\mathcal{T}}(v, ve) = +1$, or any other convention, according to convenience. We do not need to do that because we have not defined an incidence matrix for $\mathcal{T}_*(\Sigma)$.

To fix the notation, $\mathcal{T}_C(\Sigma)$ and $\mathcal{T}_S(\Sigma)$ denote the total graphs defined by the combinatorial line graph (2.1) and the spectral line graph (2.2). Accordingly, we shall call them respectively the *combinatorial total graph* and the *spectral total graph*. If we want to consider both variants, we shall write $\mathcal{T}_*(\Sigma)$ instead. We need to show that our definition, regardless of $\Sigma \in [\Sigma]$ and of its chosen orientation η, gives rise to the same signed graph up to switching equivalence.

In Figure 2 we illustrate an example of a total graph of a signed graph. The root graph and the orientation are taken from Figure 1.

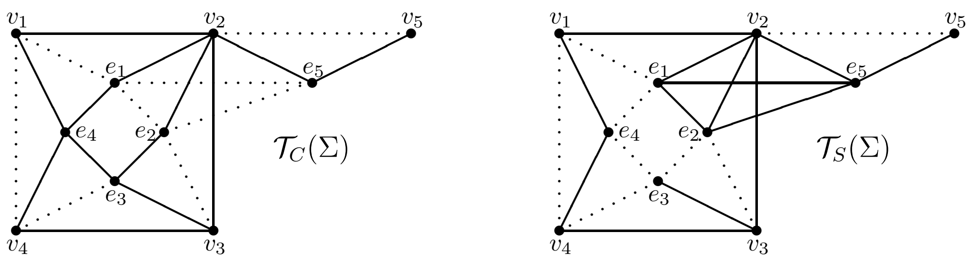

Figure 2: The combinatorial and the spectral total graphs resulting from Σ_η depicted in Figure 1.

We show that our definitions of a total graph are stable under reorientation and switching. For reorientation we have the first lemma.

Lemma 3.2. *Let $\Sigma = G_\sigma$ be a signed graph, and Σ_η and $\Sigma_{\eta'}$ two orientations of Σ. Then $\mathcal{T}_*(\Sigma_\eta)$ and $\mathcal{T}_*(\Sigma_{\eta'})$ are switching equivalent, for each $* \in \{C, S\}$.*

Proof. For the sake of readability, we will restrict the discussion to the combinatorial line graph defined by Zaslavsky. Hence, hereafter $\mathcal{L}(\Sigma) := \mathcal{L}_C(\Sigma)$ and $\mathcal{T}(\Sigma_\eta) := \mathcal{T}_C(\Sigma_\eta)$.

Let $G = (V, E)$, where $|V| = n$ and $|E| = m$. Suppose that η and η' differ on some set $F \subseteq E$, and let B_η and $B_{\eta'}$ be the corresponding vertex-edge incidence matrices, respectively. Let $S = (s_{ij})$ be the $m \times m$ diagonal matrix such that $s_{ii} = -1$ if $e_i \in F$

and $s_{ii} = 1$, otherwise. Then $B_{\eta'} = B_\eta S$. Since $S = S^\intercal = S^{-1}$, in view of (2.1), we have

$$A_{\mathcal{L}(\Sigma_{\eta'})} = 2I - B_{\eta'}^\intercal B_{\eta'} = S^\intercal(2I - B_\eta^\intercal B_\eta)S = S^\intercal A_{\mathcal{L}(\Sigma_\eta)} S.$$

Therefore,

$$\begin{aligned} A_{\mathcal{T}(\Sigma_{\eta'})} &= \begin{pmatrix} A_\Sigma & B_{\eta'} \\ B_{\eta'}^\intercal & A_{\mathcal{L}(\Sigma_{\eta'})} \end{pmatrix} \\ &= \begin{pmatrix} A_\Sigma & B_\eta S \\ S^\intercal B_\eta^\intercal & S^\intercal A_{\mathcal{L}(\Sigma_\eta)} S \end{pmatrix} \\ &= \begin{pmatrix} I & O \\ O & S^\intercal \end{pmatrix} \begin{pmatrix} A_\Sigma & B_\eta \\ B_\eta^\intercal & A_{\mathcal{L}(\Sigma_\eta)} \end{pmatrix} \begin{pmatrix} I & O \\ O & S \end{pmatrix} \\ &= \begin{pmatrix} I & O \\ O & S \end{pmatrix}^{-1} A_{\mathcal{T}(\Sigma_\eta)} \begin{pmatrix} I & O \\ O & S \end{pmatrix}. \end{aligned}$$

This completes the proof. □

Next, we prove that switching equivalent signed graphs produce switching equivalent total graphs.

Lemma 3.3. *If Σ and Σ' are switching equivalent, then $\mathcal{T}_*(\Sigma)$ and $\mathcal{T}_*(\Sigma')$ are switching equivalent as well, for each $* \in \{C, S\}$.*

Proof. The notation is the same as in Lemma 3.2. Since Σ and Σ' are switching equivalent, their adjacency matrices are switching similar. Hence, $A_\Sigma = S^{-1} A_{\Sigma'} S$ for some switching matrix S. Observe that if $B = B_\eta$ is a vertex-edge incidence matrix of Σ, then $B' = SB_\eta$ is a vertex-edge incidence matrix of Σ'. Additionally, in view of (2.1), we have $A_{\mathcal{L}(\Sigma)} = 2I - B^\intercal B$.

Therefore, (for Σ') we have

$$\begin{aligned} A_{\mathcal{T}(\Sigma')} &= \begin{pmatrix} A_{\Sigma'} & B' \\ B'^\intercal & A_{\mathcal{L}(\Sigma')} \end{pmatrix} = \begin{pmatrix} A_{\Sigma'} & B' \\ B'^\intercal & 2I - B'^\intercal B' \end{pmatrix} \\ &= \begin{pmatrix} S^{-1} A_\Sigma S & SB \\ (SB)^\intercal & 2I - B^\intercal (S^\intercal S) B \end{pmatrix} \\ &= \begin{pmatrix} S & O \\ O & I \end{pmatrix}^{-1} \begin{pmatrix} A_\Sigma & B \\ B^\intercal & A_{\mathcal{L}(\Sigma)} \end{pmatrix} \begin{pmatrix} S & O \\ O & I \end{pmatrix} \\ &= \begin{pmatrix} S & O \\ O & I \end{pmatrix}^{-1} A_{\mathcal{T}(\Sigma)} \begin{pmatrix} S & O \\ O & I \end{pmatrix}. \end{aligned}$$

Hence, $\mathcal{T}(\Sigma)$ is switching equivalent to $\mathcal{T}(\Sigma')$, and we are done. □

In view of Lemmas 3.2 and 3.3 the definition given by (3.1) can be used for spectral investigations.

Remark 3.4. A careful reader has probably noticed that the switching matrix in Lemma 3.2 is the one realizing switching equivalence between the line graphs, while the switching matrix in Lemma 3.3 is the one realizing switching equivalence between the root signed graphs. In general, if we have two switching equivalent total graphs, then the switching matrix will be obtained by combining the switching matrices of the corresponding root and line graphs.

Remark 3.5. The spectral total graph $\mathcal{T}_S(\cdot)$ does not generalize the total graph of an unsigned graph, because with the $\mathcal{T}_S$ operator the total graph of an all-positive signed graph does not have an all-positive signature, as the convention of treating unsigned graphs as all positive and the definition of the unsigned total graph would imply. On the other hand, if we consider unsigned graphs as signed graphs with the all-negative signature, then $\mathcal{T}_C(-G) = -\mathcal{T}(G)$, so that $\mathcal{T}_C$ can be considered as the generalization to signed graphs of the unsigned total graph operator. This observation lends some support to using the line graph operator $\mathcal{L}_C$ in spectral graph theory and treating unsigned graphs as all negative, though contrary to existing custom.

3.2 Properties of total graphs

Now we study some structural and spectral properties of $\mathcal{T}_C(\Sigma)$ and $\mathcal{T}_S(\Sigma)$. We begin by computing the number of triangles of $\mathcal{T}_*(\Sigma)$.

Theorem 3.6. *Let an unsigned graph G have order n, size m, degree sequence $(d_1, d_2, \dots, d_n)$, and t triangles. Then the number of triangles of $\mathcal{T}_*(G)$ is $2t + m + \sum_{i=1}^{n} \binom{d_i+1}{3}$.*

Proof. Every triangle of $\mathcal{T}_*(G)$ is one of the following four types:

(a) belongs to G,

(b) belongs to $\mathcal{L}_*(G)$,

(c) has 1 vertex in G and 2 vertices in $\mathcal{L}_*(G)$,

(d) has 2 vertices in G and 1 vertex in $\mathcal{L}_*(G)$.

Every triangle of $\mathcal{L}_*(G)$ arises from a triplet of adjacent edges of G. Such a triplet either forms a triangle or has a common vertex. Therefore, $\mathcal{L}_*(G)$ contains $t + \sum_{i=1}^{n} \binom{d_i}{3}$ triangles.

Every triangle of type (c) arises from a pair of adjacent edges of G, so their number is $\sum_{i=1}^{n} \binom{d_i}{2}$.

Every triangle of type (d) arises from an edge of G, so their number is m.

Altogether, the number of triangles is

$$t + t + \sum_{i=1}^{n} \binom{d_i}{3} + \sum_{i=1}^{n} \binom{d_i}{2} + m = 2t + m + \sum_{i=1}^{n} \binom{d_i+1}{3},$$

as claimed. □

Moreover, we can establish which triangles are either positive or negative.

Theorem 3.7. *Let $\Sigma = G_\sigma$ be a signed graph of order n, size m, degree sequence $(d_1, d_2, \dots, d_n)$, and $t = t^+ + t^-$ triangles, where t^+ (resp., t^-) denotes the number of positive (resp., negative) triangles. Then $\mathcal{T}_C(\Sigma)$ has exactly $2t^+$ positive triangles, while $\mathcal{T}_S(\Sigma)$ has exactly $t + m$ negative triangles.*

Proof. The total number of triangles is computed in Theorem 3.6.

We have the following facts that the reader can easily check. The triangles of type (a) will keep their sign in the total signed graph. Hence, we have t^+ positive triangles for $\mathcal{T}_C(\Sigma)$ and t^- negative triangles for $\mathcal{T}_S(\Sigma)$.

A positive (negative) triangle in Σ becomes a positive (negative) triangle in $\mathcal{L}_C(G)$, and a negative (positive) triangle in $\mathcal{L}_S(G)$. A set of mutually adjacent edges in G will give rise to a complete graph in $\mathcal{L}_*(G)$ whose signature is equivalent to the all-negative (resp., all-positive) one for $\mathcal{L}_C(\Sigma)$ (resp., $\mathcal{L}_S(\Sigma)$). Summing up, the triangles of type (b) will be t^+ positive for $\mathcal{T}_C(\Sigma)$ and t^+ negative for $\mathcal{T}_S(\Sigma)$.

Next, let us consider a triangle of type (c). Such a triangle of $\mathcal{T}_*(\Sigma)$ is obtained from two edges, say vu and vw, of Σ that are incident to the same vertex v. Regardless of $\sigma(vu)$ and $\sigma(vw)$, we can assign an orientation such that the arrows from the side of v are both inward (directed towards v). Hence, the edges $\{v, vw\}$ and $\{v, uv\}$ of $\mathcal{T}_*(\Sigma)$ will be positive, while the edge $\{vu, vw\}$ will be negative (resp., positive) in $\mathcal{T}_C(\Sigma)$ (resp., $\mathcal{T}_S(\Sigma)$).

Finally, a triangle of type (d) comes from a pair of adjacent vertices u and v and the joining edge uv. Again, regardless of $\sigma(uv)$ and with a similar reasoning as above, the resulting triangle will always be negative in $\mathcal{T}_*(\Sigma)$.

Now, the statement easily follows by counting the positive (negative) triangles of $\mathcal{T}_C(\Sigma)$ (resp., $\mathcal{T}_S(\Sigma)$). □

Remark 3.8. From Theorem 3.7 we easily deduce that $\mathcal{T}_C(\Sigma)$ and $\mathcal{T}_S(\Sigma)$ have in general switching inequivalent signatures which are not the opposite of each other. Hence, in contrast to the line graphs defined by (2.1) and (2.2), the total graphs derived from them have unrelated signatures.

We conclude this section by analysing the degree of imbalance of these compound graphs. A *vertex cover* of a graph is a set of vertices such that every edge has at least one end in the cover. The smallest size of a vertex cover is the *vertex cover number*, τ.

Theorem 3.9. *Let $\Sigma = G_\sigma$ be a signed graph of order n, size m, and vertex cover number τ. The following hold true:*

(i) *$\mathcal{T}_*(\Sigma)$ is balanced if and only if G is totally disconnected.*

(ii) *$\mathcal{T}_*(\Sigma)$ is antibalanced if and only if either $* = S$ and Σ has no adjacent edges, or $* = C$ and Σ is antibalanced.*

(iii) *$l(\mathcal{T}_*(\Sigma)) \geq m + l(\mathcal{L}_*(\Sigma))$, with equality when $* = S$, and also when $* = C$ and Σ is a disjoint union of paths and cycles.*

(iv) *$l(\mathcal{T}_*(\Sigma)) = m$ if and only if either $* = S$ and Σ is antibalanced, or $* = C$ and Σ is a disjoint union of paths and positive cycles.*

(v) *$\nu(\mathcal{T}_*(\Sigma)) \geq \tau$, with equality if $* = S$ and Σ is antibalanced.*

(vi) *$\nu(\mathcal{T}_S(\Sigma)) \leq \tau + \nu(\mathcal{L}_S(\Sigma))$.*

(vii) *The largest (adjacency) eigenvalue λ of $\mathcal{T}_*(\Sigma)$ satisfies*

$$\lambda \leq \max\left\{\frac{-d_i + \sqrt{5d_i^2 + 4(d_i m_i - 4)}}{2} \ : \ 1 \leq i \leq n+m\right\},$$

where d_i and m_i denote, respectively, the degree of a vertex i of $\mathcal{T}_*(\Sigma)$ and the average degree of its neighbours.

Proof. (i): Each edge of Σ leads to a negative triangle of type (d), so $\mathcal{T}_*(\Sigma)$ is balanced if and only if Σ has no edges.

(ii): Adjacent edges lead to a positive triangle of type (c) in $\mathcal{T}_S(\Sigma)$, hence it cannot be antibalanced. If there are no adjacent edges, $\mathcal{T}_S(\Sigma)$ consists only of negative triangles of type (d) and any isolated vertices of Σ, which is antibalanced.

There are four kinds of cycle to consider in $\mathcal{T}_C(\Sigma)$: triangles of types (c) and (d) and cycles in Σ and $\mathcal{L}_C(\Sigma)$. The triangles are negative, hence antibalanced. If Σ is not antibalanced, the total graph cannot be, but if Σ, thus also $\mathcal{L}_C(\Sigma)$ by Theorem 2.4(ii), is antibalanced, then it follows – from the fact that all cycles in the total graph are obtained by combining cycles of those four kinds – that the total graph is antibalanced.

(iii): The m triangles of type (d) of the proof of Theorem 3.6 are negative and independent, in the sense that no two of them share the same edge. Therefore, to eliminate each of them it is necessary to delete m edges (for example, the edges of Σ in $\mathcal{T}_*(\Sigma)$). Deleting these edges does not change the frustration index of the subgraph $\mathcal{L}_*(\Sigma)$, so at least an additional $l(\mathcal{L}_*(\Sigma))$ edges must be deleted to attain balance of $\mathcal{T}_*(\Sigma)$. Hence, we have the inequality.

Equality holds for $\mathcal{T}_S(\Sigma)$ because the triangles of type (c) are positive. In $\mathcal{T}_C(\Sigma)$ those triangles are negative. When Σ is a disjoint union of paths and positive cycles, then the negative cycles are those of type (c) and (d) which share a common edge. Deleting such independent edges (there are m of them) leads to a balanced signed graph. When Σ has a negative cycle, one edge in those triangles can be replaced by one edge each in the negative cycle in Σ and in the corresponding negative cycle in $\mathcal{L}_C(\Sigma)$ for a total of one extra edge for each negative cycle of Σ.

(iv): The equality for $\mathcal{T}_S(\Sigma)$ holds under the formulated conditions since there $\mathcal{L}_S(\Sigma)$ is balanced and then the entire $\mathcal{T}_S(\Sigma)$ becomes balanced after deleting all m edges of Σ. For $\mathcal{T}_C(\Sigma)$ the result follows from (iii).

Conversely, if $l(\mathcal{T}_*(\Sigma)) = m$, then $\mathcal{L}_*(\Sigma)$ must be balanced, i.e., it cannot contain a negative cycle. For $* = S$, this means that Σ is antibalanced. For $* = C$, this means that Σ does not contain a vertex of degree 3 or greater, as the corresponding edges produce negative triangles. Evidently, Σ cannot contain negative cycles, because this leads to additional negative cycles in $\mathcal{T}_C(\Sigma)$. If Σ is a disjoint union of paths and positive cycles, the equality follows from (iii).

(v): Consider $\mathcal{T}_*(\Sigma)$. For both variants we need to eliminate (at least) the negative triangles of type (d). Instead of deleting the edges of Σ, we can just delete a minimum vertex cover of Σ and obtain the same effect. The equality is obtained for $\mathcal{T}_S(-G)$.

(vi): If B is a minimum set of vertices of $\mathcal{L}_S(\Sigma)$ such that deleting every vertex in B leaves a balanced line graph $\mathcal{L}_S(\Sigma)$, then deleting the same vertices from the line graph in $\mathcal{T}_S(\Sigma)$ while also deleting a minimum vertex cover from Σ in $\mathcal{L}_S(\Sigma)$ as in the proof of (v) eliminates all negative cycles in the total graph.

(vii): Note that, unless G is totally disconnected, every vertex of $\mathcal{T}_*(\Sigma)$ belongs to at least one negative triangle – this triangle is again of type (d). Accordingly, the result follows by the inequality of [11]:

$$\lambda \leq \max\left\{\frac{-d_i + \sqrt{5d_i^2 + 4(d_i m_i - 4t_i^-)}}{2} \ : \ 1 \leq i \leq n+m\right\},$$

where t_i^- stands for the number of negative triangles passing through a vertex i. □

Remark 3.10. It is not the case that $\nu(\mathcal{T}_C(\Sigma)) \leq \tau + \nu(\mathcal{L}_C(\Sigma))$. A counterexample is a sufficiently long cycle of either sign, for which $\tau \approx \frac{1}{2}m$, $\nu(\mathcal{L}_C(\Sigma)) \leq 1$, and $\nu(\mathcal{T}_*(\Sigma)) \approx \frac{2}{3}m \approx \frac{4}{3}\tau > \tau + 1$ due to the negative triangles of types (c) and (d).

4 Total graphs of regular signed graphs

A signed graph $\Sigma = G_\sigma$ is said to be r-regular if its underlying graph G is an r-regular graph.

4.1 Spectrum

We infer that the spectrum of Σ lies in the real interval $[-r,\, r]$. We compute the spectrum of $\mathcal{T}_*(\Sigma)$ by means of the eigenvalues of the root (signed) graph Σ, when it is regular.

Theorem 4.1. *Let Σ be an r-regular signed graph $(r \geq 2)$ with n vertices and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then:*

(i) *The eigenvalues of $\mathcal{T}_C(\Sigma)$ are 2 with multiplicity $(\frac{r}{2} - 1)n$ and*

$$\frac{1}{2}\big(2 + 2\lambda_i - r \pm \sqrt{r^2 - 4\lambda_i + 4}\big), \ \textit{for} \ 1 \leq i \leq n.$$

(ii) *The eigenvalues of $\mathcal{T}_S(\Sigma)$ are -2 with multiplicity $(\frac{r}{2} - 1)n$ and*

$$\frac{1}{2}\big(r - 2 \pm \sqrt{(r - 2\lambda_i)^2 + 4(\lambda_i + 1)}\big), \ \textit{for} \ 1 \leq i \leq n.$$

Proof. The proof is inspired from Cvetković's proof of the theorem concerning the total graphs of regular unsigned graphs [6, Theorem 2.19]. Due to the inconsistency between the concepts of line graphs of unsigned graphs and that of spectral line graphs of signed graphs, our proof differs at some points, as do the final results.

Since Σ is r-regular, for some incidence matrix B, we have $BB^\intercal = L_\Sigma = D_G - A_\Sigma = rI - A_\Sigma$, $A(\mathcal{L}_C(\Sigma)) = 2I - B^\intercal B$, and $A(\mathcal{L}_S(\Sigma)) = B^\intercal B - 2I$.

The characteristic polynomial of $\mathcal{T}_C(\Sigma)$ is given by

$$\begin{aligned}\Phi_{\mathcal{T}_C(\Sigma)}(x) &= \begin{vmatrix} xI - A_\Sigma & -B \\ -B^\intercal & xI - \mathcal{L}_C(\Sigma) \end{vmatrix} \\ &= \begin{vmatrix} xI - rI + BB^\intercal & -B \\ -B^\intercal & xI - 2I + BB^\intercal \end{vmatrix}.\end{aligned}$$

Multiplying the first row of the block determinant by $B^\intercal$ and adding to the second, and then multiplying the second by $\frac{1}{x-2}B$ and adding to the first one, we get

$$\Phi_{\mathcal{T}_C(\Sigma)}(x) = \begin{vmatrix} (x-r)I + BB^\intercal + \frac{1}{x-2}\big((x-r-1)BB^\intercal + BB^\intercal BB^\intercal\big) & O \\ (x-r-1)B^\intercal + B^\intercal BB^\intercal & (x-2)I \end{vmatrix}.$$

Further, we compute

$$\begin{aligned}\Phi_{\mathcal{T}_C(\Sigma)}(x) &= (x-2)^{\frac{r}{2}n}\big|(x-r)I+BB^{\intercal}+\frac{1}{x-2}\big((x-r-1)BB^{\intercal}+BB^{\intercal}BB^{\intercal}\big)\big|\\ &= (x-2)^{\frac{r}{2}n}\big|xI-A_{\Sigma}+\frac{1}{x-2}\big((x-r-1)(rI-A_{\Sigma})+(rI-A_{\Sigma})^2\big)\big|\\ &= (x-2)^{(\frac{r}{2}-1)n}\big|A_{\Sigma}^2+(3-2x-r)A_{\Sigma}+(x^2+x(r-2)-r)I\big|\\ &= (x-2)^{(\frac{r}{2}-1)n}\prod_{i=1}^{n}\big(\lambda_i^2+(3-2x-r)\lambda_i+(x^2+x(r-2)-r)\big)\\ &= (x-2)^{(\frac{r}{2}-1)n}\prod_{i=1}^{n}\big(x^2+(r-2-2\lambda_i)x+\lambda_i^2+(3-r)\lambda_i-r\big).\end{aligned}$$

Since the roots of $x^2+(r-2-2\lambda_i)x+\lambda_i^2+(3-r)\lambda_i-r=0$ are given by $\frac{1}{2}\big(2+2\lambda_i-r\pm\sqrt{r^2-4\lambda_i+4}\big)$, (i) follows.

Item (ii) follows similarly, by taking the spectral variant of the line graph. □

From the above theorem we can deduce the real interval containing the eigenvalues of the total graph of a regular signed graph.

Corollary 4.2. *Let Σ be an r-regular signed graph with n vertices and eigenvalues $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$. Then:*

(i) *The spectrum of $\mathcal{T}_C(\Sigma)$, if $r\geq 4$, lies in the interval*

$$\Big[\frac{1}{2}(2+\lambda_n-r-\sqrt{r^2-4\lambda_n+4}),\ \frac{1}{2}(2+\lambda_1-r+\sqrt{r^2-4\lambda_1+4})\Big].$$

(ii) *The spectrum of $\mathcal{T}_S(\Sigma)$, if $r\geq 2$, lies in the interval*

$$\Big[\frac{1}{2}(r-2-\sqrt{(r-2\lambda_n)^2+4(\lambda_n+1)}),\ \frac{1}{2}(r-2+\sqrt{(r-2\lambda_n)^2+4(\lambda_n+1)})\Big].$$

Proof. Consider first $\mathcal{T}_C(\Sigma)$. It is routine to check that the function $f_1(\lambda)=\frac{1}{2}(2+\lambda-r+\sqrt{r^2-4\lambda+4})$ is increasing for $\lambda\in[-r,r]$ when $r\geq 4$. Hence, the maximum of f_1 is attained for λ_1. The function $f_2(\lambda)=\frac{1}{2}(2+\lambda-r-\sqrt{r^2-4\lambda+4})$ is always increasing, therefore, its minimum is achieved by λ_n. Hence, the entire spectrum of $\mathcal{T}_C(\Sigma)$ lies in $[f_2(\lambda_n),\ f_1(\lambda_1)]$, and we get (i).

Consider next $\mathcal{T}_S(\Sigma)$. Analysing the function

$$f_3(\lambda)=\sqrt{(r-2\lambda)^2+4(\lambda+1)}=\sqrt{(2\lambda-(r-1))^2+2r+3},$$

we find that it is decreasing for $\lambda\leq\frac{r-1}{2}$, increasing for $\lambda\geq\frac{r-1}{2}$, and symmetric around $\frac{r-1}{2}$. Since $\lambda_1\leq r$ and $\lambda_n\leq -1$ (this holds for every signed graph by induction on the number of edges using eigenvalue interlacing), we have $\frac{r-1}{2}-\lambda_n\geq|\frac{r-1}{2}-\lambda_1|$. Since our function is symmetric around $\frac{r-1}{2}$, the last inequality leads to $f_3(\lambda_n)\geq f_3(\lambda_1)$. Hence, $\frac{1}{2}(r-2+f_3(\lambda_n))$ is the largest eigenvalue of $\mathcal{T}_S(\Sigma)$. There are two candidates for the least eigenvalue of the same signed graph: $\frac{1}{2}(r-2-f_3(\lambda_n))$ and (according to Theorem 4.1(ii)) -2. Taking into account that $\lambda_n\leq -1$, we get $\frac{1}{2}(r-2-f_3(\lambda_n))\leq -2$, and thus the least eigenvalue is $\frac{1}{2}(r-2-f_3(\lambda_n))$, which completes (ii). □

4.2 A composition

We next consider a particular composition of spectral total graphs – those whose definition is based on the spectral line graph. Of course, similar results can be obtained in case of the combinatorial definition. Some further definitions and notation are needed. The *Cartesian product* (see also [8]) of the signed graphs $\Sigma_1 = (G_1, \sigma_1)$ and $\Sigma_2 = (G_2, \sigma_2)$ is determined in the following way: (1) Its underlying graph is the Cartesian product $G_1 \times G_2$; we state for the sake of completeness that its vertex set is $V(G_1) \times V(G_2)$, and the vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if either $u_1 = v_1$ and u_2 is adjacent to v_2 in G_2 or $u_2 = v_2$ and u_1 is adjacent to v_1 in G_1. (2) The sign function is defined by

$$\sigma((u_1, u_2), (v_1, v_2)) = \begin{cases} \sigma_1(u_1, v_1) & \text{if } u_2 = v_2, \\ \sigma_2(u_2, v_2) & \text{if } u_1 = v_1. \end{cases}$$

For the real multisets $\mathcal{S}_1$ and $\mathcal{S}_2$, we denote by $\mathcal{S}_1 + \mathcal{S}_2$ the multiset containing all possible sums of elements of $\mathcal{S}_1$ and $\mathcal{S}_2$ (taken with their repetition). Especially, if $\mathcal{S}_2$ consists of the additive identity repeated i times, then the previous sum is denoted by $\mathcal{S}_1^i$ and consists of the elements of $\mathcal{S}_1$, each with multiplicity increased by the factor i. Let further $\mathrm{Spec}(G_\sigma)$ denote the spectrum of G_σ.

Inspired by [4, 5], we consider the polynomial $p(G_\sigma) = \sum_{i=0}^{k} c_i G_\sigma^i$, where $c_0, c_1, \ldots,$ c_k are non-negative integers ($c_k \neq 0$), G_σ is a regular signed graph with a fixed orientation, G_σ^i is the ith power of G_σ with respect to the spectral total graph operation (that is, $G_\sigma^i = \mathcal{T}_S^{i-1}(G_\sigma)$, $i > 0$, and $G_\sigma^0 = K_1$), $c_i G_\sigma^i$ denotes the disjoint union of c_i copies of G_σ^i, and the sum of signed graphs is their Cartesian product.

Theorem 4.3. *For an r-regular signed graph G_σ ($r \geq 2$) with n vertices,*

$$\mathrm{Spec}(p(G_\sigma)) = \sum_{i=0}^{k} \mathrm{Spec}(G_\sigma^i)^{c_i}, \tag{4.1}$$

where, for $i \geq 2$, $\mathrm{Spec}(G_\sigma^i)$ is comprised of -2 with multiplicity $(\frac{r_{i-1}}{2} - 1)n_{i-1}$ and

$$\frac{1}{2}\Big(r_{i-1} - 2 \pm \sqrt{\big(r_{i-1} - 2\lambda_j^{(i-1)}\big)^2 + 4\big(\lambda_j^{(i-1)} + 1\big)}\ \Big), \ \textit{for}\ 1 \leq j \leq n_{i-1},$$

where $r_i = 2^{i-1}r$, $n_1 = n$, $n_i = n\prod_{j=2}^{i}(2^{j-3}r + 1)$, and with $\lambda_1^{(i-1)}, \lambda_2^{(i-1)}, \ldots, \lambda_{n_{i-1}}^{(i-1)}$ being the eigenvalues of G_σ^{i-1}.

Proof. Since, for a non-negative integer c, $\mathrm{Spec}(c\Sigma) = \mathrm{Spec}(\Sigma)^c$ and $\mathrm{Spec}(\Sigma_1 + \Sigma_2) = \mathrm{Spec}(\Sigma_1) + \mathrm{Spec}(\Sigma_2)$ (for the latter, see [8]), we arrive at (4.1), and thus it remains to compute $\mathrm{Spec}(\Sigma^i)$. The case $i \leq 1$ is clear; clearly, for $i \geq 2$, $\mathrm{Spec}(\Sigma^i)$ is as in the theorem, where r_{i-1} and n_{i-1} are the vertex degree and the number of vertices of Σ^{i-1}.

By the definition of a total graph we have $r_i = 2r_{i-1}$, which along with $r_1 = r$ leads to $r_i = 2^{i-1}r$.

By the same definition, we also have $n_i = n_{i-1} + m_{i-1}$, where $m_{i-1} = \frac{1}{2}n_{i-1}r_{i-1}$ is the number of edges of Σ^{i-1}. So, $n_i = n_{i-1} + \frac{1}{2}n_{i-1}r_{i-1} = n_{i-1}\big(\frac{1}{4}r_i + 1\big)$. Solving, we get

$$n_i = n\prod_{j=2}^{i}\Big(\frac{1}{4}r_i + 1\Big) = n\prod_{j=2}^{i}(2^{j-3}r + 1),$$

and we are done. □

Regarding the last theorem, for $r = 0$ the resulting spectrum is trivial. For $r = 1$, $\mathrm{Spec}(\Sigma^2)$ is computed directly, not as in the theorem.

4.3 Eulerian regular digraph

We conclude the paper by offering a result which applies only to a signed graph that is regular and with all edges positive. Note that, by the definition, an oriented all-positive signed graph is precisely a directed graph. An eigenvalue of a signed graph G_σ is called *main* if there is an associated eigenvector not orthogonal to the all-1 vector $\mathbf{j}$. An orientation of a (signed) graph is called *Eulerian* if the in-degree equals the out-degree at every vertex.

Theorem 4.4. *Let $\Sigma = G_\sigma$ be an r-regular signed graph with the all-positive signature and an Eulerian orientation η. Then $\mathcal{T}_S(\Sigma_\eta)$ has exactly two main eigenvalues: r and -2.*

Proof. The assumptions of positive edges and Eulerian orientation mean that the row sums of B_η are zero. Under our assumptions, every block of (3.1) has a constant row sum given in the following (quotient) matrix

$$Q = \begin{pmatrix} r & 0 \\ 0 & -2 \end{pmatrix}.$$

The spectrum of Q contains the main part of the spectrum of $\mathcal{T}_S(\Sigma_\eta)$. (The explicit proof can be found in [12], but the reader can also consult [6, Chapter 4] or [1].) By definition, every signed graph has at least one main eigenvalue. If $\mathcal{T}_S(\Sigma_\eta)$ has exactly one main eigenvalue, then the eigenspace of any other is orthogonal to $\mathbf{j}$, which implies that $\mathbf{j}$ is associated with the unique main eigenvalue, but this is impossible (for $\mathcal{T}_S(\Sigma_\eta)$, observe Q). Therefore, both eigenvalues of Q are the main eigenvalues of $\mathcal{T}_S(\Sigma_\eta)$, and we are done. □

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Domination type parameters of Pell graphs*

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Abstract

Pell graphs are defined on certain ternary strings as special subgraphs of Fibonacci cubes of odd index. In this work the domination number, total domination number, 2-packing number, connected domination number, paired domination number, and signed domination number of Pell graphs are studied. Using integer linear programming, exact values and some estimates for these numbers of small Pell graphs are obtained. Furthermore, some theoretical bounds are obtained for the domination numbers and total domination numbers of Pell graphs.

Keywords: Pell graphs, Fibonacci cube, domination number, integer linear programming.

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1 Introduction

One of the basic models for interconnection networks is the n-dimensional hypercube graph Q_n. It has 2^n vertices, represented by all binary strings of length n, and two vertices in Q_n are adjacent if they differ in exactly one coordinate. For convenience, we set

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$Q_0 = K_1$. The n dimensional *Fibonacci cube* Γ_n is defined as the subgraph of Q_n induced by the vertices whose string representations are Fibonacci strings. They were introduced by Hsu [10] as an alternative model for interconnection networks and extensively studied in the literature [13]. There are numerous subgraphs and variants of Fibonacci cubes in the literature, such as Lucas cubes [15], generalized Fibonacci cubes [11], k-Fibonacci cubes [5] and Pell graphs [14].

Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. A set $D \subseteq V$ is called a *dominating set* of G if every vertex in $V \setminus D$ is adjacent to some vertex in D. Then the *domination number* $\gamma(G)$ of G is defined as the minimum cardinality of a dominating set of G. Similarly, a set $D \subseteq V$ is called a *total dominating set* of a graph G without isolated vertices, if every vertex in V is adjacent to some vertex in D and the *total domination number* $\gamma_t(G)$ of G is defined as the minimum cardinality of a total dominating set of G.

The domination type parameters of Fibonacci and Lucas cubes are first considered in [3, 17]. Using integer linear programming, domination and total domination numbers of these cubes and some additional domination type parameters of these cubes [2, 12] and hypercubes [2] are considered in the literature. Furthermore, upper bounds and lower bounds on domination and total domination numbers of Fibonacci and Lucas cubes are obtained in [2, 3, 17, 18, 19, 20]. The domination and total domination number of k-Fibonacci cubes are considered in [6]. In this work, we studied some domination type parameters of Pell graphs.

2 Preliminaries

Let f_n denote the Fibonacci numbers defined as $f_0 = 0$, $f_1 = 1$ and $f_n = f_{n-1} + f_{n-2}$ for $n \geq 2$. Similarly, let p_n denote the Pell numbers defined as $p_0 = 1$, $p_1 = 2$ and $p_n = 2p_{n-1} + p_{n-2}$ for $n \geq 2$. Here we remark that the generating function of p_n (see, for example [9]) is

$$\sum_{n\geq 0} p_n x^n = \frac{1}{1 - 2x - x^2}. \tag{2.1}$$

Binary strings of length n not containing two consecutive 1s constitute the set of *Fibonacci strings* $\mathcal{F}_n$ of length n, that is, the binary strings $b_1 b_2 \ldots b_n$ such that $b_i \cdot b_{i+1} = 0$ for all $i = 1, 2, \ldots, n-1$.

Ternary strings over the alphabet $\{0, 1, 2\}$ where there are no maximal blocks of 2s of odd length constitute the set of *Pell strings*, $\mathcal{P}_n$. Then the n dimensional Pell graph, Π_n, is defined as the simple graph where the vertices are represented by the Pell strings of length n, and two vertices are adjacent whenever one of them can be obtained from the other by replacing a 0 with a 1 (or vice versa), or by replacing a factor 11 with 22 (or vice versa) [14]. The vertices of Π_n can be partitioned into vertices that start with 0, vertices that start with 1 and vertices that start with 22. The subgraphs induced by these vertices are isomorphic to Π_{n-1}, Π_{n-1}, and Π_{n-2}, respectively. This gives the following canonical decomposition of Pell graphs for $n \geq 2$

$$\Pi_n = 0\Pi_{n-1} + 1\Pi_{n-1} + 22\Pi_{n-2}, \tag{2.2}$$

where $\Pi_0 = K_1$ and $\Pi_1 = K_2$. Here remark that we have also to add the edges of perfect matchings between $0\Pi_{n-1}$ and $1\Pi_{n-1}$; and also between $22\Pi_{n-2}$ and $11\Pi_{n-1}$ (an induced subgraph of $1\Pi_{n-1}$).

Every Pell string decomposes uniquely into the product of the factors $0, 1$ and 22. Let $\psi\colon \mathcal{P}_n \to \mathcal{F}_{2n}$ where $\psi(0) = 10$, $\psi(1) = 00$ and $\psi(22) = 0100$. Hence, we know that ψ maps any Pell string of length n to a unique Fibonacci string of length $2n$ with no 0101 factors and without a final 1, which are called *Pell binary strings*. For a graph G, we denote a subgraph H of G by $H \subseteq G$. Then using this notation and the ψ mapping it is shown that

Theorem 2.1 ([14, Theorem 7])**.** *For $n \geq 1$, we have the inclusion $\Pi_n \subseteq \Gamma_{2n-1}$.*

Let Γ^*_{2n} be the Hamming graph generated by the set of all Pell binary strings of length $2n$ then we have the following result showing that Π_n is isomorphic to an induced subgraph of $\Gamma_{2n-1}0$.

Theorem 2.2 ([14, Theorem 8])**.** *The graphs Π_n and Γ^*_{2n} are isomorphic.*

Let $N(v)$ denote the open neighborhood of $v \in V$, that is, the set of vertices adjacent to v, and $N[v] = N(v) \cup \{v\}$. Using Theorem 2.1, we have the following Lemma.

Lemma 2.3. *Let $v \in \Pi_n \subseteq \Gamma_{2n-1}0$. For any $u \in N(v) \subseteq \Gamma_{2n-1}0$, the binary string representation of u can not have two non-overlapping 0101 factors as a substring.*

Proof. Assume that there is a vertex $u \in N(v)$ of the form $\alpha_1 0101 \alpha_2 0101 \alpha_3 0 \in \mathcal{F}_{2n-1}0$. Then we know that the distance between u and v in Γ_{2n-1} is 1. Hence, v should have a 0101 factor, which is a contradiction. □

Let $\alpha 0(0101)0\beta \in \mathcal{F}_{2n}$ for some Fibonacci strings α and β which do not have a 0101 factor. Let us define the maps ϕ_1, ϕ_2 and ϕ from $\mathcal{F}_{2n}$ into $\mathcal{F}_{2n}$ by setting

$$\begin{aligned}
\phi_1(\alpha 0(0101)0\beta) &= \alpha 0(0001)0\beta,\\
\phi_2(\alpha 0(0101)0\beta) &= \alpha 0(0100)0\beta,\\
\phi(\alpha 0(0101)0\beta) &= \alpha 0(0000)0\beta.
\end{aligned}$$

3 Main results

We first interrelate the domination and total domination numbers of Fibonacci cubes and Pell graphs using Theorem 2.1 and Lemma 2.3.

Proposition 3.1. *For any positive integer n, we have*

(i) $\gamma(\Pi_n) \leq \gamma(\Gamma_{2n-1})$

(ii) $\gamma_t(\Pi_n) \leq \gamma_t(\Gamma_{2n-1})$

Proof. (i) Let D be a minimal dominating set of Γ_{2n-1} and set

$$\begin{aligned}
D' = \{\alpha \mid \alpha \text{ is a Pell binary string from } D0\} \cup\\
\cup \{\phi(\beta 0) \mid \beta 0 \in D0 \text{ has one 0101 factor}\}.
\end{aligned}$$

Note that $|D'| \leq |D|$. Let u be a vertex of Π_n. Then the vertex $\psi(u)$ is dominated in $\Gamma_{2n-1}0$ by some $d0 \in D0$. If $d0$ is a Pell binary string then $d0$ belongs to D'. If $d0$ is not a Pell binary string then we know that it has only one 0101 factor and $\psi(u)$ must be of the form $\phi_1(d0)$ or $\phi_2(d0)$, which are also dominated by a Pell binary string $\phi(d0)$. Then we obverse that D' is a dominating set of Π_n. Hence, we have $\gamma(\Pi_n) \leq \gamma(\Gamma_{2n-1})$.

(ii) Using the same argument in the previous part, assume that D is a minimal total dominating set of Γ_{2n-1}. Then we merely need to show that D' is a total dominating set. Since D is a total dominating set in Γ_{2n-1}, we know that every vertex $v \in V(\Pi_n) \subseteq V(\Gamma_{2n-1}0)$ must be adjacent to some vertex $w \in D0$. If $w \in D'$, there is nothing to show. Otherwise, w must have one 0101 factor. Since Pell binary string representations of the vertices in Π_n do not have a 0101 factor, $v \in V(\Pi_n)$ must be of the form $\phi_1(w)$ or $\phi_2(w)$. Hence, v is also adjacent to $\phi(w) \in D'$. □

Using the canonical decomposition (2.2) of Π_n, we obtain the following results.

Proposition 3.2. *For any integer $n \geq 3$, we have*

(i) $\gamma(\Pi_n) \leq 2\gamma(\Pi_{n-1}) + \gamma(\Pi_{n-2})$

(ii) $\gamma_t(\Pi_n) \leq 2\gamma(\Pi_{n-1}) + \gamma_t(\Pi_{n-2})$

(iii) $\gamma(\Pi_n) \leq \gamma_t(\Pi_n) \leq 5\gamma(\Pi_{n-2}) + 2\gamma(\Pi_{n-3})$

Proof. (i) This follows directly from the canonical decomposition (2.2) of Pell graphs.

(ii) Let D_1 be a dominating set for Π_{n-1} and D_2 be a total dominating set for Π_{n-2}. From (2.2) we know that there is a perfect matching between $0\Pi_{n-1}$ and $1\Pi_{n-1}$. Using this perfect matching, we conclude that the set $0D_1 \cup 1D_1 \cup 22D_2$ is a total dominating set for Π_n, which gives the desired result.

(iii) This follows from using the canonical decomposition (2.2) of Pell graphs recursively and the perfect matchings between the induced subgraphs, namely 5 copies of Π_{n-2} and 2 copies of Π_{n-3}. □

Considering the vertices of high degrees, lower bounds on $\gamma(\Gamma_n)$ and $\gamma(\Lambda_n)$ are obtained in [17, Theorem 3.2] and [3, Theorem 3.5.], respectively. Using the same argument, we obtain the lower bound for $\gamma(\Pi_n)$ in Proposition 3.4. Before we introduce this lower bound, we have the following remark on the degree distribution of the vertices of Π_n.

Remark 3.3. We know that Π_n is an induced subgraph of $\Gamma_{2n-1}0$, which means that the degrees of the vertices of Π_n is at most $2n-1$. It is shown in [14, Proposition 27] that 1^n is the unique vertex having degree $2n-1$ for $n \geq 2$. Using the recursive relation in [14, Theorem 29], which gives the number of all vertices of Π_n having fixed degree, it is easy to show that for $n \geq 3$, there are only 2 vertices having degree $2n-2$ (namely, 01^{n-1} and $1^{n-1}0$), and for $n \geq 4$ there are exactly $n+1$ vertices having degree $2n-3$. The rest of the vertices of Π_n have degree at most $2n-4$ for $n \geq 4$.

Proposition 3.4. *For any $n \geq 7$, we have* $\gamma_t(\Pi_n) \geq \gamma(\Pi_n) \geq \left\lceil \dfrac{p_n - n - 8}{2n-3} \right\rceil$.

Proof. Let D be a minimum dominating set of Π_n and define the over domination of Π_n with respect to D as

$$OD(\Pi_n) = \left(\sum_{v \in D} \big(\deg(v) + 1 \big) \right) - |V(\Pi_n)|\,.$$

Let $S = \{v \in V(\Pi_n) \mid \deg(v) \geq 2n-3\}$. Using Remark 3.3, we have

$$\begin{aligned} 0 \leq OD(\Pi_n) &= 2n + 2(2n-1) + (n+1)(2n-2) - p_n + \sum_{v \in D \setminus S} \big(\deg(v)+1\big) \\ &\leq 2n^2 + 6n - 4 - p_n + (|D| - |S|)(2n-3) \\ &= n + 8 - p_n + |D|(2n-3) \end{aligned}$$

which gives the desired result. □

3.1 Integer linear programming for domination numbers

Suppose each vertex $v \in V(\Pi_n)$ is associated with a binary variable x_v. The problems of determining $\gamma(\Pi_n)$ and $\gamma_t(\Pi_n)$ can be expressed as problems of minimizing the objective function

$$\sum_{v \in V(\Pi_n)} x_v \tag{3.1}$$

subject to the following constraints for every $v \in V(\Lambda_n)$:

$$\sum_{a \in N[v]} x_a \geq 1 \text{ (for domination number)},$$

$$\sum_{a \in N(v)} x_a \geq 1 \text{ (for total domination number)}.$$

The value of the objective function (3.1) gives $\gamma(\Pi_n)$ and $\gamma_t(\Pi_n)$, respectively. Note that this problem has p_n binary variables and p_n constraints.

We implemented the integer linear programming problem (3.1) on Intel Core i7-10875H CPU @ 2.30GHz with 32GB RAM running the Ubuntu 20.04 LTS Linux operating system and using Gurobi Optimizer [8]. We obtain the exact values of $\gamma(\Pi_n)$ for $n \leq 6$ and $\gamma_t(\Pi_n)$ for $n \leq 7$. Furthermore, we obtain the estimates $60 \leq \gamma(\Pi_7) \leq 64$ (takes approximately 1 hour) and $137 \leq \gamma(\Pi_7) \leq 162$ (takes approximately 1 hour) . We collect the values of $\gamma(\Pi_n)$ and $\gamma_t(\Pi_n)$ that we obtained from (3.1) in Table 1. In Tables 2 and 3 we present examples of a minimal dominating and total dominating sets that were obtained during the computation of these values. We also present an example of a dominating set of Π_7 having cardinality 64 in Appendix (see, Table 11).

Table 1: Domination and total domination numbers for small Pell graphs.

n	1	2	3	4	5	6	7	8
$\lvert V(\Pi_n)\rvert$	2	5	12	29	70	169	408	985
$\gamma(\Pi_n)$	1	2	4	7	14	30	60−64	
$\gamma_t(\Pi_n)$	2	2	4	9	16	34	72	137−162

Using the computation results presented in Table 1, Proposition 3.2 and a simple induction argument we obtain the following results.

Theorem 3.5. *For $n \geq 6$, we have $\gamma(\Pi_n) \leq 22p_{n-4} - 40p_{n-5}$; and for $n \geq 9$, we have $\gamma_t(\Pi_n) \leq 22p_{n-4} - 40p_{n-5}$.*

Proof. From Proposition 3.2 and Table 1, we know that

$$\gamma(\Pi_n) \leq 2\gamma(\Pi_{n-1}) + \gamma(\Pi_{n-2}) \tag{3.2}$$

and $\gamma(\Pi_6) = 30$, $\gamma(\Pi_7) \leq 64$. We set $s_6 = 30$, $s_7 = 64$ and $s_n = 2s_{n-1} + s_{n-2}$ for $n \geq 8$. Using (3.2), one can easily see that $\gamma(\Pi_n) \leq s_n$ for $n \geq 6$. Let $S = \sum_{n\geq 0} s_{n+6}x^n$ be the generating function of the sequence s_{n+6}. Therefore, S satisfies

$$S - 30 - 64x = 2x(S - 30) + x^2 S$$

which gives

$$S = \frac{30 + 4x}{1 - 2x - x^2}\ .$$

Then using (2.1), we obtain $s_{n+7} = 30p_{n+1} + 4p_n$ for $n \geq 0$ and $s_6 = 30p_0$. This is equivalent to $s_n = 22p_{n-4} - 40p_{n-5}$ for all $n \geq 6$. Using a similar argument, we obtain the desired result for the total domination number. □

Remark 3.6. For any graph G of minimum degree δ, a general upper bound due to Arnautov [1] and Payan [16] is

$$\gamma(G) \leq \frac{|V(G)|}{\delta + 1} \sum_{j=1}^{\delta+1} \frac{1}{j}\ . \tag{3.3}$$

We know that $\delta(\Pi_n) = \lceil \frac{n}{2} \rceil$ (cf. [14, Proposition 27]). Computing the upper bound in Theorem 3.5 and the right-hand side of the bound (3.3) for $\gamma(\Pi_n)$, we observe that our bound from Theorem 3.5 is better than the bound from (3.3) for $n \leq 44$.

Table 2: Example of a minimal dominating set for Π_6.

000000, 000221, 001022, 001101, 001110, 001122,
010011, 010110, 012200, 022000, 022111, 022220,
100011, 100220, 101100, 102211, 110101, 110122,
111001, 111010, 111221, 112211, 112222, 122022,
122100, 220000, 220022, 220220, 221111, 222200.

Table 3: Example of a minimal total dominating set for Π_7.

0000000, 0001022, 0001122, 0001220, 0001221, 0002211, 0010000, 0010011,
0010111, 0011100, 0012211, 0022011, 0022100, 0100101, 0100111, 0101010,
0101101, 0110220, 0111220, 0122011, 0122111, 0122220, 0220111, 0220122,
0221000, 0221001, 0221122, 0222200, 0222210, 1000110, 1000111, 1001001,
1002200, 1010111, 1011001, 1011010, 1011110, 1022111, 1022122, 1022221,
1100022, 1100220, 1101010, 1102200, 1102210, 1102222, 1110001, 1110010,
1110022, 1110100, 1110220, 1111022, 1112201, 1112222, 1122000, 1122001,
1220010, 1220100, 1221111, 1221221, 2200000, 2200111, 2201000, 2201111,
2201221, 2210001, 2210111, 2211022, 2211110, 2212201, 2222110, 2222111.

3.2 Additional domination type parameters of small Pell graphs

By using the integer linear programming approach several additional parameters of small Fibonacci cubes, Lucas cubes and k-Fibonacci cubes are obtained in [2, 6, 12, 20]. In this section we use a similar approach to obtain domination type parameters of small Pell graphs. For completeness of the paper, we first give the definition of these parameters and corresponding linear optimization problems similar to (3.1).

A set $X \subseteq V$ is a 2-packing if the distance $d(u, v) \geq 3$ for any $u, v \in X$, $u \neq v$. The maximum size of a 2-packing of G is the 2-packing number of G denoted $\rho(G)$. It can be determined using the following optimization problem:

$$\begin{aligned} \rho(G) = \max \sum_{v \in V} x_v & \\ \text{subject to} \quad \sum_{u \in N[v]} x_u \leq 1, \ & \text{for all } v \in V. \end{aligned}$$

The independent domination number $i(G)$ is the minimum size of a dominating set that induces no edges (or, equivalently, the size of the smallest maximal independent set), which can be determined using the following optimization problem:

$$\begin{aligned} i(G) = \min \sum_{v \in V} x_v & \\ \text{subject to} \quad \sum_{u \in N[v]} x_u \geq 1, \ & \text{for all } v \in V \\ (|V| - 1)x_v + \sum_{u \in N(v)} x_u \leq |V| - 1, \ & \text{for all } v \in V. \end{aligned}$$

A set $X \subseteq V$ is a k-tuple dominating set of G if for every vertex $v \in V$ we have $|N[v] \cap X| \geq k$, that is, $v \in X$ and has at least $k-1$ neighbors in S or $v \in V \setminus X$ has at least k neighbors in X. The k-tuple domination number $\gamma_{\times k}(G)$ is the minimum cardinality of a k-tuple dominating set of G. Clearly, $\gamma(G) = \gamma_{\times 1}(G) \leq \gamma_{\times k}(G)$, while $\gamma_t(G) \leq \gamma_{\times 2}(G)$ and $\gamma_{\times k}(G)$ can be determined using the following optimization problem:

$$\begin{aligned} \gamma_{\times k}(G) = \min \sum_{v \in V} x_v & \\ \text{subject to} \quad \sum_{u \in N[v]} x_u \geq k, \ & \text{for all } v \in V. \end{aligned}$$

Specifically, a k-tuple dominating set where $k = 2$ is called a double dominating set and in this work we determine double domination number $\gamma_{\times 2}(\Pi_n)$ of small Pell graphs.

A function $f\colon V \to \{-1, 1\}$ is called a signed dominating function if $\sum_{u \in N[v]} f(u) \geq 1$ holds for every $v \in V$ [4]. The signed domination number $\gamma_s(G)$ of G is the minimum of $\sum_{v \in V} f(v)$ taken over all signed dominating functions f of G and it can be determined using the following optimization problem [2]:

$$\begin{aligned} \gamma_s(G) = \min \sum_{v \in V} (2x_v - 1) & \\ \text{subject to} \quad \sum_{u \in N[v]} (2x_u - 1) \geq 1, \ & \text{for all } v \in V. \end{aligned}$$

Here we note that binary variables x_v associated with every vertex $v \in V$ indicates whether v is assigned weight 1 ($x_v = 1$) or -1 ($x_v = 0$).

The connected domination number $\gamma_c(G)$ is the order of a smallest dominating set that induces a connected graph. We used the Miller-Tucker-Zemlin constraints to find a minimal connected domination set for Pell graphs [7].

The paired domination number $\gamma_p(G)$ is the order of a smallest dominating set $S \subseteq V$ s.t. the graph induced by S contains a perfect matching. We associate to each edge $e = uv \in E$ a binary variable $x_e = x_{uv}$ indicating whether e is present in the graph induced by a paired dominating set. Then the following optimization problem determines $\gamma_p(G)$ [2]:

$$\begin{aligned} \gamma_p(G) &= 2 \cdot \min \sum_{e \in E} x_e \\ \text{subject to} \quad & \sum_{u \in N(v)} x_{uv} \leq 1, \text{ for all } v \in V \\ & \sum_{u \in N(v)} \sum_{w \in N(u)} x_{uw} \geq 1, \text{ for all } v \in V. \end{aligned}$$

Using the integer linear programming approaches described in this section, we obtain the values and estimates of $\rho(\Pi_n)$, $i(\Pi_n)$, $\gamma_{\times 2}(\Pi_n)$, $\gamma_s(\Pi_n)$, $\gamma_c(\Pi_n)$, $\gamma_p(\Pi_n)$ for some small values of n and collect these results in Table 4. Furthermore, in Tables 5, 6, 7, 9 and 10 in Appendix, we present example of a set of vertices giving $\rho(\Pi_n)$ and $\gamma_p(\Pi_n)$ for $n = 7$, $\gamma_c(\Pi_n)$ for $n = 5$, and $i(\Pi_n)$ and $\gamma_{\times 2}(\Pi_n)$ for $n = 6$ that were obtained during the computation of these values. In Table 8, we also present the set of vertices $v \in V(\Pi_6)$ for which $f(v) = -1$, where f is a signed dominating function giving $\gamma_s(\Pi_6) = 45$.

Table 4: Values of additional domination type parameters for small Pell graphs.

n	1	2	3	4	5	6	7
$\lvert V(\Pi_n)\rvert$	2	5	12	29	70	169	408
$\rho(\Pi_n)$	1	2	3	6	11	22	46
$i(\Pi_n)$	1	2	4	7	15	31	60−69
$\gamma_{\times 2}(\Pi_n)$	2	4	7	13	27	56	113−121
$\gamma_s(\Pi_n)$	2	3	4	11	20	45	88−102
$\gamma_c(\Pi_n)$	1	2	4	9	18	35−38	66−82
$\gamma_p(\Pi_n)$	2	2	4	10	16	34	72

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Appendix

Table 5: Example of a 2-packing set for Π_7.

0000110, 0001001, 0010000, 0010122, 0011221, 0012201, 0022022, 0022110, 0100022, 0100221, 0101100, 0102222, 0110101, 0111011, 0122000, 0220010, 0221122, 0221220, 0222200, 1000101, 1001022, 1002210, 1010011, 1010220, 1011100, 1012222, 1022001, 1100010, 1101111, 1122122, 1122220, 1220022, 1220100, 1220221, 1221001, 1222211, 2200122, 2200220, 2201000, 2202201, 2210001, 2211022, 2211221, 2212210, 2222010, 2222101.

Table 6: Example of a minimal independent dominating set for Π_6.

000000, 000221, 001011, 001122, 001220, 002200, 010011, 010110, 010122, 011101, 012211, 022000, 022022, 022220, 100022, 100101, 100110, 101000, 102211, 111001, 111010, 111100, 111221, 112222, 122111, 220000, 220111, 220220, 221022, 222201, 222210.

Table 7: Example of a minimal double dominating set for Π_6.

000000, 000022, 000111, 000220, 001022, 001100, 001101, 001110, 002211, 010000, 010010, 010101, 010220, 011011, 011101, 011122, 011221, 012210, 012211, 022000, 022011, 022022, 022110, 022220, 100001, 100110, 100111, 101001, 101010, 101221, 102200, 102211, 102222, 110022, 110100, 110122, 111010, 111022, 111122, 111220, 111221, 112200, 122000, 122101, 122111, 220001, 220011, 220100, 220220, 220221, 221001, 221010, 221110, 221122, 222201, 222211.

Table 8: The set of vertices $v \in V(\Pi_6)$ for which $f(v) = -1$, where f is a signed dominating function giving $\gamma_s(\Pi_6) = 45$.

000001, 000010, 000101, 000110, 000122, 001010, 001022, 001101,
001110, 001221, 002222, 010001, 010100, 010122, 010220, 011001,
011011, 011100, 011111, 011221, 012200, 012211, 022010, 022022,
022100, 022122, 022220, 100000, 100011, 100111, 100221, 101000,
101022, 101101, 101110, 102201, 102210, 102222, 110000, 110011,
110100, 110111, 110220, 111011, 111110, 111111, 122001, 122010,
122101, 122220, 220010, 220022, 220101, 220122, 220220, 221001,
221010, 221101, 221221, 222200, 222210, 222222.

Table 9: Example of a minimal connected dominating set for Π_5.

00011, 00101, 00111, 00221, 01000, 01111,
01122, 02201, 02211, 10011, 11000, 11100,
11110, 11111, 11122, 11220, 22011, 22111.

Table 10: Example of a minimal paired dominating set for Π_7.

0000000, 0000100, 0000220, 0001022, 0001122, 0001220, 0010111, 0011001,
0011010, 0011100, 0011111, 0012200, 0022001, 0022220, 0100011, 0100111,
0101101, 0102201, 0110022, 0111110, 0112222, 0122011, 0122111, 0220000,
0220111, 0221000, 0221110, 0221111, 1000011, 1000111, 1001101, 1002210,
1002211, 1010010, 1011010, 1011101, 1022022, 1022122, 1022220, 1101000,
1101010, 1101221, 1102210, 1110001, 1110010, 1110022, 1110100, 1110101,
1110122, 1110220, 1110221, 1111221, 1112222, 1122000, 1122100, 1220220,
1221011, 1221022, 1222200, 1222201, 2200110, 2200111, 2201000, 2201022,
2201122, 2202201, 2210001, 2211110, 2211220, 2212201, 2222011, 2222111.

Table 11: Example of a dominating set having 64 vertices for Π_7.

0000010, 0001001, 0002211, 0010022, 0010101, 0010221, 0011100, 0011110,
0022010, 0022122, 0100000, 0100111, 0101022, 0101220, 0102200, 0110000,
0111100, 0111110, 0112222, 0122001, 0122221, 0220000, 0220122, 0220220,
0221011, 0222201, 1000001, 1000100, 1000122, 1000220, 1001122, 1001221,
1002210, 1011000, 1011011, 1012201, 1022101, 1022220, 1101010, 1101101,
1110010, 1110011, 1110110, 1110111, 1112222, 1122000, 1122022, 1220101,
1221000, 1221022, 1221221, 1222210, 2200022, 2200100, 2200221, 2201010,
2202211, 2210001, 2211001, 2211122, 2211220, 2212200, 2222110, 2222111.

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Finitizable set of reductions for polyhedral quadrangulations of closed surfaces

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Abstract

In this paper, we discuss generating theorems of polyhedral quadrangulations of closed surfaces. We prove that the set of the eight reductional operations $\{R_1, \dots, R_8\}$ defined for polyhedral quadrangulations is finitizable for any closed surface F^2, that is, there exist finitely many minimal polyhedral quadrangulations of F^2 using such operations $R_1, \dots, R_7$ and R_8. Furthermore, we show that any proper subset of $\{R_1, \dots, R_8\}$ is not finitizable for polyhedral quadrangulations of the torus.

Keywords: Generating theorem, reduction, finitizable set, polyhedral quadrangulation.

Math. Subj. Class. (2020): 05C10

1 Introduction

In this paper, we consider simple connected graphs embedded on closed surfaces. Although we follow the standard graph theory terminology, for some technical terms without description here, refer to Section 2. Sometimes, such an embedded graph is expected to be a "*good*" one, that is, every facial walk is a cycle, and any two of them are disjoint, intersect in one vertex, or intersect in one edge. It is known that a graph G embedded on the sphere satisfies the above good conditions if and only if G is 3-connected. However, if G is embedded on a non-spherical closed surface, then G is required to be *polyhedral*, i.e., 3-connected and 3-representative; note that 3-connected graphs on the sphere are also polyhedral.

For example, a simple graph G cellularly embedded on a closed surface F^2 each of whose face is bounded by a cycle of length 3 is polyhedral if G is not a 3-cycle on the sphere. Such a graph triangulating a closed surface F^2 is known as a *triangulation* of

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F^2. On the other hand, following the convention in topological graph theory, a 4-cycle embedded on the sphere is regarded as a *quadrangulation*, which is a graph cellularly embedded on a closed surface F^2 so that each face is bounded by a cycle of length 4. In this paper, our main subject is the set of polyhedral quadrangulations of closed surfaces.

In topological graph theory, we sometimes discuss *generating theorems* of graphs embedded on closed surfaces (i.e., constructing all graphs in a certain class $\mathcal{C}$ from $\mathcal{C}_0 \subset \mathcal{C}$ by a repeated applications of certain expanding operations only through $\mathcal{C}$). This notion is equivalent to that every graph in $\mathcal{C}$ can be reduced to one in $\mathcal{C}_0$ by a repeated applications of the reductional operations (or *reductions*, simply), which are inverses of the above expanding operations; we denote the set of such reductions by X here. In a generating theorem of graphs, $|X|$ and $|\mathcal{C}_0|$ are expected to be small. In particular, X is called *finitizable* for $\mathcal{C}$ if $|\mathcal{C}_0|$ is finite. If X' is not finitizable for any proper subset $X' \subset X$, then the finitizable set X is *minimal*. For example, if $\mathcal{C}$ is the set of simple triangulations of the sphere, then $X = \{\text{contraction}\}$ is finitizable and $\mathcal{C}_0 = \{\text{tetrahedron}\}$. (See [19]. A *contraction* of e in a triangulation G is to remove e, identify the two ends of e and replace two pairs of multiple edges by two single edges respectively.) In fact, it was proved in [2, 3, 7, 16] that for every closed surface F^2, $\{\text{contraction}\}$ is finitizable for the set of simple triangulations of F^2. Furthermore, see [1, 9, 10, 20, 21] for the complete lists of minimal triangulations on fixed non-spherical closed surfaces with low genera. Moreover, finitizable sets of reductions for even triangulations, i.e., triangulations such that each vertex has even degree, are discussed in literatures; e.g., see [6, 18].

As mentioned above, in this paper, we focus on quadrangulations of closed surfaces. Figure 1 shows the eight reductions, denoted by $R_1, \dots, R_7$ and R_8 simply for our purpose, defined for quadrangulations of closed surfaces. In fact, R_1, R_2 and R_3 are typical ones which were first given by Batagelj [4] (see e.g., [23] for the formal definition); especially, R_1 and R_2 are called a *face-contraction* and a 4-*cycle removal*, respectively, in the literature. Further, the fourth reduction R_4 was defined and discussed in [22]; which is called a *cube-contraction* in the paper. The other four reductions will be defined in the next section.

Let $\mathcal{C}$ be a set of quadrangulations of a closed surface F^2 with some certain conditions, and let $G \in \mathcal{C}$. For a subset $X \subseteq \{R_1, \dots, R_8\}$, G is X-*irreducible* if we cannot apply any reduction in X without violating the condition of $\mathcal{C}$; i.e., the resulting graph is no longer in $\mathcal{C}$. In particular, an $\{R_1\}$-irreducible quadrangulation in the set of simple quadrangulations of a closed surface F^2 is known as just a *irreducible* quadrangulation of F^2. In [16], it was proved that for any closed surface F^2 there exist only finitely many irreducible quadrangulations of F^2, that is, $\{R_1\}$ is finitizable for the set of simple quadrangulations of every closed surface. Actually, the complete lists of irreducible quadrangulations of the sphere, the projective plane, the torus and the Klein bottle were obtained in [4, 5, 14, 17] and [13], respectively; for example, a 4-cycle is the unique irreducible quadrangulation of the sphere, and the unique quadrangular embeddings of K_4 and $K_{3,4}$ are irreducible quadrangulations of the projective plane. (Note that a restricted R_1 was used in [5].)

The situation for 3-connected (and simple) quadrangulations of closed surfaces is a little bit complicated in comparison with the above case of irreducible quadrangulations. Throughout the researches in [4, 5, 12, 15], it had been proved that for any closed surface F^2, $\{R_1, R_2, R_3\}$ is finitizable for 3-connected quadrangulations of F^2; note that the minimal one on the sphere is the cube, and for any non-spherical closed surface F^2, the set of the minimal graphs coincides with the set of irreducible quadrangulations of F^2. Further-

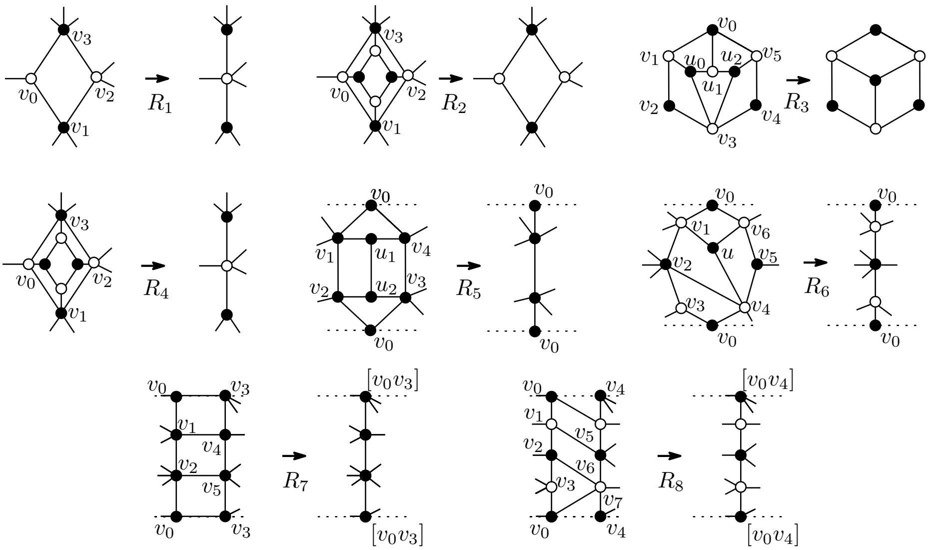

Figure 1: Reductional operations for quadrangulations.

more, it was shown that $\{R_1, R_2, R_3\}$ is minimal for those graphs on the sphere and the projective plane while it is not minimal on the other closed surfaces; in fact, R_3 is unnecessary and hence $\{R_1, R_2\}$ is minimal and finitizable for those closed surfaces. Moreover, it was proved in [22] that $\{R_1, R_3, R_4\}$ is minimal and finitizable for 3-connected quadrangulations of the sphere and the projective plane, and $\{R_1, R_4\}$ is minimal and finitizable for those graphs on the other closed surfaces.

As mentioned above, in this paper, we deal with polyhedral quadrangulations of closed surfaces. Recently in [23], the generating theorem for such polyhedral quadrangulations of the projective plane was discussed using three reductions R_1, R_2 and R_3, and they obtained 26 families of $\{R_1, R_2, R_3\}$-irreducible quadrangulations of the projective plane. However, such families contains infinite series of graphs; i.e., unfortunately, $\{R_1, R_2, R_3\}$ is not finitizable for those graphs. The following is our main result in the paper:

Theorem 1.1. *For every closed surface F^2, $\{R_1, \ldots, R_8\}$ is finitizable for polyhedral quadrangulations of F^2.*

Since every reduction in the above theorem preserves bipartiteness of quadrangulations and each of R_5 and R_7 requires an essential cycle of length 3, we obtain the following corollary.

Corollary 1.2. *For every closed surface F^2, $\{R_1, R_2, R_3, R_4, R_6, R_8\}$ is finitizable for bipartite polyhedral quadrangulations of F^2.*

One might think that the eight reductions in Theorem 1.1 are a little bit too many. However, at least those on the torus, we can show the necessity of such eight reductions as follows.

Theorem 1.3. *For polyhedral quadrangulations of the torus, $\{R_1, \ldots, R_8\}$ is minimal finitizable.*

Furthermore, R_7 (resp., R_8) requires an annular region on the closed surface which is bounded by two 2-sided 3-cycles (resp., 4-cycles). Therefore, in particular on the projective plane, $\{R_1, \ldots, R_6\}$ is finitizable by Theorem 1.1. As well as the previous case on the torus, we can show the following.

Theorem 1.4. *For polyhedral quadrangulations of the projective plane, $\{R_1, \ldots, R_6\}$ is minimal finitizable.*

This paper is organized as follows. In the next section, we define terminology and the remaining four new reductions for our argument in the paper. Next, we show some propositions and lemmas holding for polyhedral quadrangulations for our purpose, some of which are quoted from [23]. Section 4 is devoted to prove our main result in the paper. In Section 5, we discuss the minimality of the set of eight reductions by showing some infinite series of polyhedral quadrangulations.

2 Basic definitions

We denote the vertex set and the edge set of a graph G embedded on a closed surface F^2 by $V(G)$ and $E(G)$, respectively. A *k-path* (resp., *k-cycle*) in a graph G is a path (resp., cycle) of length k. (The *length* of a path (or cycle) is the number of its edges in this paper.) We denote the set of vertices of degree 3 by V_3 in our argument, and $\langle V_3 \rangle_G$ represents the subgraph induced by V_3 in G.

Let G be a graph embedded on a closed surface F^2. Then, a connected component of $F^2 - G$ is a *face* of G, and we denote the face set of G by $F(G)$. If every face of G is homeomorphic to an open 2-cell (or an open disc), then, G is a 2-*cell embedding* or 2-*cell embedded graph* on F^2. Clearly, every quadrangulation (or triangulation) of a closed surface is a 2-cell embedded graph. A *facial cycle* C of a face f is a cycle bounding f in G; i.e., $C = \partial f$. Then, $\bar{f}$ denotes a closure of f, i.e., $\bar{f} = f \cup \partial f$. For brevity, we sometimes denote like $f = v_0v_1v_2v_3$ where $v_0v_1v_2v_3$ is a facial cycle of $f \in F(G)$. Furthermore in our argument, we often discuss the interior of a 2-cell region D bounded by a closed walk W of G, i.e., $W = \partial D$, which contains some vertices and edges. (Note that a 2-cell region implies an "open" 2-cell region in this paper.) Similarly, $\bar{D}$ denotes a closure of D, i.e., $\bar{D} = D \cup \partial D$. Let $f_1, \ldots, f_k$ denote the faces of G incident to $v \in V(G)$ where $\deg(v) = k$. Then, the boundary walk of $\bar{f}_1 \cup \cdots \cup \bar{f}_k$ is the *link walk* of v and denoted by $lw(v)$. Clearly, $lw(v)$ bounds a 2-cell region containing a unique vertex v.

A simple closed curve γ on a closed surface F^2 is *trivial* if γ bounds a 2-cell region on F^2, and *essential* otherwise. Among essential simple closed curves, one with an annular neighborhood is called 2-*sided* while one whose tubular neighborhood forms a Möbius band is called 1-*sided*. Since cycles in graphs embedded on surfaces can be regarded as simple closed curves, we use the above terminology for them; e.g., we say that a cycle is essential and 2-sided.

The *representativity* of G, denoted by $r(G)$, is the minimum number of intersecting points of G and γ, where γ ranges over all essential simple closed curves on the surface. A graph G embedded on F^2 is *r-representative* if $r(G) \geq r$. Note that the "representativity" is also called the "*face-width*" in the literature; see e.g., [11] for the details. A graph G embedded on a non-spherical closed surface F^2 is *polyhedral* if G is 3-connected and 3-representative. Observe that for every vertex v of a polyhedral graph, the link walk of v forms a cycle.

Let G be a quadrangulation of a closed surface F^2 and let $f = v_0v_1v_2v_3$ be a face of G. Then a pair $\{v_i, v_{i+2}\}$ is called a *diagonal pair* of f in G for each $i \in \{0, 1\}$. A closed curve γ on F^2 is a *diagonal k-curve* for G if γ passes only through distinct k faces $f_0, \ldots, f_{k-1}$ and distinct k vertices $x_0, \ldots, x_{k-1}$ of G such that for each i, f_i and f_{i+1} share x_i, and that for each i, $\{x_{i-1}, x_i\}$ forms a diagonal pair of f_i of G, where the subscripts are taken modulo k. Furthermore, we call a simple closed curve γ on F^2 a *semi-diagonal k-curve* if in the above definition $\{x_{i-1}, x_i\}$ is not a diagonal pair for exactly one i; note that $x_{i-1}x_i$ is an edge of ∂f_i in this case. Each simple curve β_i along γ joining x_{i-1} and x_i in f_i is called a *γ-segment*; where $\bigcup_{i=0}^{k-1} \beta_i = \gamma$.

For a simple closed curve ℓ on F^2, when ℓ intersects with G at only vertices of G, that is, $G \cap \ell$ is a subset $S \subset V(G)$, then we say that ℓ *passes* S; observe that ℓ does not pass through any vertex in $V(G) \setminus S$ in this case. For example, in the above definition of a diagonal (or semi-diagonal) k-curve, we say that γ passes $\{x_0, \ldots, x_{k-1}\}$. On the other hand, when we say that ℓ *passes through* a vertex v (or some vertices) of G, then ℓ probably passes through other vertices of G.

Let G be a simple quadrangulation of a non-spherical closed surface F^2. Assume that G has a hexagonal 2-cell region D bounded by a closed walk $\partial D = v_0v_1v_2v_0v_3v_4$ containing exactly two vertices u_1 and u_2 such that $v_0v_1u_1v_4, v_1v_2u_2u_1, v_3v_4u_1u_2$ and $v_2v_0v_3u_2$ are faces of G in D, and that $v_0v_1v_2$ is an essential cycle of length 3. Furthermore, we assume that v_0, v_1, v_2, v_3 and v_4 are different vertices, and that each of v_1, v_2, v_3 and v_4 has degree at least 4 ; otherwise, G would not be polyhedral under the condition. A reduction R_5 of D is to eliminate u_1 and u_2, and identify v_1 (resp., v_2) and v_4 (resp., v_3), and replace three pairs of multiple edges by three single edges, respectively, as shown in Figure 1. Throughout the paper, the vertex obtained by the identification of two vertices a and b is denoted by $[ab]$. That is, $v_0[v_1v_4][v_2v_3]$ is an essential 3-cycle in the resulting graph.

Secondly, assume that G has an octagonal 2-cell region D bounded by a closed walk $W = v_0v_1v_2v_3v_0v_4v_5v_6$ containing exactly one vertex u such that $v_0v_1uv_6, v_1v_2v_4u$, $v_4v_5v_6u$ and $v_2v_3v_0v_4$ are faces of G in D, and that $v_0v_1v_2v_3$ is an essential cycle of length 4. Furthermore, we assume that $v_0, v_1, v_2, v_3, v_4, v_5$ and v_6 are different vertices. Note that v_1 and v_4 has degree at least 4 under the condition. (If $\deg(v_1) = 3$, then G is representativity at most 2. On the other hand, $\deg(v_4) = 3$ implies that $v_0 = v_5$, a contradiction.) A reduction R_6 of D is to eliminate u and an edge v_2v_4, and identify v_1 (resp., v_2, v_3) and v_6 (resp., v_5, v_4), and replace four pairs of multiple edges by four single edges, respectively, as shown in Figure 1. Then, $v_0[v_1v_6][v_2v_5][v_3v_4]$ is an essential 4-cycle in the resulting graph.

Thirdly, assume that G has an annular region A bounded by two essential cycles $C = v_0v_1v_2$ and $C' = v_3v_4v_5$ such that $f_1 = v_0v_1v_4v_3, f_2 = v_1v_2v_5v_4$ and $f_3 = v_2v_0v_3v_5$ are faces of G in A. (Sometimes, $f_1f_2f_3(= W_F)$ is called a *face walk* of length 3 in G, which corresponds to a 3-cycle in the dual of G.) Here, note that C_1 and C_2 are essential 2-sided cycles of G on F^2; if C_1 is trivial, then it contradicts Proposition 3.2 in the next section. The seventh reduction R_7 of A (or the above face walk W_F) is to contract edges v_0v_3, v_1v_4 and v_2v_5 simultaneously, and replace three pairs of multiple edges by three single edges, respectively, as shown in Figure 1. Note that $C = [v_0v_3][v_1v_4][v_2v_5]$ is also an essential 2-sided 3-cycle in the resulting graph.

Fourthly, assume that G has an annular region A bounded by two essential cycles $C_1 = v_0v_1v_2v_3$ and $C_2 = v_4v_5v_6v_7$ such that $f_1 = v_0v_1v_6v_5, f_2 = v_1v_2v_7v_6, f_3 = v_2v_3v_0v_7$ and $f_4 = v_0v_5v_4v_7$ are faces of G in A. (As well as the previous reduction,

$f_1 f_2 f_3 f_4 (= W_F)$ is a face walk of length 4.) Furthermore, we assume that C_1 and C_2 are essential cycles of G on F^2; observe that they are 2-sided. The eighth reduction R_8 of A (or the face walk W_F) is to eliminate edges v_0v_5, v_1v_6, v_2v_7 and v_0v_7, and identify v_i and v_{i+4} for each $i \in \{0, 1, 2, 3\}$, and replace four pairs of multiple edges by four single edges, respectively, as shown in Figure 1. Note that $C = [v_0v_4][v_1v_5][v_2v_6][v_3v_7]$ is also an essential 2-sided 4-cycle in the resulting graph.

As mentioned in the introduction, for R_1, R_2, R_3 and R_4, see e.g., [22, 23] for formal definitions. Note that the boundary of the hexagon of the graph in R_3 in the figure is a cycle. Furthermore, every quadrangulation of a closed surface is locally bipartite, and hence we color vertices of graphs in R_1, R_2, R_3, R_4, R_6 and R_8 by black and white; however, graphs in the reductions R_5 and R_7 contain short odd cycles, and hence we cannot do so.

3 Lemmas

First of all, we introduce the following two propositions for quadrangulations of closed surfaces; these are well-known in topological graph theory, and hence we omit the proofs.

Proposition 3.1. *The length of two essential cycles in a quadrangulation of a closed surface have the same parity if they are homotopic to each other on* F^2.

Proposition 3.2. *A quadrangulation of a closed surface has no separating odd cycle.*

It was shown in [23] that many facts hold for $\{R_1, R_2, R_3\}$-irreducible polyhedral quadrangulations of non-spherical closed surfaces. First, we show some of them, which will be used in our later argument in the paper. In the following lemmas, G represents a $\{R_1, R_2, R_3\}$-irreducible polyhedral quadrangulations of a non-spherical closed surface F^2 otherwise specified. (The assertions are a little bit changed so as to suit for this paper.)

Lemma 3.3 (Lemmas 3.5, 3.13 and 3.15 in [23])**.** *Every connected component of* $\langle V_3 \rangle_G$ *is a* 4*-cycle bounding a face of G or a path of length at most* 2.

Lemma 3.4 (Lemmas 3.8, 3.10 and 3.12 in [23])**.** *Let* $f = v_0v_1v_2v_3$ *be a face of G with* $\deg(v_0), \deg(v_2) \geq 4$. *Then, there exists*

(i) *an essential* 4*-cycle* $v_0v_1xv_3$ *for* $x \notin \{v_0, v_1, v_2, v_3\}$,

(ii) *an essential diagonal* 3*-curve passing through* v_1 *and* v_3*, or*

(iii) *an essential semi-diagonal* 3*-curve passing through* v_1 *and* v_3.

Lemma 3.5. *Let* $f = v_0v_1v_2v_3$ *be a face of G with* $\deg(v_0), \deg(v_2) \geq 4$. *Then, there exists an essential cycle passing through* v_0, v_1 *and* v_3 *with length* 4, 5 *or* 6.

Proof. It is clear by Lemma 3.4. (For example, if (ii) in the previous lemma holds, then there exists an essential cycle of length 6 along the essential diagonal 3-curve.) □

Lemma 3.6 (Lemma 3.14 in [23])**.** *Let* $P = u_0u_1u_2$ *be a* 2*-path in* $\langle V_3 \rangle_G$ *as shown in the left-hand side of* R_3 *in* Figure 1 *where* $\deg(v_4) \geq 4$. *Then, there is an essential diagonal* 3*-curve or an essential semi-diagonal* 3*-curve passing* $\{v_1, u_1, v_5\}$.

Assume that G has a 4-cycle $C = u_0u_1u_2u_3$ in $\langle V_3\rangle_G$ bounding a face of G such that u_i is adjacent to a third vertex $v_i \notin \{u_0, u_1, u_2, u_3\}$ for each $i \in \{0, 1, 2, 3\}$. Under the situation, a 4-cycle $v_0v_1v_2v_3$ bounds a 2-cell region which contains exactly four vertices u_0, u_1, u_2 and u_3. We call the subgraph H isomorphic to a cube with eight vertices u_i, v_i for $i \in \{0, 1, 2, 3\}$ an *attached cube*. We denote $\partial(H) = v_0v_1v_2v_3$, and we call C an *attached* 4*-cycle* of H.

Lemma 3.7 (Lemma 3.16 in [23]). *Assume that G has an attached cube H with* $\partial(H) = v_0v_1v_2v_3$*, an attached* 4*-cycle* $C = u_0u_1u_2u_3$ *and* $u_iv_i \in E(G)$ *for each* $i \in \{0, 1, 2, 3\}$*. Then there is an essential diagonal (or semi-diagonal)* 3*-curve* γ *passing* $\{v_0, u_1, v_2\}$ *or* $\{v_1, u_2, v_3\}$.

Next, we show three lemmas holding for $\{R_1, R_2, R_3, R_4\}$-irreducible polyhedral quadrangulations of non-spherical closed surfaces.

Lemma 3.8. *Let G be an* $\{R_1, R_2, R_3, R_4\}$*-irreducible polyhedral quadrangulation of a non-spherical closed surface* F^2 *having an attached cube H with* $\partial(H) = v_0v_1v_2v_3$*, an attached* 4*-cycle* $C = u_0u_1u_2u_3$ *and* $u_iv_i \in E(G)$ *for each* $i \in \{0, 1, 2, 3\}$*. By* Lemma 3.7*, we may assume that there exists an essential simple closed curve* γ_1 *passing* $\{v_0, u_1, v_2\}$*. Then, there exists an essential simple closed curve* γ_2 *passing either* $\{v_1, u_2, v_3\}$ *or* $\{v_1, u_2, v_3, x\}$ *where* $x \notin V(H)$*. In particular, if* γ_1 *is 2-sided, then* γ_2 *is not homotopic to* γ_1.

Proof. Let G' denote the quadrangulation obtained from G by applying an R_4 of H so as to identify v_1 and v_3. We denote the 2-path $v_0[v_1v_3]v_2$ in G' by P. By our assumption, G' is not polyhedral. If G' has a loop e, then e is incident to $[v_1v_3]$ such that e and P cross transversally at $[v_1v_3]$; otherwise, G would have a loop, a contradiction. Further, this e is essential by Proposition 3.2. Thus in this case, we find an essential semi-diagonal 3-curve γ_2 passing $\{v_1, u_2, v_3\}$ in G, half of which is along e.

Secondly, we suppose that G' has a pair of multiple edges. Similar to the previous case, we may assume that such multiple edges join $[v_1v_3]$ and another vertex $x \notin \{v_0, v_2\}$; otherwise, G would have multiple edges. Then, the 2-cycle $C = [v_1v_3]x$ formed by the above multiple edges crosses P transversally, similar to the previous case. Thus, C cannot be trivial by the above observation and the existence of γ_1, and hence we have our desired simple closed curve γ_2 passing $\{v_1, u_2, v_3, x\}$ in G; note that if v_1xv_3 forms a corner of a face of G, then we can take an essential diagonal 3-curve passing $\{v_1, u_2, v_3\}$. In the following argument, we assume that G' is simple and hence G' is 2-connected and 2-representative.

By the above argument, we may assume that G' has a diagonal (or semi-diagonal) 2-curve γ' passing $\{[v_1v_3], x\}$ such that γ' and P cross at $[v_1v_3]$ transversally; note that if G' has a 2-cut, then G' also has a surface separating diagonal 2-curve by Lemma 3.6 in [23]. Observe that at least one of two γ'-segments β_0 and β_1, say β_0 without loss of generality, joins the diagonal pair of $f_0 = [v_1v_3]sxt$ for $s, t \in V(G')$. Here, suppose that x is either v_0 or v_2, say v_0. Then, let $\tilde{\beta}_0$ denote a simple closed curve obtained from β_0 by joining $[v_1v_3]$ and v_0 by a simple curve along the edge $[v_1v_3]v_0$. In this case, $\tilde{\beta}_0$ must be essential by Proposition 3.2. Under the situation, we can take an essential simple closed curve intersecting with G at exactly two vertices v_0 and either v_1 or v_3, which corresponds to $\tilde{\beta}_0$, a contradiction. Thus, we conclude that x is neither v_0 nor v_2.

Observe that even when γ_1 is an essential diagonal 3-curve passing through a face $f = v_0pv_2q$ for $p, q \in V(G)$, we have $\{v_0, v_2\} \cap \{p, q\} = \emptyset$ since G is simple. This implies that the γ_1-segment in f and γ' cannot cross transversally, and hence we conclude that γ' is essential. Therefore, we have an essential diagonal (or semi-diagonal) 4-curve γ_2 passing $\{v_1, u_2, v_3, x\}$ in the statement, half of which is along γ', and the other half is inside the quadrangular region bounded by $\partial(H)$.

Finally, assume that γ_1 is 2-sided. Suppose, for a contradiction, that γ_2 is homotopic to γ_1. Under the condition, γ_2 must cross γ_1 even times, i.e., twice here. However, this is not the case by the above argument. □

Lemma 3.9. *Let G be an $\{R_1, R_2, R_3, R_4\}$-irreducible polyhedral quadrangulation of non-spherical closed surface. Then any 2-cell region bounded by a 4-cycle is either a face of G or contains exactly four vertices which is of an attached cube.*

Proof. Using the above Lemma 3.8 and Lemma 4.3 in [23], we immediately have the conclusion of the lemma. □

Furthermore in [23], Suzuki determined configurations in a 2-cell region bounded by a 6-cycle in $\{R_1, R_2, R_3\}$-irreducible polyhedral quadrangulations of non-spherical closed surfaces. By combining the results of Lemmas 3.7, 3.8 and 3.9, we can easily obtain the following lemma; so, we omit the proof.

Lemma 3.10. *Let G be an $\{R_1, R_2, R_3, R_4\}$-irreducible polyhedral quadrangulation of a non-spherical closed surface F^2. Then the number of vertices inside a 2-cell region bounded by a 6-cycle (resp., 4-cycle) is at most 16 (resp., 4).*

In the latter half of the section, we discuss reductions R_5, R_6, R_7 and R_8 applied to polyhedral quadrangulations in turn.

Lemma 3.11. *Let G be a polyhedral quadrangulation of a closed surface F^2 having a 2-cell region D with $\partial D = v_0v_1v_2v_0v_3v_4$ containing two vertices u_1 and u_2 as shown in the left-hand side of R_5 in* Figure 1*, and let G' denote a quadrangulation obtained from G by an R_5 of D. If G' is not polyhedral, then there exists an essential simple closed curve γ' such that*

(i) *γ' intersects exactly two vertices of G',*

(ii) *γ' passes through at least one vertex of $[v_1v_4]$ and $[v_2v_3]$, and*

(iii) *γ' does not pass through v_0.*

In particular, if $C = v_0[v_1v_4][v_2v_3]$ is 2-sided, then γ' is not homotopic to C.

Proof. Some similar arguments as in Lemma 3.8 will appear, and we omit the long explanation at that time for brevity. If G' has a loop e with a vertex u, then u must be one of $[v_1v_4]$ and $[v_2v_3]$, say $[v_1v_4]$ up to symmetry, such that e and $C = v_0[v_1v_4]v_2v_3$ cross transversally at $[v_1v_4]$. Clearly e is essential, and we can take an essential simple closed curve intersecting G at only v_1 and v_4, a contradiction.

Next, assume that G' has a pair of multiple edges, which joins $[v_1v_4]$ and another vertex $x \neq v_0$. If the 2-cycle $C' = [v_1v_4]x$ formed by the multiple edges is essential, then we can take our desired simple closed curve along C'. Thus, we suppose that C' is trivial below.

If $x \notin V(C)$, then G would have multiple edges joining x and either v_1 or v_4; observe that C and C' do not cross transversally, otherwise $x \in V(C)$ since C' is trivial. If $x \in V(C)$, then x must be $[v_2v_3]$. Also in this case, G would have multiple edges joining either v_1 and v_2 or v_3 and v_4, a contradiction. Therefore, we assume that G' is 2-connected and 2-representative below.

Now, G' has a diagonal (or semi-diagonal) 2-curve γ' passing $\{[v_1v_4], x\}$ such that γ' and C cross at $[v_1v_4]$ transversally. We consider the γ'-segment β_0 and $\tilde{\beta}_0$ which play the same role as in the argument in Lemma 3.8. If $x = v_0$, then $\tilde{\beta}_0$ is essential by Proposition 3.2, and hence G is not polyhedral as well, a contradiction. If γ' is trivial, then x must be $[v_2v_3]$ since $x \neq v_0$. However, this contradicts Proposition 3.2 for $\tilde{\beta}_0$. Therefore, γ' is essential and satisfying the conditions in the statement. Similar to the argument in Lemma 3.8, if C is 2-sided, then C and γ' are not homotopic. □

Lemma 3.12. *Let G be a polyhedral quadrangulation of a closed surface F^2 having a 2-cell region D with $\partial D = v_0v_1v_2v_3v_0v_4v_5v_6$ containing a unique vertex u as shown in the left-hand side of R_6 in* Figure 1*, and let G' denote a quadrangulation obtained from G by an R_6 of D. If G' is not polyhedral, then there exists an essential simple closed curve γ' such that*

(i) *γ' intersects at most two vertices of G',*

(ii) *γ' passes through at least one vertex of $[v_1v_6], [v_2v_5]$ and $[v_3v_4]$, and*

(iii) *γ' does not pass through v_0.*

In particular, if $C = v_0[v_1v_6][v_2v_5][v_3v_4]$ is 2-sided, then γ' is not homotopic to C.

Proof. The most part is same as the argument in Lemma 3.11, and hence we implicitly omit the argument which had already done before. First, observe that there does not exist a face $f \notin D$ such that $v_0, v_2 \in \partial f$; otherwise, we can find a simple closed curve intersecting with G at exactly two vertices, which passes through the face $v_2v_3v_0v_4$ and f. Similarly, there is no face $f \notin D$ of G such that $v_4, v_6 \in \partial f$. Further, in the case when G' is not simple, a loop of a vertex $[v_2v_5]$ might exist, unlike the argument in Lemma 3.11, and then, it is essential by Proposition 3.2.

Thus, we assume that G' has a diagonal (or semi-diagonal) 2-curve γ' passing $\{x, y\}$, and we may assume that y is one of $[v_1v_6], [v_2v_5]$ and $[v_3v_4]$ such that γ' and $C = v_0[v_1v_6][v_2v_5][v_3v_4]$ cross at y transversally. If $x = v_0$, then y must be $[v_2v_5]$ by the same argument as in the previous lemma; recall the argument of $\tilde{\beta}_0$. However, under the condition, G would have a face $f \notin D$ such that $v_0, v_2 \in \partial f$, which is passed by a γ'-segment, a contradiction. Thus, γ' does not pass through v_0 in the following argument. If γ' is trivial, then $\{x, y\} = \{[v_1v_6], [v_3v_4]\}$, and γ' crosses C exactly twice by the former argument. Similarly, there exists a face $f \notin D$ such that $v_4, v_6 \in \partial f$ and f is passed by a γ'-segment, a contradiction. Therefore, γ' is essential. Further, it is not difficult to see that γ' is not homotopic to C when C is 2-sided. □

Lemma 3.13. *Let G be a polyhedral quadrangulation of a closed surface F^2 having an annular region A formed by three faces $v_0v_1v_4v_3, v_1v_2v_5v_4$ and $v_2v_0v_3v_5$ as shown in the left-hand side of R_7 in* Figure 1*, and let G' be a quadrangulation obtained from G by an R_7 of A. If G' is not polyhedral, then there exists an essential simple closed curve γ' such that*

(i) *γ' intersects exactly two vertices of G',*

(ii) *γ' passes through exactly one vertex of $[v_0v_3]$, $[v_1v_4]$ and $[v_2v_5]$, and*

(iii) *$C = [v_0v_3][v_1v_4][v_2v_5]$ and γ' are not homotopic.*

Proof. Almost the same argument as in the proofs of Lemmas 3.11 and 3.12 holds, and hence we omit the proof. (This is easier than those proofs.) Since any two homotopic 2-sided simple closed curves on a closed surface cross even times, (iii) immediately holds from (ii). □

Lemma 3.14. *Let G be a polyhedral quadrangulation of a closed surface F^2 having an annular region A formed by four faces $v_0v_1v_6v_5, v_1v_2v_7v_6, v_2v_3v_0v_7$ and $v_0v_5v_4v_7$ as shown in the left-hand side of R_8 in* Figure 1*, and let G' be a quadrangulation obtained from G by an R_8 of A. If G' is not polyhedral, then there exists an essential simple closed curve γ' such that*

(i) *γ' intersects exactly two vertices of G',*

(ii) *γ' passes through at least one vertex of $[v_0v_4]$, $[v_1v_5]$, $[v_2v_6]$ and $[v_3v_7]$, and*

(iii) *$C = [v_0v_4][v_1v_5][v_2v_6][v_3v_7]$ and γ' are not homotopic.*

Proof. Note that there does not exist a face $f \notin A$ (resp., $f' \notin A$) such that $v_0, v_2 \in \partial f$ (resp., $v_5, v_7 \in \partial f'$), similar to the argument in the proof of Lemma 3.12. Furthermore, for example, there might be an edge v_2v_5 in G such that 2-cycle $C' = [v_1v_5][v_2v_6]$ formed by a pair of multiple edges is essential in G'; this is different from the previous lemma. The argument is almost same, and hence we omit it as well. □

4 Main result

First, we refer to the following lemma, which plays an important role in the proof of our main result.

Lemma 4.1 (Juvan, Malnič and Mohar [8])**.** *For any closed surface F^2 and any non-negative integer k, there exists a constant $f(k, F^2)$ such that if $\mathcal{L}$ is a set of pairwise non-homotopic simple closed curves on F^2 such that any two elements of $\mathcal{L}$ cross at most k times, then $|\mathcal{L}| \leq f(k, F^2)$.*

In the next lemmas, we show that there is an upper bound of the maximum degree (resp., the diameter) of $\{R_1, \dots, R_6\}$-irreducible (resp., $\{R_1, \dots, R_8\}$-irreducible) polyhedral quadrangulations of a non-spherical closed surface F^2.

Lemma 4.2. *Let G be an $\{R_1, \dots, R_6\}$-irreducible polyhedral quadrangulation of a non-spherical closed surface F^2. Then the maximum degree of G is bounded by a constant depending only on F^2.*

Proof. We prove that $\Delta(G) \leq 640f(5, F^2) + 79$, where $f(\cdot, F^2)$ is the function in Lemma 4.1. Suppose, for a contradiction, that G has a vertex v with $\deg(v) \geq$

$640f(5, F^2) + 80$. Let L_v be the link walk of v in G. Give a direction to L_v and denote the directed cycle by $\overrightarrow{L}_v$. Let

$$a_1^1, \ldots, a_{16}^1, b_1^1, \ldots, b_7^1, c_1^1, \ldots, c_{17}^1, a_1^2, \ldots, a_{16}^2, b_1^2, \ldots, b_7^2, c_1^2, \ldots, c_{17}^2, \quad \ldots, \\ a_1^l, \ldots, a_{16}^l, b_1^l, \ldots, b_7^l, c_1^l, \ldots, c_{17}^l$$

be $40l$ consecutive vertices of L_v taken along $\overrightarrow{L}_v$, where $l \geq 16f(5, F^2)+2$. Then, we may assume that $vb_1^1b_2^1b_3^1$ is a face of G; note that $vb_1^ib_2^ib_3^i$ is also a face for each $i \in \{2, \ldots, l\}$ under the assumption. Let $P(a, b)$ denote the path in L_v starting at $a \in V(L_v)$ and ending at $b \in V(L_v)$ along $\overrightarrow{L}_v$.

In the former half of the proof, we show the following fact: For each $i \in \{1, \ldots, l\}$, there exists either (A) a cycle of length at most 6 containing a path $b_s^ivb_t^i$ $(1 \leq s < t \leq 6)$, or (B) a cycle of length at most 4 containing a path b_s^ivu $(1 \leq s \leq 6)$ where $u \in V(L_v)$. We call the cycle having the above property (A) (resp., (B)) a *type-A cycle* (resp., *type-B cycle*). Note that there might be a cycle having both properties (A) and (B); in that case, we can classify it into either.

In the following argument, we discuss several cases around vertices $b_1^i, \ldots, b_6^i$ and b_7^i. To simplify notation, we put $b_j^i = b_j$ for each $j \in \{1, \ldots, 7\}$ by omitting the upper subscript "i". First of all, assume that $\deg(b_2) \geq 4$. In this case, we apply an R_1 of $vb_1b_2b_3$ at $\{b_1, b_3\}$, i.e., identifying b_1 and b_3. By Lemma 3.4, we can easily find our desired cycle containing a path b_1vb_3; take such a path using edges of faces passed by the diagonal 3-curve or the semi-diagonal 3-curve. The same fact holds for b_4 and b_6, and hence we assume that $\deg(b_h) = 3$ for each $h \in \{2, 4, 6\}$ below.

Next, assume $\deg(b_3) = 3$. Then, there exist faces $b_1b_2xy, b_2b_3b_4x$ and b_4b_5zx for $x, y, z \in V(G)$. If $\deg(x) \geq 4$, then we can find our desired cycle containing a path b_1vb_5 by Lemma 3.6 as a type-A cycle. On the other hand, if $\deg(x) = 3$, i.e., $y = z$ in this case, then $b_2b_3b_4x$ is an attached 4-cycle. In this case, there exists either a type-A cycle or a type B cycle, both of which contain vb_1, by Lemma 3.7. Thus, we assume that $\deg(b_3) \geq 4$ and $\deg(b_5) \geq 4$ in the following argument.

For the face $vb_3b_4b_5$, there is

(i) an essential 4-cycle vb_3b_4x for $x \notin \{v, b_3, b_4, b_5\}$,

(ii) an essential diagonal 3-curve γ passing through v and b_4, or

(iii) an essential semi-diagonal 3-curve γ passing through v and b_4, by Lemma 3.4.

First, we discuss (i). In this case, x is a vetex of L_v such that $xv \in E(G)$, and hence there exists our desired type-B cycle. Secondly, assume (ii), and let $f_1 = vb_3b_4b_5, f_2 = b_4pqr$ and $f_3 = vsqt$ be faces passed by γ where $q, s, t \in V(L_v)$ (see the left-hand side of Figure 2). Since $\deg(v_4) = 3$, we have $|\{b_3, b_5\} \cap \{p, r\}| = 1$. Without loss of generality, we may assume that $p = b_3$, and we find our desired type-B 4-cycle vb_3qs.

Thirdly, we discuss (iii). We further divide this case into the following two subcases:

(1) γ passes through $f_1 = vb_3b_4b_5, f_2 = b_4pqr$ and $f_3 = vqst$ where $q, s, t \in V(L_v)$, and

(2) γ passes through $f_1 = vb_3b_4b_5, f_2 = b_4pqr$ and $f_3 = vsrt$ where $s, r, t \in V(L_v)$.

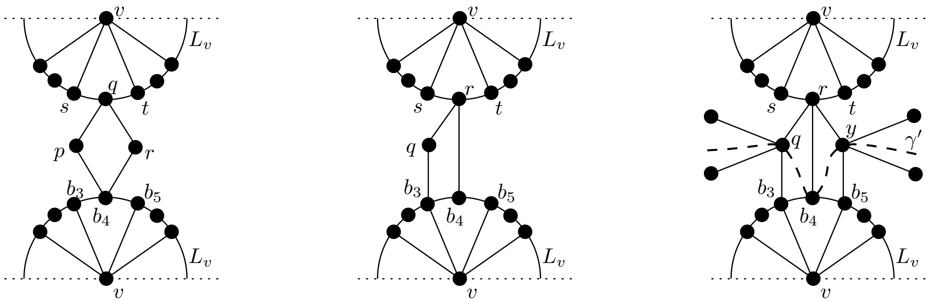

Figure 2: Configurations around L_v.

First, assume the former case (iii)(1). Similar to the above argument, we have $|\{b_3, b_5\} \cap \{p, r\}| = 1$ since $\deg(v_4) = 3$, and we may assume that $p = b_3$ here. In this case, we find a type-B cycle vb_3q of length 3.

Next, suppose the latter case (iii)(2). Similarly, we have $\deg(v_4) = 3$, and hence we may assume that $p = b_3$ (see the center of Figure 2). Furthermore, if $\deg(r) = 3$, then q must be either s or t, and hence we find our desired type-B cycle vb_3q of length 3. Thus, we assume $\deg(r) \geq 4$ in the following argument. By applying Lemma 3.4 to $f_2 = b_3b_4rq$ since $\deg(b_3) \geq 4$ and $\deg(r) \geq 4$, we find either a 2-path P joining q and b_4 such that the cycle b_4b_3qP is essential, or an essential simple closed curve γ' passing $\{q, b_4, x\}$ for $x \in V(G)$. If the former holds, then $P = qb_5b_4$ since $\deg(b_4) = 3$. In this case, there exists our desired type-A cycle vb_3qb_5 of length 4. Next, we assume the latter, and suppose that γ' is an essential diagonal 3-curve. If γ' passes through rb_4b_5y for $y \in V(G)$, then there exists a 2-path P' joining y and q along γ' (see the right-hand side of Figure 2). That is, there exists a type-A cycle $vb_3qP'yb_5$ of length 6. If γ' passes through $b_3b_4b_5v$, then $q \in V(L_v)$ and γ' passes $\{v, b_4, q\}$. In this case, there exists a type-B cycle vb_3qq' of length 4 where $qq' \in E(L_v)$. When γ' is an essential semi-diagonal 3-curve, similar argument holds, and we have either a type-A cycle of length 5 or a type-B cycle of length 3.

In the latter half of the proof, we lead to a contradiction. For our purpose, let C_A^l denote a type-A cycle containing $b_s^l v b_t^l$ where $1 \leq s < t \leq 6$, and let $C_B^{i,j}$ denote a type-B cycle containing a 2-path $b_s^i vu$ where $1 \leq s \leq 6$ such that $u \in \{a_1^j, \dots, a_{16}^j, b_1^j, \dots, b_7^j, c_1^j, \dots, c_{17}^j\}$; i.e., $C_B^{i,j}$ was obtained by the argument above when discussing vertices $b_1^i, \dots, b_7^i$. (Note that $C_B^{i,i}$ might exist for some i.) Then, any two type-A cycles cross at most 5 times, since they cannot cross at a vertex v. Clearly, the number of crossing points of a type-B cycle and another type-A or type-B cycle is at most 4.

First, assume that there exist at least $2f(5, F^2) + 1$ type-A cycles. By the definition of the function, F^2 admits at most $f(5, F^2)$ simple closed curves which are pairwise non-homotopic and cross at most 5 times, and hence there exist three such homotopic cycles C_A^i, C_A^j and C_A^k $(i < j < k)$ by the Pigeonhole Principle. Let $\tilde{D}$ denote the configuration which is the union of the closed disk $\bar{D}$ bounded by L_v and the three cycles C_A^i, C_A^j and C_A^k. First, suppose that $\tilde{D}$ is an embedding on F^2 such that C_A^i, C_A^j and C_A^k are 2-sided. Moreover, assume that C_A^i (resp., C_A^j) contains $b_s^i v b_t^i$ with $1 \leq s < t \leq 6$ (resp., $b_{s'}^j v b_{t'}^j$ with $1 \leq s' < t' \leq 6$).

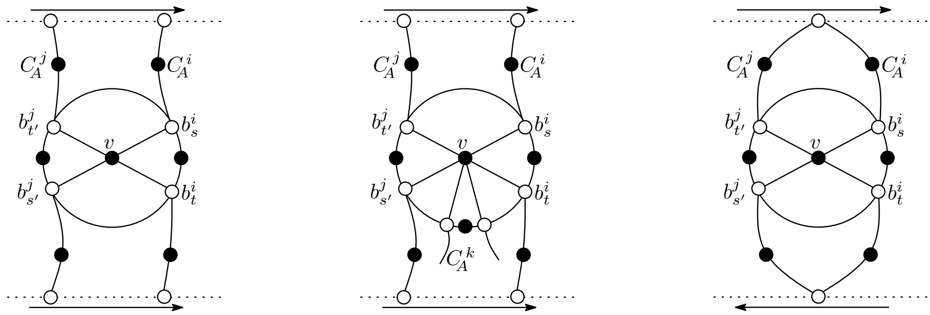

Figure 3: Type-A cycles around v.

Observe that in $\tilde{D}$, C_A^i and C_A^j bound a pinched annulus A (i.e., an annulus where the two boundary components might touch several times) having a pinched point v (see the left-hand side of Figure 3). If C_A^i and C_A^j have a common vertex other than v, then there exists a 2-cell region R in A bounded by a cycle of length either 4 or 6 such that $\bar{R}$ contains $P(b_t^i, b_{s'}^j)$ or $P(b_{t'}^j, b_s^i)$. However, this contradicts Lemma 3.10 since $P(b_t^i, b_{s'}^j)$ (resp., $P(b_{t'}^j, b_s^i)$) contains vertices $c_1^i, \ldots, c_{17}^i, a_1^j, \ldots, a_{15}^j$, and a_{16}^j (resp., $c_1^j, \ldots, c_{17}^j, a_1^i, \ldots,$ a_{15}^i, and a_{16}^i). In the following argument, we call a region like the above R a *dense quadrangle* or a *dense hexagon*, which contains at least 5 or 17 inner vertices, respectively. Thus, we conclude that C_A^i and C_A^j have the unique common vertex v. However, under the situation, the third type-A cycle C_A^k must cross transversally either C_A^i or C_A^j (see the center of Figure 3), contradicting the same argument as above. In the case when each of C_A^i, C_A^j and C_A^k is 1-sided, any two of them must cross, and hence there exists a dense quadrangle or a dense hexagon, as well as the previous case (see the right-hand side of Figure 3).

Next, we discuss type-B cycles. Under our definition, for some $i \neq j$, $C_B^{i,j}$ and $C_B^{j,i}$ might exist; as an extreme example, $C_B^{i,j}$ might coincide with $C_B^{j,i}$. If so, i.e., there exist $C_B^{i,j}$ and $C_B^{j,i}$, then we choose one from them. By the above argument, we may assume that there exist at most $2f(5, F^2)$ type-A cycles. That is, there exist at least $7f(5, F^2) + 1$, which is the half of $14f(5, F^2) + 2$, distinct type-B cycles around v, such that the set of those cycles contains no pair of two cycles $C_B^{i,j}$ and $C_B^{j,i}$ for $1 \leq i \leq j \leq l$.

Similar to the argument for type-A cycles, there exist eight such homotopic cycles simply denoted by $\Gamma_1, \Gamma_2, \ldots, \Gamma_8$ having a common vertex v such that they are placed on F^2 as shown in the left-hand side of Figure 4. Note that the lengths of those cycles are same, which is either 3 or 4, by Proposition 3.1. Furthermore, note that if Γ_i and Γ_{i+1} have a common vertex other than v for some $i \in \{1, \ldots, 7\}$, then we can easily find a dense quadrangle or a dense hexagon, contradicting Lemma 3.10; only Γ_1 and Γ_8 might have a common vertex other than v. Therefore, $\Gamma_i \cup \Gamma_{i+1}$ bounds an octagonal (resp., a hexagonal) 2-cell region for each $i \in \{1, \ldots, 7\}$ if $|\Gamma_i| = 4$ (resp., if $|\Gamma_i| = 3$).

Let $D_{i,j}$ denote an octagonal (or a hexagonal) region bounded by $\Gamma_i \cup \Gamma_j$ for $1 \leq i < j \leq 8$. By Euler's formula, $\Gamma_{4,5}$ contains a vertex u of degree 3; e.g., see Lemma 4.1 in [23]. By Lemma 3.3, u belongs to a connected component of $\langle V_3 \rangle_G$ which is

(i) a 4-cycle,

(ii) a 2-path,

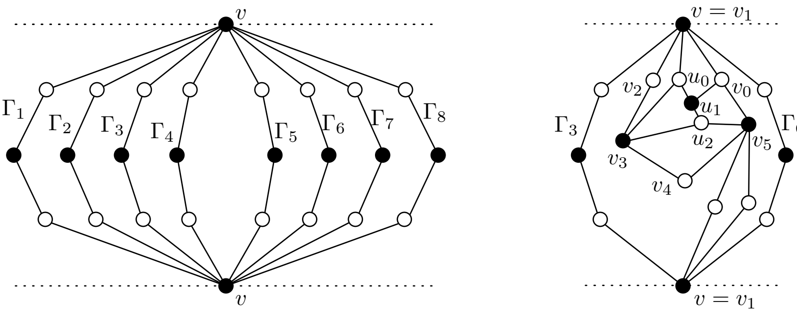

Figure 4: Type-B cycles around v.

(iii) a K_2 or

(iv) an isolated vertex.

First, we assume that $|\Gamma_i| = 4$, and discuss the above four cases in order.

Case (i): In this case, an attached cube H with $\partial(H) = v_0v_1v_2v_3$ containing u as an vertex of the attached 4-cycle is in $\bar{D}_{3,6}$. (Observe that faces incident to u are in $D_{4,5}$, and the other two faces in the 2-cell region bounded by $\partial(H)$ are at least in $D_{3,6}$.) Then, by Lemma 3.7 and the existence of Γ_2 and Γ_7, one of v_0, v_1, v_2 and v_3, say v_0 without loss of generality, must be v; we call the above Γ_2 and Γ_7 *obstructions* throughout the proof. However, Lemma 3.8 requires one more essential simple closed curve which does not pass through $v = v_0$, a contradiction; by the existence of obstructions again.

Case (ii): We assume that u belongs to a 2-path $P = u_0u_1u_2$ and the configuration around P is given by the left-hand side of R_3 in Figure 1. Similarly, the hexagon bounded by $v_0v_1v_2v_3v_4v_5$ is contained in $\bar{D}_{3,6}$, and hence the obstructions, which are Γ_2 and Γ_7, play the same role in this argument. By Lemma 3.6, one of v_1 and v_5, say v_1 without loss of generality, must be v (see the right-hand side of Figure 4). Since $\deg(v_3) \geq 4$ and $\deg(v_5) \geq 4$, there is an essential diagonal 3-curve passing $\{v_4, u_2, v_0\}$ or $\{v_4, u_2, u_0\}$ by Lemma 3.4. However, in each case, such three vertices are inner vertices of $D_{2,7}$, a contradiction.

Case (iii): We assume that $u_0u_1 \in E(G)$ is a connected component of $\langle V_3 \rangle_G$, and there are four faces $v_0v_1u_1v_4, v_1v_2u_2u_1$ and $u_1u_2v_3v_4$ and $u_2v_2v_0'v_3$ contained in $D_{3,6}$. Here, we locally color vertices in $\bar{D}_{3,6}$ by two colors black and white; we assume that v is colored by black. Further, we may assume that v_0' is colored by black without loss of generality; note that v_0, v_2 and v_3 are white vertices. When considering a face $v_0v_1u_1v_4$, there is an essential diagonal 3-curve passing either $\{v_0, u_1, v_2\}$ or $\{v_0, u_1, v_3\}$ by Lemma 3.4, since we have $\deg(v_1) \geq 4$ and $\deg(v_4) \geq 4$. By the existence of obstructions, one of v_0, v_2 and v_3 must be v under the situation. However, it contradicts the above bipartition.

Case (iv): Assume that u is incident to three faces $v_0v_1uv_6, v_1v_2v_4u$ and $uv_4v_5v_6$, which are in $D_{4,5}$, and note that $\deg(v_i) \geq 4$ for each $i \in \{1, 4, 6\}$. As well as the previous case, we locally color vertices in $\bar{D}_{3,6}$; assume that v is colored by black. If u is a white vertex, then it contradicts Lemma 3.4 by the existence of obstructions; note that there should be a diagonal 3-curve passing three white vertices including u. Therefore, u is a black vertex below. By Lemma 3.4 again, exactly one of v_0, v_2 and v_5, say v_0 without loss

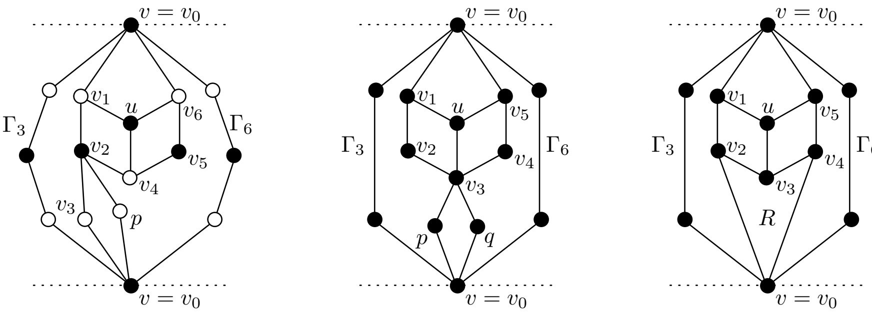

Figure 5: Configurations in the 2-cell region bounded by Type-B cycles.

of generality, coincides with v, and there exists a diagonal 3-curve passing through three faces $v_0v_1uv_6, v_1v_2v_4u$ and $v_2v_3v_0p$ for $v_3, p \in V(G)$, up to symmetry (see the left-hand side of Figure 5). If $\deg(v_2) \geq 4$, then Lemma 3.4 works for $v_2v_3v_0p$, and it contradicts the existence of the obstructions. Thus, we conclude that $|\{v_1, v_4\} \cap \{v_3, p\}| = 1$, and we may suppose $v_4 = p$ since $\{v_1, v_4\} \cap \{v_3, p\} \neq \{v_1\}$; otherwise, G would have multiple edges. Then, G has an octagonal region bounded by $v_0v_1v_2v_3v_0v_4v_5v_6$ satisfying the condition of a reduction R_6. However, it contradicts Lemma 3.12 by the existence of the obstructions.

Next, we assume that $|\Gamma_i| = 3$. We implicitly omit the same argument as in the case assuming $|\Gamma_i| = 4$. (That is, we give only the different and important points below.)

Case (i): The same argument as in the case of $|\Gamma_i| = 4$ works.

Case (ii): We may assume that $v_1 = v$, and there is an essential semi-diagonal 3-curve passing $\{v_4, u_2, v_0\}$, $\{v_4, u_2, u_1\}$ or $\{v_4, u_2, u_0\}$ by Lemma 3.4. However, in any case, such three vertices are inner vertices of $D_{2,7}$, a contradiction.

Case (iii): In this case, the similar argument (not using the bipartition) leads us to the conclusion that $v_0 = v_0' = v$ such that the 3-cycle $v_0v_1v_2$ is homotopic to Γ_i. However, it contradicts Lemma 3.11 by the existence of the obstructions.

Case (iv): Assume that u is incident to three faces $v_0v_1uv_5, uv_1v_2v_3$ and $uv_3v_4v_5$, which are in $D_{4,5}$, and note that $\deg(v_i) \geq 4$ for each $i \in \{1, 3, 5\}$. For a face $v_0v_1uv_5$, there exists a semi-diagonal 3-curve passing either $\{v_0, u, v_3\}$ or $\{v_0, u, v_4\}$, up to symmetry, by Lemma 3.4. Fist assume the former case. If $v = v_0$, then there is a face $f = v_3pvq$ for $p, q \in V(G)$ (see the center of Figure 5). For f, Lemma 3.4 works and we conclude a contradiction by the existence of the obstructions since $\deg(v_3) \geq 4$. On the other hand, if $v = v_3$, then there is a face vsv_0t for $s, t \in V(G)$. As well as the previous case, we can apply Lemma 3.4 for vsv_0t since $\deg(v_0) \geq 4$; if $\{v_1, v_5\} \cap \{s, t\} \neq \emptyset$, then G would not become 3-representative.

Next, we assume the latter case. In this case, v is either v_0 or v_4, say v_0, up to symmetry. By the assumption, there exists an edge v_4v_0 such that $v_0v_5v_4$ is homotopic to Γ_i. Furthermore, applying Lemma 3.4 for a face $v_1v_2v_3u$, there must be a semi-diagonal 3-curve passing $\{v_0, u, v_2\}$; note that v_2, u, v_4 and v_5 are vertices in $\bar{D}_{4,5}$, i.e., inner vertices of $D_{3,6}$. That is, we have $v_2v_0 \in E(G)$ such that $v_2v_0v_4v_3$ bounds a 2-cell region R inside $D_{4,5}$ (see the right-hand side of Figure 5). By the above argument of (i), we may assume that $D_{4,5}$ does not contain a vertex of degree 3 belonging to an attached 4-cycle, and hence

R is a face of G by Lemma 3.9. However, v_3 has degree 3, contrary to u being an isolated vertex of $\langle V_3 \rangle_G$. Therefore, we got our desired conclusion. □

Lemma 4.3. *Let G be an $\{R_1, R_2, R_3\}$-irreducible polyhedral quadrangulation of a non-spherical closed surface F^2. For any vertex $v \in V(G)$, there exists an essential cycle of length at most 6 either*

(i) *containing v, or*

(ii) *containing $u \in V(G)$ such that $uv \in E(G)$.*

Proof. First, assume that $\deg(v) = 3$, and let u_0, u_1 and u_2 be vertices adjacent to v. If two of u_0, u_1 and u_2, say u_0 and u_1 without loss of generality, have degree at least 4, then we can easily find our desired cycle by Lemma 3.5. Thus, by Lemma 3.3, we may assume that $\deg(u_0) = \deg(u_1) = 3$ and $\deg(u_2) \geq 4$ below. If v is contained in a 4-cycle of $\langle V_3 \rangle_G$, then there exists such a cycle by Lemma 3.7. On the other hand, if v is not contained in the above 4-cycle in $\langle V_3 \rangle_G$, that is, if a 2-path $u_0 v u_1$ is a connected component of $\langle V_3 \rangle_G$, then G also has our desired cycle by Lemma 3.6.

Next, we assume $\deg(v) \geq 4$, and let u_0 and u_1 be vertices adjacent to v such that $u_0 v u_1$ forms a corner of a face of G. If one of u_0 and u_1, say u_0 without loss of generality, has degree 3, then G has a cycle of length at most 6 passing through u_0 by the above argument, and hence it satisfies (ii) of the statement in the lemma. If $\deg(u_0) \geq 4$ and $\deg(u_1) \geq 4$, then there exists our desired cycle by Lemma 3.5 again. □

Lemma 4.4. *Let G be an $\{R_1, \ldots, R_8\}$-irreducible polyhedral quadrangulation of a non-spherical closed surface F^2. Then the diameter of G is bounded by a constant depending only on F^2.*

Proof. In this proof, we prove that $\mathrm{diam}(G) \leq 50 f(0, F^2) - 1$ where $\mathrm{diam}(G)$ is a *diameter* of G and $f(\cdot, F^2)$ is the function in Lemma 4.1. Suppose, for a contradiction, that G has two vertices x and y with distance at least $50 f(0, F^2)$. Let P be a path from x to y attaining the distance, and let $x = v_1, v_2, \ldots, v_k$ be the vertices on P lying in this order, where $k \geq 5 f(0, F^2) + 1$, so that the distance between v_i and v_{i+1} is exactly 10 on P, for each $i \in \{1, \ldots, k-1\}$. Then, there exists a cycle C_i of length at most 6 passing through either v_i or a vertex u_i adjacent to v_i for each $i \in \{1, \ldots, k\}$ by Lemma 4.3. Since the distance between v_i and v_j is at least 10 for any $i < j$, two cycles C_i and C_j are mutually disjoint. Since F^2 admits only $f(0, F^2)$ pairwise non-crossing non-homotopic essential cycles, and since we assumed $k \geq 5 f(0, F^2) + 1$, we can take six pairwise homotopic cycles from $\{C_1, \ldots, C_k\}$ by the Pigeonhole Principle. Let $\Gamma_1, \ldots, \Gamma_6$ be such six cycles of length at most 6, which are mutually homotopic. Note that those cycles are 2-sided since any two of them are disjoint, and that the parities of those cycles are pairwise same. We may assume that these $\Gamma_1, \ldots, \Gamma_6$ lie on an annulus in this order.

Let $A_{i,j}$ denote the annular region bounded by Γ_i and Γ_j for $1 \leq i < j \leq 6$; similarly, $\bar{A}_{i,j}$ contains its two boundaries Γ_i and Γ_j. Note that there is no edge joining vertices on Γ_i and Γ_{i+1} for each $i \in \{1, \ldots, 5\}$; for otherwise, the distance between v_i and v_{i+1} would be at most 9, contradicting that P is a shortest path joining x and y in G. Similar to the argument in Lemma 4.2, we call Γ_1 and Γ_6 obstructions for our purpose.

First, we discuss the case when G has a vertex u of degree 3 in $\bar{A}_{3,4}$. By Lemma 3.3, u belongs to a connected component of $\langle V_3 \rangle_G$ which is

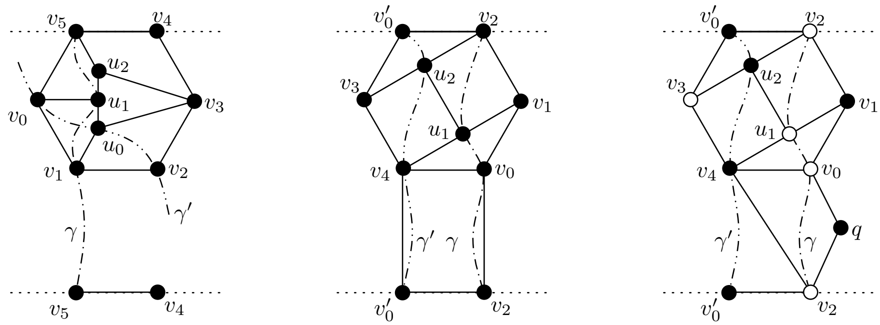

Figure 6: Configurations around connected components of $\langle V_3 \rangle_G$.

(i) a 4-cycle,

(ii) a 2-path,

(iii) a K_2 or

(iv) an isolated vertex.

We discuss the above four cases in order.

Case (i): Under the assumption, an attached cube containing u as an vertex of an attached 4-cycle is in $\bar{A}_{2,5}$. (For example, even if u is on Γ_3, then there is no face f such that ∂f contains both u and a vertex on Γ_2, since there is no edge joining vertices on Γ_2 and Γ_3, and since $\deg(u) = 3$.) Similar argument in Case (i) in the proof of Lemma 4.2 works, and we conclude that this is not the case; i.e, we cannot take two essential simple closed curves γ_1 and γ_2 in Lemma 3.8 by the existence of the obstructions.

Case (ii): We assume that u belongs to a 2-path $P = u_0u_1u_2$ and the configuration around P is given by the left-hand side of R_3 in Figure 1. Similarly, the hexagonal region R bounded by $v_0v_1v_2v_3v_4v_5$ is contained in $\bar{A}_{2,5}$. By Lemma 3.6, there exists an essential diagonal (or a semi-diagonal) 3-curve γ passing $\{v_1, u_1, v_5\}$ (see the left-hand side of Figure 6). On the other hand, since $\deg(v_1) \geq 4$ and $\deg(v_3) \geq 4$ hold, there exists an essential diagonal (or semi-diagonal) 3-curve γ' passing $\{v_0, u_0, v_2\}$ by Lemma 3.4. Observe that both γ and γ' are homotopic to Γ_i by the existence of obstructions. Under the situation, γ and γ' cross transversally in R, and it must cross transversally one more time since these two curves are 2-sided. This implies that there should be a face incident to four vertices v_0, v_1, v_2 and v_5, in which γ and γ' pass through. However, it contradicts that G is simple.

Case (iii): Assume that $u_1u_2 \in E(G)$ is a connected component of $\langle V_3 \rangle_G$, and there are four faces $v_0v_1u_1v_4, v_1v_2u_2u_1, u_1u_2v_3v_4$ and $u_2v_2v_0'v_3$ incident to u_1 and u_2. Note that $\deg(v_i) \geq 4$ for any $i \in \{1, 2, 3, 4\}$. When considering a face $v_0v_1u_1v_4$, there exists an essential diagonal (or semi-diagonal) 3-curve γ passing either $\{v_0, u_1, u_2\}$ or $\{v_0, u_1, v_2\}$ by Lemma 3.4, up to symmetry. Note that γ is homotopic to Γ_i. In the former case, we have $v_0 = v_0'$, and hence we discuss an R_5 to the hexagonal region containing u_1 and u_2. However, it immediately contradicts that G is $\{R_1, \ldots, R_8\}$-irreducible by the existence of obstructions and by Lemma 3.11.

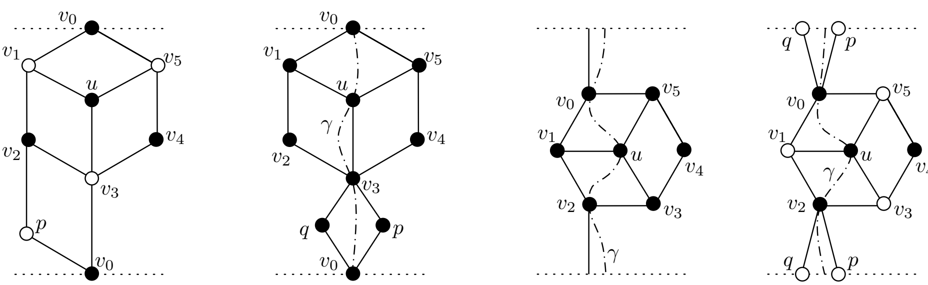

Figure 7: Configurations around connected components of $\langle V_3 \rangle_G$.

Therefore, we assume the latter case. In this case, we may assume that there exists an essential diagonal (or semi-diagonal) 3-curve γ' passing $\{v_0', u_2, v_4\}$ by the same argument as above. Note that γ' is homotopic to γ under the condition. If γ and γ' are both essential semi-diagonal 3-curves (by Proposition 3.1) then, there exists a face $v_0v_4v_0'v_2$ by Lemma 3.9 and our former argument (see the center of Figure 6). However, since $\deg(v_2) \geq 4$ and $\deg(v_4) \geq 4$, we apply Lemma 3.4, and conclude a contradiction.

Thus, we suppose that γ is an essential diagonal 3-curve, and there is a face $f = v_0pv_2q$ for $p, q \in V(G)$ which is passed by γ. Here, observe that $v_1 \notin \{p, q\}$ by the simplicity of G, and hence we have $\deg(v_2) \geq 4$. For f, if $\deg(v_0) \geq 4$, then it is contrary to G being $\{R_1, \ldots, R_8\}$-irreducible by the existence of obstructions and by Lemma 3.4. Therefore, we assume that $\deg(v_0) = 3$ below. Without loss of generality, we may assume that $p = v_4$ (see the right-hand side of Figure 6). Under the situation, we can apply Lemma 3.12 to the octagonal region bounded by $v_2v_1v_0qv_2v_4v_3u_2$, and obtain a contradiction.

Case (iv): Assume that u is incident to three faces $v_0v_1uv_5, v_1v_2v_3u$ and $uv_3v_4v_5$. Note that $\deg(v_i) \geq 4$ for any $i \in \{1, 3, 5\}$. Hence, for a face $v_0v_1uv_5$, we have

(a) an essential 4-cycle $v_0v_1uv_3$, or

(b) an essential diagonal 3-curve or semi-diagonal 3-curve γ passing

  (1) $\{v_0, u, v_3\}$ or

  (2) $\{v_0, u, v_2\}$

  by Lemma 3.4, up to symmetry.

First, assume (a). In this case, for a face $v_1v_2v_3u$, there must be an essential diagonal 3-curve passing $\{v_0, u, v_2\}$ by Lemma 3.4; it is not difficult to check that this is the unique case by Proposition 3.1 and the existence of obstructions. Furthermore, by Lemma 3.9, there exists a face $v_2pv_0v_3$ for $p \in V(G)$, and it contradicts Lemma 3.12 for an octagonal region bounded by $v_0v_1v_2pv_0v_3v_4v_5$ by the similar argument as above (see the first figure of Figure 7).

Secondly, we assume (b)(1). In this case, γ is an essential semi-diagonal 3-curve, and hence there exists a face v_0pv_3q for $p, q \in V(G)$ which γ passes through (see the second figure of Figure 7). Then, we have $\deg(v_0) \geq 4$ since $\{p, q\} \cap \{v_1, v_5\} = \emptyset$; otherwise, G would become representativity at most 2. Therefore, for v_0pv_3q, we apply Lemma 3.4, and obtain a contradiction as well as former cases.

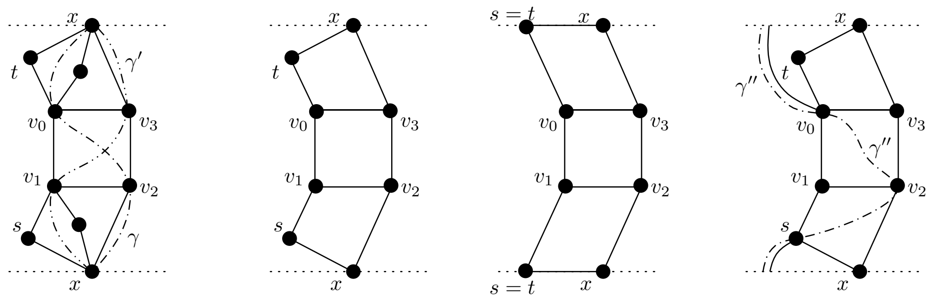

Figure 8: Configurations of Case (I) in Lemma 4.4.

Thirdly, we discuss the case (b)(2). First, assume that γ is an essential semi-diagonal 3-curve; i.e., $v_0v_2 \in E(G)$ which is along γ (see the third figure of Figure 7). Then, for a face $uv_3v_4v_5$, there exists either v_4v_0 or v_4v_2, say v_4v_0 without loss of generality, as an edge of G such that $v_0v_5v_4$ is homotopic to Γ_i. Under the situation, there exists a 2-cell region R bounded by $v_0v_4v_3v_2$, which is a face of G by Lemma 3.9 and the former argument. However, we obtain a contradiction since $\deg(v_3) \geq 4$. Therefore, we suppose that γ is an essential diagonal 3-curve; i.e., there exists a face bounded by v_0pv_2q for $p, q \in V(G)$ (see the last figure of Figure 7). If $\{p, q\} \cap \{v_3, v_5\} \neq \emptyset$, then it gives rise to the above case (a), which had already discussed. On the other hand, if $v_1 \in \{p, q\}$, then G would have multiple edges, a contradiction. Thus, we have $\deg(v_0) \geq 4$ and $\deg(v_2) \geq 4$, and conclude a contradiction by Lemma 3.4, similar to the former cases.

Therefore, in the following argument, we discuss the case when $\deg(u) \geq 4$ for any vertex u in $\bar{A}_{3,4}$. In this case, we focus on a face $f = v_0v_1v_2v_3$ in $\bar{A}_{3,4}$ with $\deg(v_i) \geq 4$ for each $i \in \{0, 1, 2, 3\}$. By Propositions 3.1 and 3.2, Lemma 3.4 and the existence of obstructions, it suffices to discuss the following two cases (I) and (II), up to symmetry.

Case (I): There exist two essential semi-diagonal 3-curves γ and γ' passing $\{v_0, v_2, x\}$ and $\{v_1, v_3, x\}$, respectively, for $x \in V(G)$ such that γ and γ' are homotopic to Γ_i (see the first figure of Figure 8). Then, there are two faces $f = v_0v_3xt$ and $f' = v_1sxv_2$ for $s, t \in V(G)$ by Lemma 3.9 (see the second figure of Figure 8). Under the situation, if $s = t$, then there exists an annular region A bounded by two 3-cycles sv_0v_1 and xv_3v_2 which contains exactly three edges dividing it into three faces (see the third figure of Figure 8). Then, we apply Lemma 3.13 to A and obtain a contradiction by the existence of the obstructions.

Thus, we assume $s \neq t$ below, and hence s, t, v_2 and v_3 are distinct vertices; i.e., we have $\deg(x) \geq 4$. Then, we apply Lemma 3.4 to f' and find an essential semi-diagonal 3-curve γ'' passing $\{s, v_2, z\}$ for $z \in V(G)$. By the existence of the obstructions, γ' and γ'' should be homotopic. That is, γ' and γ'' cross even times (actually twice), and hence we have $z = v_0$ and $sv_0 \in E(G)$ (see the last figure of Figure 8). Then, there exists a 2-cell region bounded by sv_0v_3x, and it contradicts Lemma 3.9 since $s \neq t$.

Case (II): There exists an essential diagonal 3-curve γ passing $\{v_1, v_3, x\}$ for $x \in V(G)$, and $v_0x, v_2x \in E(G)$ such that γ and the 4-cycle $v_0v_1v_2x$ are homotopic to Γ_i (see the left-hand side of Figure 9). Then, there are two faces $f = v_2v_1sx$ and $f' = v_0v_3tx$ for $s, t \in V(G)$ by Lemma 3.9 (see the center of Figure 9). By the simplicity of G, $s, t \notin \{v_0, v_1, v_2, v_3\}$, and hence $\deg(x) \geq 4$. Thus, for f, there exists an essential diagonal

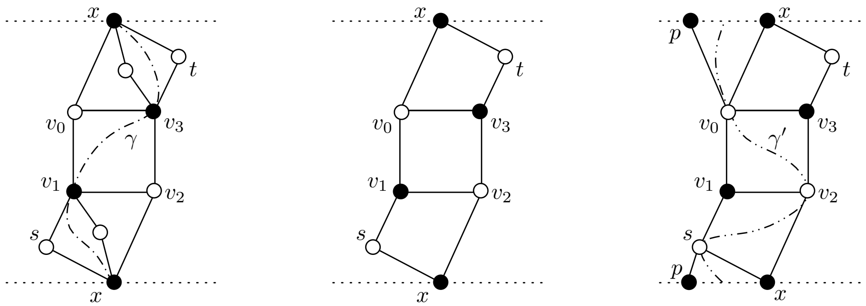

Figure 9: Configurations of Case (II) in Lemma 4.4.

3-curve γ' passing $\{v_0, v_2, s\}$ by Lemma 3.4; this is a unique case by the same argument as in Case (I). Then, by Lemma 3.9, there is a face $f'' = spv_0x$ for $p \in V(G)$ which γ' passes through (see the right-hand side of Figure 9). Apply Lemma 3.14 to the annular region bounded by two 4-cycles v_0v_1sp and v_3v_2xt, and obtain a contradiction. □

Now, we prove our main result as follows.

Proof of Theorem 1.1. Let G be a graph with maximum degree Δ and diameter d. Then, the following inequality holds.

$$|V(G)| \leq 1 + \sum_{k=1}^{d} \Delta(\Delta - 1)^{k-1} = 1 + \frac{\Delta((\Delta - 1)^d - 1)}{\Delta - 2}.$$

Therefore, every $\{R_1, \ldots, R_8\}$-irreducible quadrangulation G of F^2 has a finite number of vertices, since its maximum degree and diameter are bounded by Lemmas 4.2 and 4.4, respectively. Thus, F^2 admits only finitely many $\{R_1, \ldots, R_8\}$-irreducible quadrangulations, up to homeomorphism. □

5 Minimality of reductions

In the previous section, we proved that $\{R_1, \ldots, R_8\}$ is sufficient to finitize the number of minimal quadrangulations of any closed surface. However, one might think that the eight reductions are little too much. As mentioned in the introduction, Theorem 1.3 describes more accurate facts for the torus.

Proof of Theorem 1.3. See Figure 10. Each J_i represents an infinite series of $\{R_1, \ldots, R_8\} \setminus \{R_i\}$-irreducible quadrangulations of the torus. (To obtain the torus, identify two horizontal segments and two vertical segments of the rectangle, respectively.) In each gray colored quadrangular region in figures contains exactly four vertices which is of an attached 4-cycle. We can construct only J_6 and J_8 as bipartite quadrangulations since the others require essential cycles of length 3. Observe that we cannot apply R_8 to J_6, since the dual of J_6 has no essential cycle of length at most 4. Moreover, each of J_7 and J_8 is an infinite series of 4-regular quadrangulations of the torus. □

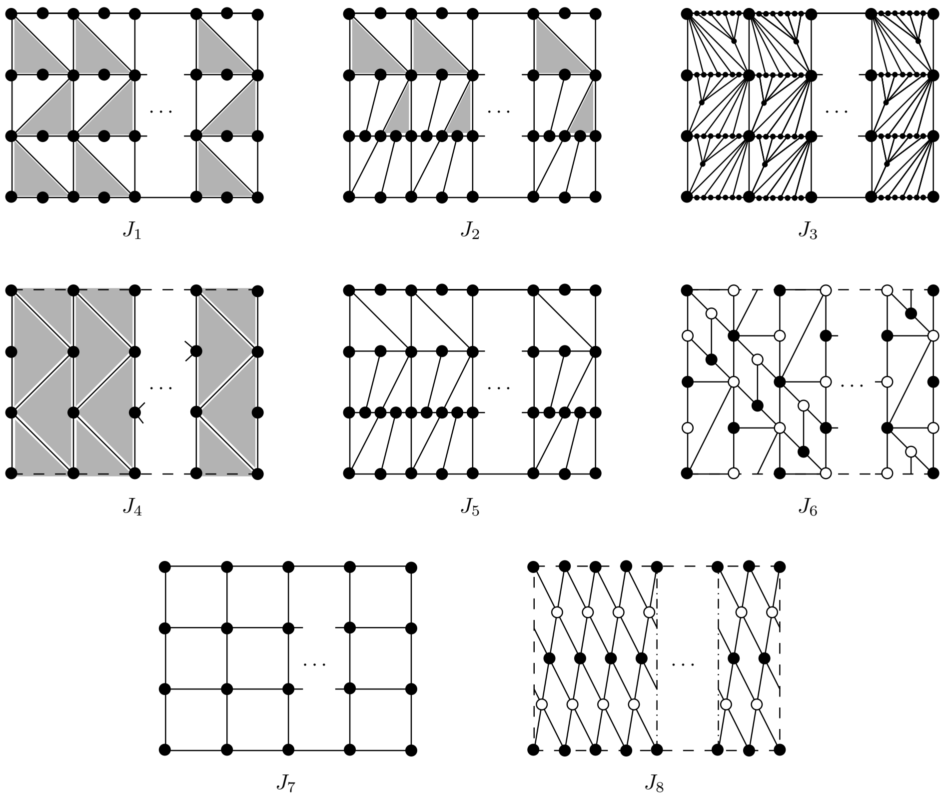

Figure 10: Infinite series of quadrangulations of the torus.

Proof of Theorem 1.4. As mentioned in the introduction, the projective plane does not admit 2-sided essential simple closed curves and hence $\{R_1, \ldots, R_6\}$ is finitizable for polyhedral quadrangulations of the projective plane by Theorem 1.1. The infinite series of minimal graphs can be obtained in a similar way as those of torus; we leave it for readers. For example, an infinite series of polyhedral quadrangulations denoted by $I_{26}(2n+1)$ $(n \geq 2)$, which can be found in [23], is $\{R_1, \ldots, R_5\}$-irreducible quadrangulations of the projective plane. □

In the end of the paper, we pose the following problem.

Problem 5.1. For any closed surface F^2 other than the sphere, the projective plane and the torus, is $\{R_1, \ldots, R_8\}$ a minimal finitizable set of reductions for polyhedral quadrangulations of F^2?

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The fullerene graphs with a perfect star packing*

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Abstract

Fullerene graph G is a connected plane cubic graph with only pentagonal and hexagonal faces, which is the molecular graph of carbon fullerene. A spanning subgraph of G is called a perfect star packing in G if its each component is isomorphic to $K_{1,3}$. For an independent set $D \subseteq V(G)$, if each vertex in $V(G) \setminus D$ has exactly one neighbor in D, then D is called an efficient dominating set of G. In this paper we show that the number of vertices of a fullerene graph admitting a perfect star packing must be divisible by 8. This answers an open problem asked by Došlić et al. and also shows that a fullerene graph with an efficient dominating set has $8n$ vertices. In addition, we find some counterexamples for the necessity of Theorem 14 of paper of Došlić et al. from 2020 and list some subgraphs that preclude the existence of a perfect star packing of type $P0$.

Keywords: Fullerene graph, perfect star packing, efficient dominating set.

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1 Introduction

A chemical graph is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. Perfect matchings of a chemical graph correspond to Kekulé structures of the molecule, which feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules [20]. Alternating sextet faces (sextet patterns) also play a meaningful role in the prediction of molecular stability, in particular, but not only, in benzenoid compounds. Although for fullerenes, the above two structures do not play the same role as in benzenoid compounds, they have received considerable attention in recent years, see [1, 4, 8, 13, 17, 21, 32, 33] etc..

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A perfect matching in a graph G may be viewed as a collection of subgraphs of G, each of which is isomorphic to K_2, whose vertex sets partition the vertex set of G. This is naturally generalized by replacing K_2 by an arbitrary graph H. For a given graph H, an *H-packing* of G is the set of some vertex disjoint subgraphs, each of which is isomorphic to H. From the optimization point of view, the maximum H-packing problem is to find the maximum number of vertex disjoint copies of H in G called the *packing number*. An H-packing in G is called *perfect* if it covers all the vertices of G. If H is isomorphic to K_2, the maximum (perfect) H-packing problem becomes the familiar maximum (perfect) matching problem. If H is the cycle C_6 of length 6, for a fullerene or a hexagonal system G, the packing number is related to the Clar number (the maximum number of mutually disjoint sextet patterns) of G. If H is the star graph $K_{1,3}$, it is the maximum star packing problem. If a $K_{1,3}$-packing covers all the vertices of G, we call it being a *perfect star packing*. For a given family $\mathcal{F}$ of graphs, an H-packing concept can also be generalized to an $\mathcal{F}$-packing (we refer the reader to [29] for the definition).

Packing in graphs is an effective tool as it has lots of applications in applied sciences. H-packing, is of practical interest in the areas of scheduling [5], wireless sensor tracking [6], wiring-board design, code optimization [23] and many others. Packing problems were already studied for carbon nanotubes [2]. Packing lines in a hypercube had been studied in [15]. H-packing was determined for honeycomb [29] and hexagonal network [28]. For representing chemical compounds or to problems of pattern recognition and image processing, P_3-packing has some applications in chemistry [30]. Packing stars in fullerene graph have been investigated in [14] by Doslić et al.. For any integer $n \geq 5$, they found a fullerene graph of order $8n$ which has a perfect star packing. So they raised an open problem "Is there a fullerene on $8n + 4$ vertices with a perfect star packing?".

In the following section we introduce necessary preliminaries and characterize the classical fullerenes which have a perfect star packing. Section 3 gives a negative answer to the open problem asked by Doslić et al. [14]. This implies that a fullerene graph with an efficient dominating set must has $8n$ vertices. In Section 4, we generalize the Proposition 1 in reference [14] and give three counterexamples for the necessity of Theorem 14 in the same paper. We also list some subgraphs that preclude the existence of a perfect star packing of type $P0$.

2 Characterization of fullerenes with a perfect star packing

A *fullerene* graph (simply fullerene) is a cubic 3-connected plane graph with only pentagonal and hexagonal faces. By the Euler formula, each fullerene graph has exactly 12 pentagons. Such graphs are suitable models for carbon fullerene molecules: carbon atoms are represented by vertices, whereas edges represent chemical bonds between two atoms (see [16, 26]). For all even $n \geq 24$ and $n = 20$, Grünbaum and Motzkin [19] showed that there exists a fullerene graph with n vertices. Using a similar approach, Klein and Liu [24] proved that a fullerene graph with isolated pentagons of order n exists for $n = 60$ and for each even $n \geq 70$. We refer the reader to the reference [16] for more details on fullerene graphs.

A cycle of a fullerene graph G is a *facial cycle* if it is the boundary of a face in G, otherwise, it is a *non-facial* cycle. Clearly, each pentagon and hexagon in G is a facial cycle since G is 3-connected and any 3-edge-cut is trivial [31]. In paper [14], the authors obtained the following basic conclusions.

Proposition 2.1 ([14]). *Let S be a perfect star packing of fullerene graph G. Then each pentagon of G can contain at most one center of a star in S.*

Lemma 2.2 ([14]). *Let S be a perfect star packing of fullerene graph G. Then a vertex shared by two pentagons of G cannot be the center of a star in S.*

Recall that a vertex set X of a graph G is said to be *independent* if any two vertices in X are not adjacent in G. A cycle $C = v_1v_2 \cdots v_kv_1$ in G is called *induced* if v_i has only two adjacent vertices v_{i+1} and v_{i-1} around the k vertices $v_1, v_2, \cdots, v_k$ (note that $i + 1 := 1$ if $i = k$, and $i - 1 := k$ if $i = 1$). Otherwise, there exists some i and $j \notin \{i-1, i+1\}$ such that v_i and v_j are adjacent in G, the edge v_iv_j is a *chord* of C and C is not induced. A subgraph R of a graph G is *spanning* if R covers all the vertices of G. For a vertex v of a graph G, we call vertex u being a *neighbor* of v in G if u is adjacent to v in G.

Theorem 2.3. *Let G be a fullerene graph. Then G has a perfect star packing if and only if G has an independent vertex set S^* such that each component of $G - S^*$ is an induced cycle in G.*

Proof. If G has a perfect star packing S, then S is a spanning subgraph of G and any component in S is isomorphic to a star graph $K_{1,3}$. Let S^* be the set of all 3-degree vertices in S. Clearly, S^* is an independent vertex set in G and any vertex in $G - S^*$ has degree 2. So each component of $G - S^*$ is an induced cycle in G.

Let S^* be an independent vertex set of G such that each component of $G - S^*$ is an induced cycle in G. Clearly, each vertex in S^* and its three neighbors induce a star graph $K_{1,3}$. We collect all these star graphs and denote this set by $\mathcal{H}$. For any vertex x on a cycle C in $G - S^*$, x has exactly one neighbor in S^* since G is 3-regular and induced cycle C is a component of $G - S^*$. So $\mathcal{H}$ is a spanning subgraph of G and each component of $\mathcal{H}$ is a star graph $K_{1,3}$, that is, $\mathcal{H}$ is a perfect star packing of G. □

We note that star graph $K_{1,3}$ has exactly one *center* (the vertex of degree 3) and three leaves. For a perfect star packing S of fullerene graph G, each 1-degree vertex in S is a *leaf*. In the following, we denote by $C(S)$ the set of all the centers of stars in S.

Remark 2.4. Let S be a perfect star packing of fullerene graph G. Then

(1) $C(S)$ is an independent vertex set in G.

(2) Any leaf in S has exactly one neighbor belonging to $C(S)$ and has exactly two neighbors being leaves in S.

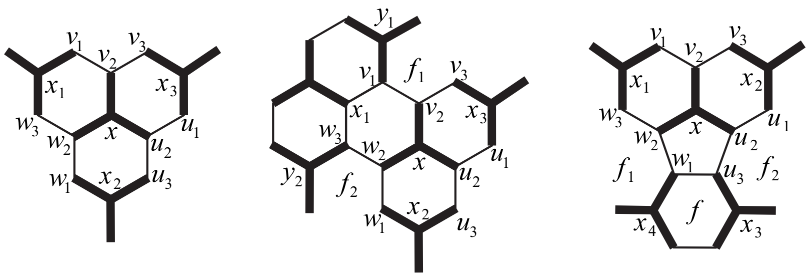
(3) Each cycle in $G - C(S)$ does not have a chord.

Proposition 2.5. *Each hexagon can contain at most two centers of a perfect star packing of fullerene graph G. If a hexagon h contains two such centers, then they are antipodal points on the hexagon h.*

Proof. Let h be a hexagon in G. We denote the six vertices of h by $v_1, v_2, \ldots, v_6$ in the clockwise direction. If vertex v_1 is the center of a star H in a perfect star packing S of G, then v_2 and v_6 are two leaves in H. Hence both v_3 and v_5 are leaves in S by Remark 2.4(2). Clearly, v_4 could be the center of a star in S. Hence h has at most two centers of S and if h contains two such centers, then they are antipodal points on h. □

3 The order of fullerenes with a perfect star packing

To show the main conclusion, we need to prepare as follows.



(a) (*b*) (*c*)

Figure 1: (a) Type 1; (b) Type 2; (c) Type 3.

Lemma 3.1. *Let S be a perfect star packing of fullerene graph G. Then for any vertex $x \in C(S)$, all the vertices on the three faces sharing x are covered by S as Type* 1*, Type* 2 *or Type* 3 (*see* Figure 1*, S are depicted in bold lines*).

Proof. By the Lemma 2.2, at most one of the three faces sharing x is a pentagon since $x \in C(S)$. There are two cases as follows.

Case 1: The three faces sharing x are all hexagons.

Clearly, x has three antipodal points on the three hexagons sharing x, denoted by x_1, x_2 and x_3 respectively as depicted in Figure 1(a). By Remark 2.4(2), the two neighbors v_1 and v_3 of v_2 are leaves in S. Similarly, u_1, u_3, w_1 and w_3 are also leaves in S. We claim that at least two of x_1, x_2 and x_3 are centers of stars in S. If x_1 is not the center of a star in S, then x_1 is a leaf in S. So the third neighbor of v_1, say y_1, is the center of a star in S (see Figure 1(b)). Similarly, the third neighbor of w_3, say y_2, is also the center of a star in S. Since the three vertices v_1, v_2 and v_3 are leaves in S and $y_1 \in C(S)$, the face f_1 has only one center of S by Propositions 2.5 and 2.1. Hence the two neighbors of v_3 on f_1 are leaves. By Remark 2.4(2), x_3 is the center of a star in S, that is, $x_3 \in C(S)$. Similarly, w_1 is a leaf in S and the two neighbors of w_1 on f_2 are all leaves in S. Hence $x_2 \in C(S)$. So at least two of x_1, x_2 and x_3 belong to $C(S)$. If exactly two of x_1, x_2 and x_3 belong to $C(S)$, without loss of generality, we suppose that $x_2, x_3 \in C(S)$, then all the vertices on the three faces sharing x are covered by S as Type 2. If all the three vertices x_1, x_2 and x_3 belong to $C(S)$ (see Figure 1(a)), then all the vertices on the three faces sharing x are covered by S as Type 1.

Case 2: Exactly one of the three faces sharing x is a pentagon.

By Proposition 2.1, w_1 and u_3 are leaves in S (see Figure 1(c)). Hence $x_4, x_3 \in C(S)$ and f is a hexagon by Remark 2.4(2) and Proposition 2.5. By Remark 2.4(2), the neighbor w_3 of w_2 is a leaf in S since the neighbor x of w_2 belongs to $C(S)$. Hence the other vertices on f_1 except for x_4 are all leaves in S by Propositions 2.1 and 2.5. This follows that the neighbor x_1 of w_3 is the center of a star in S by Remark 2.4(2). Similarly, we can show

$x_2 \in C(S)$. Hence all the vertices on the three faces sharing x are covered by S as Type 3 (see Figure 1(c)). □

Corollary 3.2. *Let S be a perfect star packing of fullerene graph G. If a pentagon P of G has a vertex $x \in C(S)$, then $G - C(S)$ has a non-facial cycle C of G such that the path $P - x$ is a subgraph of C.*

Proof. By Proposition 2.2, x is shared by this pentagon P and two hexagons. So all the vertices on the three faces sharing x are covered by S as Type 3 (see Figure 1(c)). Clearly, the path $P - x$ is a subgraph of a cycle C in $G - C(S)$ and C is a non-facial cycle of G. □

We note that 3-connected graphs have only one embedding up to equivalence [12]. If we embed a fullerene graph G in the plane, then any non-facial cycle C of G as a Jordan curve separates the plane into two regions, denoted by R_1^* and R_2^*, each of which has the entire C as its frontier. We denote the subgraph of G induced by the vertices lying in the interior of R_i^* by G_i, $i = 1, 2$. Here we note that $\{V(G_1), V(G_2), V(C)\}$ is a partition of all the vertices of G. We say that C *divide* the graph G into two *sides* G_1 and G_2.

Theorem 3.3. *Let S be a perfect star packing of fullerene graph G and C be a cycle in $G - C(S)$. Then $C(S)$ does not have a vertex which has three neighbors on C.*

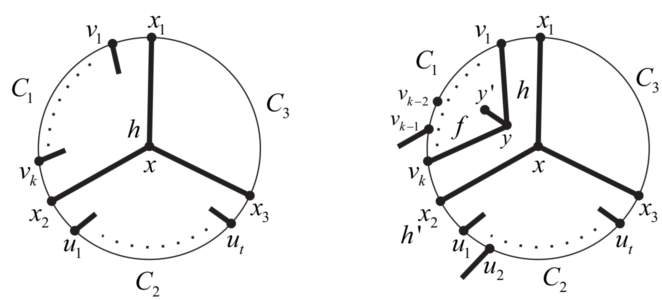


Figure 2: $x \in C(S)$ has three neighbors on C.

Proof. If C is a facial cycle of G, then C is a pentagon or a hexagon. The conclusion clearly holds. Now, let C be a non-facial cycle of G. Then C divides G into two sides, denoted by H_1 and H_2 respectively. We note that all vertices on C are leaves in S since C is a cycle in $G - C(S)$. On the contrary, we suppose that there is a vertex $x \in C(S)$ which has three neighbors on C, denoted by x_1, x_2 and x_3 respectively. Without loss of generality, we suppose that $x \in V(H_1)$ (see Figure 2(a)). The three vertices separate the circle C into three sections, denoted by C_1, C_2 and C_3 respectively, each of which is a path with x_i and x_{i+1} as two terminal ends, $i = 1, 2, 3$ (if $i = 3$, then $i + 1 := 1$). From Lemma 3.1 we know that at most one of $x_1C_1x_2x$, $x_2C_2x_3x$ and $x_3C_3x_1x$ is a facial cycle of G since C is a cycle in $G - C(S)$. Next, we suppose that $x_1C_1x_2x$ and $x_2C_2x_3x$ are non-facial cycles of G. Let $C_1 = x_1v_1v_2 \cdots v_kx_2$, $C_2 = x_2u_1u_2 \cdots u_tx_3$. So $k \geq 5$ and

$t \geq 5$ since any non-facial cycle of G has length at least 8. By Remark 2.4(3), C does not have a chord. So $v_1v_k \notin E(G)$ and $u_1u_t \notin E(G)$. This implies that h is a hexagon face of G, and x_1, x, x_2 and v_1, v_k are five vertices on h. We denote the sixth vertex of h by y. Clearly, $y \in V(H_1)$ by the planarity of G (see Figure 2(b)). Similarly, both u_1 and u_t have a common neighbor in H_1.

Since S is a perfect star packing of G and the two neighbors x_1 and v_2 of v_1 are leaves in S, y is the center of a star in S. If the third neighbor of y is on C, then it is on C_1, denoted it by v_r. The three neighbors of y separate the circle C into three sections, two of which are subgraphs of C_1, denoted by C_1^1 and C_1^2 respectively. As the above discussion, we know that one of $v_1C_1^1v_ry$ and $v_rC_1^2v_ky$ is a non-facial cycle of G. By the recursive process and the finiteness of the order of G, we can suppose that the third neighbor of y is not on C, and denoted it by y'.

See Figure 2(b), the five vertices $v_{k-1}, v_k, x_2, u_1, u_2$ belong to a common facial cycle h' of G. Since C does not have a chord by Remark 2.4(3), v_{k-1} and u_2 are not adjacent in G. So h' is a hexagon. By the planarity of G, v_{k-1} and u_2 have a common neighbor in H_2. so v_{k-2}, v_{k-1}, v_k, y and y' are on a face of G, say f. If f is a pentagon, then v_{k-2} is adjacent to y'. So all the three neighbors of v_{k-2} are leaves in S. This implies a contradiction since v_{k-2} is also a leaf in S. If f is a hexagon, then v_{k-2} and y' have a common neighbor, denoted by z. Clearly, z is v_{k-3} or not. For $z = v_{k-3}$, the three neighbors of v_{k-3} are all leaves in S, a contradiction. For $z \neq v_{k-3}$, by Remark 2.4(2), z is a leaf in S since y' has a neighbor $y \in C(S)$. So the three neighbors of v_{k-2} are all leaves in S, a contradiction. All these contradictions imply that $C(S)$ does not have a vertex which has three neighbors on C. □

Let S be a perfect star packing of fullerene graph G and C be a cycle in $G - C(S)$ which is a non-facial cycle of G. C divides G into two sides, denoted by H_1 and H_2 respectively. Set C^i be the set of all the vertices on C each of which has a neighbor in H_i, $i = 1, 2$. Clearly, $\{C^1, C^2\}$ is a partition of $V(C)$. $G[C^i]$ is a vertex induced subgraph of G which has vertex set C^i and any two vertices of C^i are adjacent if and only if they are adjacent in G. See Figure 4, $G[C^1]$ is depicted as red and $G[C^2]$ is depicted as blue. In the following, we use these symbols no longer explaining.

Lemma 3.4. *For $i = 1, 2$, if a vertex x on C has a neighbor in H_i, then the component of the induced subgraph $G[C^i]$ which contains x is a path with 2 or 3 vertices.*

Proof. We suppose that x on C has a neighhbor in H_1. For the convenience of the following description, set $C := xv_1v_2 \cdots v_kx$. Since C is a cycle in $G - C(S)$ which is a non-facial cycle of G, the length of C is at least 8. So $k \geq 7$. There are three cases for the two neighbors v_1 and v_k of x on C.

Case 1: Both v_1 and v_k have neighbors in H_2.

In this case, the three vertices v_1, x and v_k lie on the same face f of G (see Figure 3(a)). Since all the vertices on C are leaves in S, the other neighbor of v_1 (resp. v_k) which is not on C is the center of a star in S. So f has two vertices in $C(S)$ which are the centers of two stars in S covered v_1 and v_k, respectively. So f is a hexagon by Proposition 2.1. But the case cannot hold by Propositions 2.5.

Case 2: Both v_1 and v_k have neighbors in H_1.

In this case, the five vertices $v_2, v_1, x, v_k, v_{k-1}$ belong to a facial cycle h of G (see Figure 3(b)). We claim that both v_2 and v_{k-1} have neighbors in H_2. Otherwise, at least

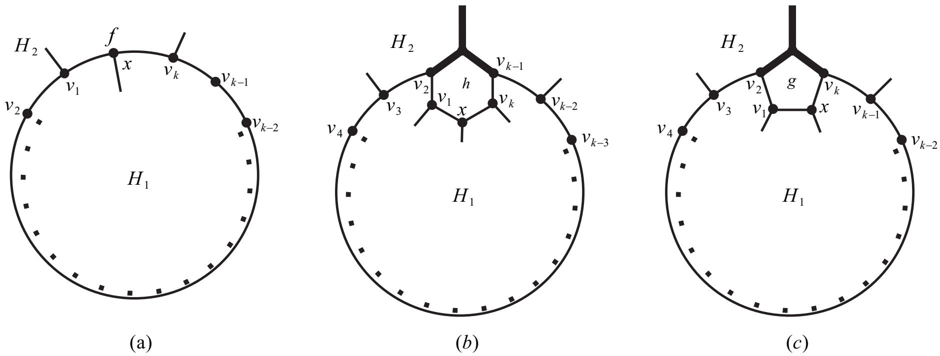


Figure 3: (a) v_1 and v_k have neighbors in H_2; (b) v_1 and v_k have neighbors in H_1; (c) v_1 has a neighbor in H_1, v_k has one in H_2.

one of v_2 and v_{k-1} has a neighbor in H_1. If v_2 has a neighbor in H_1 and v_{k-1} has a neighbor in H_2, then the six vertices $v_3, v_2, v_1, x, v_k, v_{k-1}$ lie on a face h of G. So h is a hexagon and C has a chord v_3v_{k-1}, a contradiction. For v_2 having a neighbor in H_2 and v_{k-1} having a neighbor in H_1, we can also obtain a chord of C, a contradiction. If both v_2 and v_{k-1} have neighbors in H_1, then the seven vertices $v_3, v_2, v_1, x, v_k, v_{k-1}, v_{k-2}$ belong to a common face h of G. This implies that G has a facial cycle of length at least 7, a contradiction. So both v_2 and v_{k-1} have neighbors in H_2, and $v_2, v_1, x, v_k, v_{k-1}$ lie on a hexagon h of G (see Figure 3(b)). Since C does not have a chord, the path v_1xv_k is a connected component of the induced subgraph $G[C^1]$.

Case 3: v_1 has a neighbor in H_1 and v_k has a neighbor in H_2, or v_1 has a neighbor in H_2 and v_k has a neighbor in H_1.

By symmetry, it is sufficient to consider that v_1 has a neighbor in H_1 and v_k has a neighbor in H_2. If v_2 has a neighbor in H_1, then v_3 must have a neighbor in H_2, otherwise, C has a chord or G has a facial cycle of length at least seven, a contradiction. As the proof of Case 2, v_3, v_2, v_1, x, v_k lie on a hexagonal facial cycle. So the path v_2v_1x is a connected component of the induced subgraph $G[C^1]$. Now, we suppose that v_2 has a neighbor in H_2. Then the four vertices v_k, x, v_1, v_2 lie on the same face g of G. Since v_k, x, v_1, v_2 are all leaves in S, g is a pentagon and v_2, v_k have a common neighbor in H_2 which is the center of a star in S (see Figure 3(c)). So the path xv_1 is a connected component of the induced subgraph $G[C^1]$.

In summary, the component of the induced subgraph $G[C^1]$ which contains x is a path with 2 or 3 vertices since C does not have a chord. □

In addition, we have the following Lemma.

Lemma 3.5. *Each component of* $G[C^i]$ *is a path with* 2 *or* 3 *vertices,* $i = 1, 2$.

Proof. For any vertex x on C, x must have exactly one neighbor in H_1 or H_2 since G is 3-regular and C does not have a chord. Without loss of generality, we suppose that x has exactly one neighbor in H_1. By Lemma 3.4, the component of the induced subgraph $G[C^1]$ which contains x is a path with 2 or 3 vertices. We note that the choice of x is arbitrary. So the conclusion holds. □

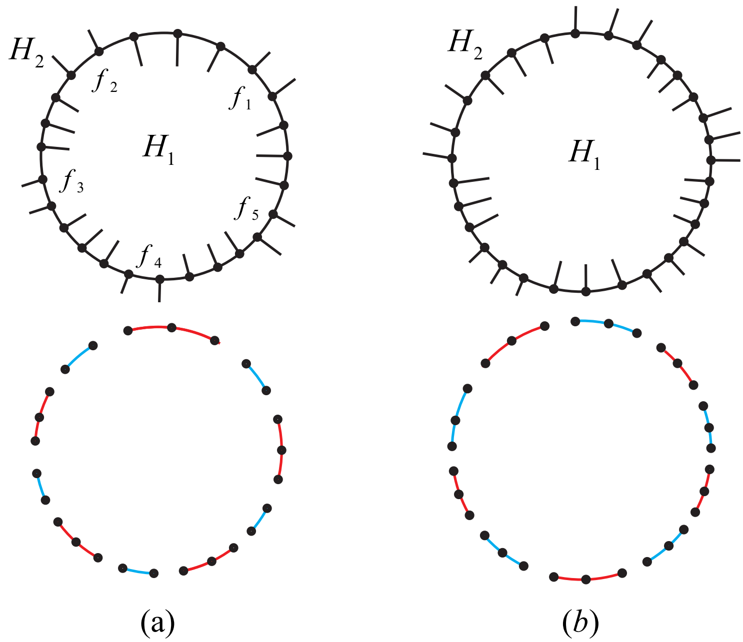


Figure 4: (a) A cycle C of length 25; (b) A cycle C of length 30. ($G[C^1]$ is red and $G[C^2]$ is blue.)

Proposition 3.6. *Let $C = v_0v_1 \cdots v_{k-1}$ be a non-facial cycle in $G - C(S)$ (In the following, the subscript is modulo k).*

(i) *If both v_i and v_{i+1} have neighbors in H_1 (resp. H_2) and v_{i-1} and v_{i+2} have neighbors in H_2 (resp. H_1), then the four vertices v_{i-1}, v_i, v_{i+1} and v_{i+2} lie on a pentagon of G.*

(ii) *If v_i, v_{i+1}, v_{i+2} have neighbors in H_1 (resp. H_2) and v_{i-1} and v_{i+3} have neighbors in H_2 (resp. H_1), then the five vertices $v_{i-1}, v_i, v_{i+1}, v_{i+2}$ and v_{i+3} lie on a hexagon of G.*

(iii) *For $j = 1, 2$, if both v_i and v_{i+1} have neighbors in H_j (we denote the two edges incident to v_i and v_{i+1} not lie in C by e_i and e_{i+1}, respectively), then the facial cycle containing both e_i and e_{i+1} is a hexagon, and two antipodal points on this hexagon are centers of two stars in the perfect star packing S.*

Proof. Cases (i) and (ii) can be easily obtained from the proof of the Cases 2 and 3 of Lemma 3.4 (see Figure 3). Since all the vertices on C are leaves in the perfect star packing S, the other end of e_i (resp. e_{i+1}) which is not on C, denoted by u_i (resp. u_{i+1}), is the center of a star in S. We know that any facial cycle of G is a pentagon or a hexagon. So u_i and u_{i+1} are distinct. By Lemmas 2.1 and 2.5, the facial cycle containing both e_i and e_{i+1} is a hexagon, and u_i and u_{i+1} are antipodal points on this hexagon. □

For example, in Figure 4, except for $f_i, i \in \{1, 2, 3, 4, 5\}$ the other faces sharing edges with C are all hexagons. Moreover, how the vertices on C being covered by S is determined.

We recall that the union of two graphs G_1 and G_2 is denoted by $G_1 \cup G_2$, which has vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. Let n_3 be the number of the components of $G[C^1] \cup G[C^2]$ each of which is isomorphic to a path with 3 vertices. Similarly, n_2 is the number of the components of $G[C^1] \cup G[C^2]$ each of which is isomorphic to a path with 2 vertices. For example, $n_3 = n_2 = 5$ in Figure 4(a) and $n_3 = 10$, $n_2 = 0$ in Figure 4(b).

Observation 1. $n_2 + n_3$ is even.

Proposition 3.7. *Let S be a perfect star packing of fullerene graph G and C a cycle in $G - C(S)$ which is a non-facial cycle of G. Then the length of C is $3n_3 + 2n_2$, and the length of C has the the same parity with n_2 and n_3.*

Proof. Clearly, the length of C is $3n_3 + 2n_2$ by Lemma 3.5. So n_3 is odd if and only if the length of C is odd. Since $n_2 + n_3$ is even by Observation 1, the parity of n_2 and n_3 are same. Then we are done. □

Theorem 3.8. *Let S be a perfect star packing of fullerene graph G. Then $G - C(S)$ has even number of odd cycles.*

Proof. If $G - C(S)$ does not have a non-facial cycle of G, then any pentagon of G does not have a vertex in $C(S)$ by Corollary 3.2. So all the vertices on pentagons are leaves in S. It implies that $G - C(S)$ has exactly twelve odd cycles, each of which is a pentagon. Next, we suppose that $G - C(S)$ has a non-facial cycle of G, denoted by C.

Claim 1: If C is an even cycle, then G has even number of pentagons which share edges with C. If C is an odd cycle, then G has odd number of pentagons which share edges with C.

By Proposition 3.6, the number of pentagons which share edges with C is equal to n_2. By Proposition 3.7, n_2 and the length of C have the same parity. So the Claim holds.

Claim 2: Any pentagon of G shares edges with at most one non-facial cycle in $G - C(S)$.

Let P be a pentagon of G. By Proposition 2.1, P has at most one vertex which is the center of a star in S. If P does not have a vertex in $C(S)$, then P is a cycle in $G - C(S)$. By Theorem 2.3, each component of $G - C(S)$ is an induced cycle of G. So P does not share edges with any non-facial cycle in $G - C(S)$. If P has a vertex $x \in C(S)$, then by Corollary 3.2 $P - x$ is a subgraph of a non-facial cycle in $G - C(S)$. So P shares edges with exactly one non-facial cycle in $G - C(S)$.

Now, we consider the following two cases for the non-facial cycles in $G - C(S)$.

Case 1: $G - C(S)$ does not have a non-facial cycle of odd length.

Then any non-facial cycle C in $G - C(S)$ is of even length. By the above Claims, there are even number of pentagons in G such that they share edges with C. Since G has exactly twelve pentagons, there are even number of pentagons in G each of which does not share edges with non-facial cycles in $G - C(S)$. These pentagons must be cycles in $G - C(S)$ by Corollary 3.2. Hence $G - C(S)$ has even number of odd cycles.

Case 2: $G - C(S)$ has some non-facial cycle of odd length.

Suppose that $G - C(S)$ has exactly k non-facial cycles of odd length. We denote the number of pentagons in G each of which does not share edges with non-facial cycles in

$G - C(S)$ by p. These p pentagons must be cycles in $G - C(S)$ by Corollary 3.2. So $G - C(S)$ has $p + k$ odd length cycles. Next, we show that p and k have the same parity. If p is odd, then G has odd number of pentagons each of which share edges with exactly one non-facial cycle in $G - C(S)$ since G has exactly 12 pentagons. By the above Claims, for each even length non-facial cycle in $G - C(S)$, G has even number of pentagons which share edges with the cycle, and for each odd length non-facial cycle in $G - C(S)$, G has odd number of pentagons which share edges with the cycle. So $G - C(S)$ has odd number of non-facial cycles of odd length. This means that k is odd. For p being even, we can similarly show that k is even. So k and p have the same parity and $p + k$ is even. □

Clearly, for a fullerene graph G with a perfect star packing, its order must be divisible by 4. So the order of G is $8k$ or $8k+4$ for some positive integer k. Now, we can obtain the following main theorem which illustrates that the order of G can not be $8k + 4$.

Theorem 3.9. *If fullerene graph G has a perfect star packing, then the order of G is divisible by* 8.

Proof. We suppose that S is a perfect star packing of G and $\mathcal{C}_o$ and $\mathcal{C}_e$ are the collections of all the odd cycles and even cycles in $G - C(S)$, respectively. Then we have the following equation.

$$\begin{aligned} |V(G)| &= |C(S)| + \sum_{C \in \mathcal{C}_o} |C| + \sum_{C \in \mathcal{C}_e} |C| \\ &= \frac{|V(G)|}{4} + \sum_{C \in \mathcal{C}_o} |C| + even. \end{aligned} \tag{3.1}$$

By Theorem 3.8, $\mathcal{C}_o$ has even number of elements. Combining the above equation, we know that $\frac{|V(G)|}{4} \times 3$ is even. Hence $\frac{|V(G)|}{4}$ is even, that is, the order of G is divisible by 8. □

This theorem is equivalent to the following corollary.

Corollary 3.10. *A fullerene graph with order $8n + 4$ does not have a perfect star packing.*

We recall that a *dominating set* of a graph G is a set D of vertices such that each vertex in $V(G) - D$ is adjacent to a vertex in D. Moreover, if each vertex in $V(G) - D$ is adjacent to exactly one vertex in D and D is an independent vertex set, then D is called *efficient*. The problem of determining the existence of efficient dominating sets in some families of graphs was first investigated by Biggs [7] and Kratochvil [25]. Later Livingston and Stout [27] studied the existence and construction of efficient dominating sets in families of graphs arising from the interconnection networks of parallel computers. It is algorithmically hard to find an efficient dominating set [3]. For more results and some historical background regarding efficient dominating set, we refer the reader to [9, 10, 11, 22] etc..

From the definitions of the efficient dominating set and the perfect star packing of a fullerene graph, the following proposition is a natural result.

Proposition 3.11 ([14]). *A fullerene graph G with n vertices has a perfect star packing if and only if G has an efficient dominating set of cardinality $\frac{n}{4}$.*

Combining Theorem 3.9 and Proposition 3.11, we get the following theorem.

Theorem 3.12. *The order of a fullerene graph with an efficient dominating set is $8n$.*

4 Some other conclusions

Došlić et al. gave the following necessary condition in terms of graph spectra.

Proposition 4.1 ([14]). *If a fullerene graph G has a perfect star packing, then -1 must be an eigenvalue of the adjacency matrix of G.*

The proof of this Theorem can be translate to a simple r-regular graph. Here for completeness, we prove as follows. For the definition of eigenvalues of the adjacency matrix of a graph, we refer the reader to [18].

Theorem 4.2. *If a simple r-regular graph G has a perfect $K_{1,r}$-packing S, then -1 must be an eigenvalue of the adjacency matrix of G.*

Proof. Let $C(S)$ be the set of centers of stars $K_{1,r}$ in S. We define the characteristic vector $\overrightarrow{c} \in \mathbb{R}^{|V(G)|}$ of $C(S)$ as follows: $c_i = 1$ if $i \in C(S)$, otherwise $c_i = 0$. Since G is a r-regular graph, we have $A\overrightarrow{u} = r\overrightarrow{u}$, where A is the adjacency matrix of G and $\overrightarrow{u}$ is the all one vectors. Let $\overrightarrow{w} = \overrightarrow{u} - (r+1)\overrightarrow{c}$. As $A\overrightarrow{c} = \overrightarrow{u} - \overrightarrow{c}$, we have

$$A\overrightarrow{w} = A\overrightarrow{u} - (r+1)A\overrightarrow{c} = r\overrightarrow{u} - (r+1)\overrightarrow{u} + (r+1)\overrightarrow{c} = (r+1)\overrightarrow{c} - \overrightarrow{u} = -\overrightarrow{w} \quad (4.1)$$

This means that -1 is an eigenvalue of A. □

For a perfect star packing S of fullerene graph G, if for each center $x \in C(S)$, all the three faces of G sharing x are hexagons, then we call S being *type* $P0$. For such perfect star packing, the following corollary holds.

Corollary 4.3. *If a fullerene graph G has a perfect star packing S of type $P0$, then $G - C(S)$ does not have a non-facial cycle of odd length.*

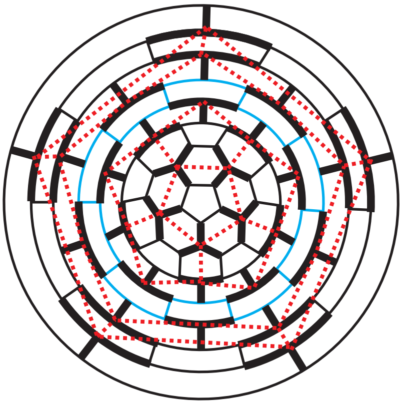
Proof. By the contrary, we suppose that $G - C(S)$ has a non-facial cycle C of odd length. By the Claim 1 of Theorem 3.8, G has a pentagon P which share edges with C. This implies that P contains the center y of a star in S. So one of the three faces of G sharing y is not a hexagon. This contradicts that S is of type $P0$. So $G - C(S)$ does not have a non-facial cycle of odd length. □

In the above Corollary, we note that $G - C(S)$ may have non-facial cycles of even lengths (see Figure 5, the blue cycle in C_{120}).

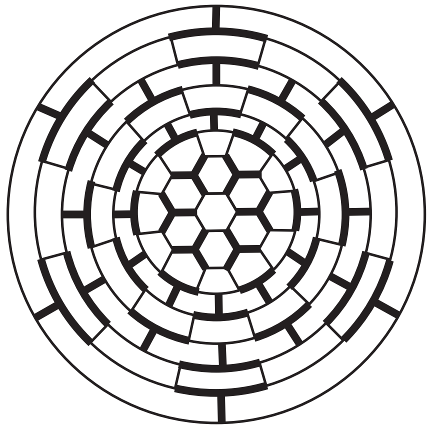
Now, we point out the flaw of the Theorem 14 in [14].

Theorem 4.4 ([14]). *A fullerene graph on $8n$ vertices has a perfect star packing of type $P0$ if and only if it arises from some other fullerene via the chamfer transformation.*

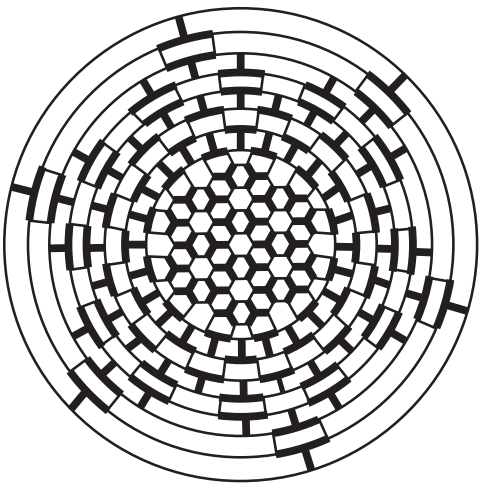
Readers can consult reference [14] to see the chamfer transformation. Here for completeness, we introduce it as follows. Let F be a fullerene graph. In each face g of F, we draw a polygon with the same number of sides as g. For each vertex $v \in V(F)$, we connect v with three new vertices each of which is inside exactly one face of F incident with v (see Figure 6, the vertices of original fullerene C_{20} are black, the new vertices are blue, each black vertex are connected to three blue vertices). We notice that each new vertex must be adjacent to exactly one vertex of F in this process, and the edges do not intersect inside. Finally, we remove all the edges of F. The resulting graph is called arising from F via the *chamfer transformation*. For example, (see Figure 6) the graph $C_{80}(I_h)$ arises from C_{20}



C_{120}



C_{144}



C_{384}

Figure 5: Each of $C_{120}, C_{144}, C_{384}$ has a unique perfect star packing of type $P0$ which is depicted in bold edges.

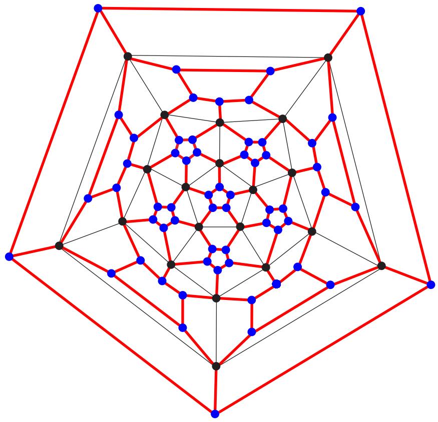


Figure 6: C_{20} is drawn in black line, $C_{80}(I_h)$ is drawn in red line.

via the chamfer transformation, and all the black vertices are the centers of stars in a perfect star packing of type $P0$ of $C_{80}(I_h)$.

For a perfect star packing S of type $P0$ in fullerene graph G, we construct a new graph with respect to S, and denoted it by G^S. $V(G^S) := C(S)$ and any two vertices in $V(G^S)$ are adjacent if and only if they belong to the same hexagon of G. In the proof of the necessity of the Theorem 4.4, there exist the following problem. G^S is planar, but does not have to be 3-regular, 3-connected and have only pentagonal and hexagonal faces. For example, it is easy to check that the fullerene graph C_{120} (resp. C_{144}, C_{384}) has a unique perfect star packing S_1 (resp. S_2, S_3) of type $P0$ (as depicted in bold edges in Figure 5). $C_{120}^{S_1}$, $C_{144}^{S_2}$ and $C_{384}^{S_3}$ are planar and not connected (the red dashed line in Figure 5 is the $C_{120}^{S_1}$, and here we omit the $C_{144}^{S_2}$ and $C_{384}^{S_3}$). In fact, we have Lemma 4.5.

I would like to thank Tomislav Došlić for conversations and email exchanges related to the contents of this paragraph.

Lemma 4.5. *The three fullerene graphs C_{120}, C_{144} and C_{384} as depicted in* Figure 5 *cannot arise from some other fullerene via the chamfer transformation.*

Proof. On the contrary, we suppose that C_{120} can arise from some fullerene F via the chamfer transformation. Then C_{120} has a perfect star packing S of type $P0$ which corresponds to the chamfer transformation of F, that is, all the vertices of F are the centers of stars in S. This means that $C_{120}^S = F$.

We can check that C_{120} has a unique perfect star packing of type $P0$, denoted by S_1 (as depicted in bold edges in Figure 5). So $S_1 = S$. However, $C_{120}^{S_1}$ is not connected (as depicted by red dotted lines in Figure 5). So $S_1 \neq S$, a contradiction.

For the other two fullerenes C_{144} and C_{384}, we can also check that each of them has a unique perfect star packing of type $P0$ (as depicted in bold edges in Figure 5). As the above proof, they also cannot arise from any fullerene graphs via the chamfer transformations. □

From Lemma 4.5 we know that the necessity of Theorem 4.4 does not hold, however, its sufficiency is right. So it can be corrected as follows.

Theorem 4.6. *A fullerene graph that arises from some other fullerene via the chamfer transformation must have a perfect star packing of type* $P0$*.*

If fullerene graph G has two pentagons sharing an edge xy, then x (resp. y) can not be center of a star in a perfect star packing of G by Lemma 2.2. Since all the three neighbors of x belong to pentagons of G, G does not have a perfect star packing of type $P0$. Hence if a fullerene graph has a perfect star packing of type $P0$, then all its pentagons are isolated. Next we list some other forbidden subgraphs for guaranteeing a fullerene graph to own a perfect star packing of type $P0$.

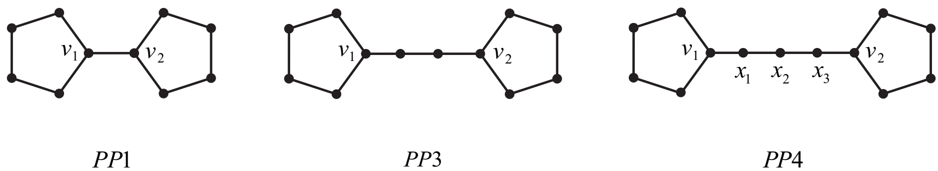


Figure 7: Three forbidden configurations.

Proposition 4.7. *If a fullerene graph* G *contains a subgraph* $PP1, PP3$ *or* $PP4$ *(see* Figure 7*), then it cannot have a perfect star packing of type* $P0$*.*

Proof. By the contrary, we suppose that G has a perfect star packing of type $P0$, denoted by S. Clearly, the vertices v_1 and v_2 (see Figure 7) are leaves in S. If $PP4$ is a subgraph of G, then x_1 is the center of a star in S since all vertices on a pentagon are leaves in S. So x_2 is a leaf in S. By Remark 2.4(2), the neighbor x_3 of x_2 is also a leaf in S. This implies that all the three neighbors of v_2 are leaves in S, a contradiction. For subgraphs $PP1$ and $PP3$, we can similarly show that v_1 or v_2 have all its three neighbors being leaves in S, a contradiction. □

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On the A_α-spectral radius of connected graphs*

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Abstract

For a simple graph G, the generalized adjacency matrix $A_\alpha(G)$ is defined as $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G), \alpha \in [0,1]$, where $A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of the vertex degrees. It is clear that $A_0(G) = A(G)$ and $2A_{\frac{1}{2}}(G) = Q(G)$ implying that the matrix $A_\alpha(G)$ is a generalization of the adjacency matrix and the signless Laplacian matrix. In this paper, we obtain some new upper and lower bounds for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of vertex degrees, average vertex 2-degrees, the order, the size, etc. The extremal graphs attaining these bounds are characterized. We will show that our bounds are better than some of the already known bounds for some classes of graphs. We derive a general upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and positive real numbers b_i. As application, we obtain some new upper bounds for $\lambda(A_\alpha(G))$. Further, we obtain some relations between clique number $\omega(G)$, independence number $\gamma(G)$ and the generalized adjacency eigenvalues of a graph G.

Keywords: Adjacency matrix, signless Laplacian matrix, generalized adjacency matrix, spectral radius, degree sequence, clique number, independence number.

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1 Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The *order* of G is the number $n = |V(G)|$ and its *size* is the number $m = |E(G)|$. The set of vertices adjacent to $v \in V(G)$, denoted by $N(v)$, refers to the *neighborhood* of v. The *degree* of v, denoted by $d_G(v)$ (we simply write d_v if it is clear from the context) means the cardinality of $N(v)$. A graph is called *regular* if all vertices have the same degree. The graph $\overline{G}$ is the *complement* of the graph G. Moreover, the complete graph K_n, the complete bipartite graph $K_{s,t}$, the path P_n, the cycle C_n and the star S_n are defined in the conventional way. The *distance* between two vertices $u, v \in V(G)$, denoted by d_{uv}, is defined as the length of a shortest path between u and v in G. The *diameter* of G is the maximum distance between any two vertices of G. Let m_i be the average degree of the adjacent vertices of vertex v_i in G. If v_i is an isolated vertex in G, then we assume that $m_i = 0$. Hence we can write

$$m_i = \begin{cases} 0 & d_i = 0. \\ \frac{1}{d_i} \sum_{j: j\sim i} d_j & \text{otherwise.} \end{cases}$$

Let p_i be the average degree of the vertices non-adjacent to vertex v_i in G. If v_i is adjacent to all the remaining vertices, then we assume that $p_i = 0$. Then we can write

$$p_i = \begin{cases} 0 & d_i = n-1. \\ \frac{\sum_{j: j\nsim i,\, j\neq i} d_j}{n - d_i - 1} & \text{otherwise.} \end{cases}$$

Let $D(G)$ be the diagonal matrix of vertex degrees and $A(G)$ be the adjacency matrix of G. The signless Laplacian matrix of G is $Q(G) = D(G) + A(G)$. Its eigenvalues can be arranged as: $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G)$. In [20], Nikiforov proposed the following matrix:

$$A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G), \quad 0 \leq \alpha \leq 1,$$

calling it the *generalized adjacency matrix* of G. Obviously, $A_0(G) = A(G)$, $2A_{\frac{1}{2}}(G) = Q(G)$, $A_1(G) = D(G)$ and $A_\alpha(G) - A_\beta(G) = (\alpha - \beta)L(G)$, where $L(G)$ is the well-studied Laplacian matrix of G, defined as $L(G) = D(G) - A(G)$. Therefore, the family $A_\alpha(G)$ can extend both $A(G)$ and $Q(G)$. The matrix $A_\alpha(G)$ is a real symmetric matrix, therefore we can arrange its eigenvalues as $\lambda_1(A_\alpha(G)) \geq \lambda_2(A_\alpha(G)) \geq \cdots \geq \lambda_n(A_\alpha(G))$, where $\lambda_1(A_\alpha(G))$ is called the *generalized adjacency spectral radius* of G. Afterwards, we will denote $\lambda_1(A_\alpha(G))$ by $\lambda(A_\alpha(G))$. If G is a connected graph and $\alpha \neq 1$, then the matrix $A_\alpha(G)$ is non-negative and irreducible. Therefore by the Perron-Frobenius theorem, $\lambda(A_\alpha(G))$ is the simple eigenvalue and there is a unique positive unit eigenvector $\mathbf{x}$ corresponding to $\lambda(A_\alpha(G))$, which is called the *generalized adjacency Perron vector* of G.

A column vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex v_i to x_i, i.e., $\mathbf{x}(v_i) = x_i$ for $i = 1, 2, \ldots, n$. Then,

$$\langle \mathbf{x}, A_\alpha \mathbf{x} \rangle = \mathbf{x}^T A_\alpha(G)\mathbf{x} = \alpha \sum_{i=1}^{n} d_i x_i^2 + 2(1-\alpha) \sum_{i\sim j} x_i x_j,$$

and λ is an eigenvalue of $A_\alpha(G)$ corresponding to the eigenvector $\mathbf{x}$ if and only if $\mathbf{x} \neq \mathbf{0}$ and

$$\lambda x_i = \alpha d_i x_i + (1-\alpha)\sum_{j\sim i} x_j,\ i = 1, 2, \ldots, n.$$

These equations are called the (λ, x)-*eigenequations* of G. For a normalized column vector $\mathbf{x} \in \mathbb{R}^n$, by the Rayleigh's principle, we have

$$\lambda(A_\alpha(G)) \geq \mathbf{x}^T A_\alpha(G)\mathbf{x}$$

with equality if and only if $\mathbf{x}$ is the generalized adjacency Perron vector of G.

The research on the (adjacency, signless Laplacian) spectrum is an intriguing topic during past two decades [4, 10, 22]. At the same time, the adjacency or signless Laplacian spectral radius have attracted many interests among the mathematical literature including linear algebra and graph theory. An interesting problem in the spectral graph theory is to obtain bounds for the (adjacency, signless Laplacian) spectral radius connecting it with different parameters associated with the graph. Another interesting problem which is worth to mention is to characterize the extremal graphs for the (adjacency, signless Laplacian) spectral radius among all graphs of order n or among a special class of graphs of order n. The spectral radius $\lambda(G)$ of the adjacency matrix $A(G)$, called the spectral radius (or adjacency spectral radius) of the graph G and the spectral radius $q_1(G)$ of the signless Laplacian matrix $Q(G)$, called signless Laplacian spectral radius of the graph G, are both well studied and their spectral theories are well developed. Various papers can be found in the literature regarding the establishment of bounds for $\lambda(G)$ and $q_1(G)$ connecting them with different parameters associated with the structure of the graph G. Since the matrix $A_\alpha(G)$ is a generalization of the matrices $A(G)$ and $Q(G)$, therefore it will be interesting to see whether the results which already hold for the spectral radius of the matrices $A(G)$ and/or $Q(G)$ can be extended to the spectral radius of the $A_\alpha(G)$. This is one of the motivation to study the spectral radius of the matrix $A_\alpha(G)$.

Let $A(G)$ be the adjacency matrix of the graph G and let B be a real diagonal matrix of order n. In 2002, Bapat et al. [1] defined the matrix $L' = B - A(G)$ and called it the perturbed Laplacian matrix of the graph G. The aim of introducing this matrix was to generalize the results that hold for the adjacency matrix and the Laplacian matrix $L(G)$ of the graph to some general class of matrices. For $\alpha \neq 1$, it is easy to see that

$$A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G) = (\alpha - 1)\Big(\frac{\alpha}{\alpha-1}D(G) - A(G)\Big).$$

Clearly $\frac{\alpha}{\alpha-1}D(G)$ is a diagonal matrix with real entries, giving that the matrix $A_\alpha(G)$ is a scaler multiple of a perturbed Laplacian matrix. This is another motivation to study the spectral properties of the matrix $A_\alpha(G)$.

Although the generalized adjacency matrix $A_\alpha(G)$ of a graph G was introduced in 2017, but a large number of papers can be found in the literature regarding the spectral properties of this matrix. Like other graph matrices, most of these papers are regarding the generalized spectral radius $\lambda(A_\alpha(G))$. In fact, various upper and lower bounds connecting $\lambda(A_\alpha(G))$ with different graph parameters and the graphs attaining these bounds can be found in the literature. For some recent works regarding the spectral properties of $A_\alpha(G)$, we refer to [8, 9, 11, 13, 14, 15, 16, 17, 21, 23, 24].

The rest of this paper is organized as follows. In Section 2, we obtain some new upper and lower bounds for $\lambda(A_\alpha(G))$, in terms of vertex degrees, average vertex 2-degrees, the order, the size, etc. The extremal graphs attaining these bounds are characterized. We will show that our bounds are better than some of the already known bounds for some classes of graphs. In Section 3, we derive a general upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and positive real numbers b_i. As application, we obtain some new upper bounds for $\lambda(A_\alpha(G))$. In Section 4, we obtain some relations between clique number $\omega(G)$, independence number $\gamma(G)$ and the generalized adjacency eigenvalues. We conclude this paper by a remark in Section 5.

2 Bounds on generalized adjacency spectral radius

The average 2-degree of a vertex $v_i \in V(G)$ is denoted by $m_i = m(v_i)$ and is defined as $m_i = \sum_{k:k\sim i} \frac{d_k}{d_i}$, where d_k is the degree of the vertex v_k.

The following gives an upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$ of a graph in terms of the vertex degrees, the average vertex 2-degrees and the parameter α.

Theorem 2.1. *Let G be a graph of order n having vertex degrees d_i, vertex average 2-degrees m_i, $1 \le i \le n$, and let $\alpha \in [0,1]$. Then*

$$\lambda(A_\alpha(G)) \le \max_{1\le i\le n} \left\{\alpha d_i + (1-\alpha)\sqrt{d_i m_i}\right\}.$$

Moreover, the equality holds if G is a k-regular graph.

Proof. Let $\mathbf{x} = (x_1, \dots, x_n)$ be the generalized adjacency Perron vector of G and let $\|\mathbf{x}\| = 1$. For any $v_i \in V(G)$, we have $\lambda(A_\alpha(G))x_i = \alpha d_i x_i + (1-\alpha)\sum_{j:j\sim i} x_j$. Hence

$$\lambda^2(A_\alpha(G))x_i^2 = \alpha^2 d_i^2 x_i^2 + 2\alpha(1-\alpha)d_i x_i \sum_{j:j\sim i} x_j + (1-\alpha)^2 \left(\sum_{j:j\sim i} x_j\right)^2. \tag{2.1}$$

By Cauchy-Schwarz inequality, we obtain

$$\left(\sum_{j:j\sim i} x_j\right)^2 \le d_i \sum_{j:j\sim i} x_j^2. \tag{2.2}$$

Therefore from (2.1) and (2.2), we get

$$\lambda^2(A_\alpha(G))x_i^2 \le \alpha^2 d_i^2 x_i^2 + 2\alpha\, d_i x_i \Big[\lambda(A_\alpha(G))x_i - \alpha d_i x_i\Big] + (1-\alpha)^2 d_i \sum_{j:j\sim i} x_j^2.$$

Thus, taking sum over all $v_i \in V(G)$, we get

$$\begin{aligned}
&\sum_{v_i\in V(G)} \lambda^2(A_\alpha(G))x_i^2\\
&\le \sum_{v_i\in V(G)} \Big[2\alpha d_i\lambda(A_\alpha(G)) - \alpha^2 d_i^2\Big]x_i^2 + (1-\alpha)^2 \sum_{v_i\in V(G)} d_i \sum_{j:j\sim i} x_j^2\\
&= \sum_{v_i\in V(G)} \Big[2\alpha d_i\lambda(A_\alpha(G)) - \alpha^2 d_i^2\Big]x_i^2 + (1-\alpha)^2 \sum_{v_i\in V(G)} d_i m_i x_i^2\\
&= \sum_{v_i\in V(G)} \Big[2\alpha d_i\lambda(A_\alpha(G)) - \alpha^2 d_i^2 + (1-\alpha)^2 d_i m_i\Big]x_i^2
\end{aligned}$$

as

$$\sum_{v_i\in V(G)} d_i \sum_{j:j\sim i} x_j^2 = \sum_{v_i\in V(G)} x_i^2 \sum_{j:j\sim i} d_j = \sum_{v_i\in V(G)} d_i m_i x_i^2.$$

From the above result, we obtain

$$\sum_{v_i\in V(G)} \Big(\lambda^2(A_\alpha(G)) - 2\alpha d_i \lambda(A_\alpha(G)) + \alpha^2 d_i^2 - (1-\alpha)^2 d_i m_i\Big) x_i^2 \le 0.$$

This is only true if there exist a vertex, say $v_j \in V(G)$, such that

$$\lambda^2(A_\alpha(G)) - 2\alpha d_j \lambda(A_\alpha(G)) + \alpha^2 d_j^2 - (1-\alpha)^2 d_j m_j \le 0,$$

hence, we get

$$\lambda(A_\alpha(G)) \le \alpha d_j + (1-\alpha)\sqrt{d_j m_j} \le \max_{1\le i\le n} \Big\{\alpha d_i + (1-\alpha)\sqrt{d_i m_i}\Big\}.$$

Now, suppose that G is a k-regular graph. So, for $i = 1, \ldots, n$, we have $d_i = m_i = k$, then $\alpha d_i + (1-\alpha)\sqrt{d_i m_i} = k$ and $\lambda(A_\alpha(G)) = k$. This shows that equality occurs for a regular graph. □

For $\alpha = 0$, the upper bound given by Theorem 2.1 reduces to the upper bound in the following corollary.

Corollary 2.2 ([5]). *Let G be a graph of order n having vertex degrees d_i, vertex average 2-degrees m_i, $1 \le i \le n$. Then*

$$\lambda(A(G)) \le \max_{1\le i\le n} \sqrt{d_i\, m_i}.$$

The following upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of vertex degrees and average vertex 2-degrees was obtained in [20]:

Theorem 2.3. *If G is a graph with no isolated vertices, then*

$$\lambda(A_\alpha(G)) \le \max_{v_j\in V} \Big\{\alpha d_j + (1-\alpha) m_j\Big\}.$$

If $\alpha \in \left(\frac{1}{2}, 1\right)$ and G is connected, equality holds if and only if G is regular.

Remark 2.4. For non-regular graphs the upper bound given by Theorem 2.1 and the upper bound given by Theorem 2.3 are incomparable for different values of α. For example, consider the graph $G = K_4 - e$. For this graph we have $d_1 = 2, d_2 = 3, d_3 = 2, d_4 = 3, m_1 = 3, m_2 = \frac{7}{3}, m_3 = 3$ and $m_4 = \frac{7}{3}$. By Theorem 2.3, we have

$$\lambda(A_\alpha(G)) \le \max\Big\{3-\alpha, \frac{7}{3} + \frac{2}{3}\alpha\Big\}.$$

It is easy to see that

$$\max\Big\{3-\alpha, \frac{7}{3} + \frac{2}{3}\alpha\Big\} = \begin{cases} \frac{7}{3} + \frac{2}{3}\alpha & \text{for } \alpha > 0.4, \\ 3-\alpha & \text{for } \alpha \le 0.4. \end{cases}$$

Also, by Theorem 2.1, we have

$$\lambda(A_\alpha(G)) \le \max\Big\{\sqrt{6}+(2-\sqrt{6})\alpha, \sqrt{7}+(3-\sqrt{7})\alpha\Big\} = \sqrt{7}+(3-\sqrt{7})\alpha.$$

For $\alpha \le 0.4$, we have $3-\alpha > \sqrt{7}+(3-\sqrt{7})\alpha$ giving that $\alpha < \frac{5-\sqrt{7}}{9} \approx 0.2615$. This gives that for $0 \le \alpha < \frac{5-\sqrt{7}}{9}$, the upper bound given by Theorem 2.1 is better than the upper bound given by Theorem 2.3; while as for $\frac{5-\sqrt{7}}{9} \le \alpha \le 0.4$, the upper bound given by Theorem 2.3 is better than the upper bound given by Theorem 2.1 for the graph $K_4 - e$.

For the graph $G = K_{1,3}$, we have $d_1 = 3, d_2 = 1, d_3 = 1, d_4 = 1, m_1 = 1, m_2 = 3, m_3 = 3$ and $m_4 = 3$. By Theorem 2.3, we have

$$\lambda(A_\alpha(G)) \le \max\Big\{1+2\alpha, 3-2\alpha\Big\}.$$

It is easy to see that

$$\max\Big\{1+2\alpha, 3-2\alpha\Big\} = \begin{cases} 3-2\alpha & \text{for } \alpha < 0.5, \\ 1+2\alpha & \text{for } \alpha \ge 0.5. \end{cases}$$

Also, by Theorem 2.1, we have

$$\lambda(A_\alpha(G)) \le \max\Big\{\sqrt{3}+(3-\sqrt{3})\alpha, \sqrt{3}+(1-\sqrt{3})\alpha\Big\} = \sqrt{3}+(3-\sqrt{3})\alpha.$$

For $\alpha < 0.5$, we have $3-2\alpha > \sqrt{3}+(3-\sqrt{3})\alpha$ giving that $\alpha < \frac{3-\sqrt{3}}{5-\sqrt{3}} \approx 0.38799$. This gives that for $0 \le \alpha < \frac{3-\sqrt{3}}{5-\sqrt{3}}$, the upper bound given by Theorem 2.1 is better than the upper bound given by Theorem 2.3; while as for $\frac{3-\sqrt{3}}{5-\sqrt{3}} \le \alpha < 0.5$, the upper bound given by Theorem 2.3 is better than the upper bound given by Theorem 2.1 for the graph $K_{1,3}$.

The following gives another upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$ of a graph G in terms of the vertex degrees, the average vertex 2-degrees and the unknown parameter β.

Theorem 2.5. *Let G be a connected graph of order n having vertex degrees d_i, average vertex 2-degrees m_i, $1 \le i \le n$, and let $\alpha \in [0, 1)$. Then*

$$\lambda(A_\alpha(G)) \le \max_{1\le i\le n}\left\{\frac{-\beta+\sqrt{\beta^2+4d_i(\alpha d_i+(1-\alpha)m_i+\beta)}}{2}\right\}, \tag{2.3}$$

where $\beta \ge 0$ is an unknown parameter. Equality occurs if and only if G is a regular graph.

Proof. Let $\mathbf{x} = (x_1, \dots, x_n)$ be the generalized adjacency Perron vector of G and let

$$x_i = \max_{1\le j\le n} x_j.$$

Since

$$\begin{aligned}\lambda^2(A_\alpha(G))\mathbf{x} &= (A_\alpha(G))^2\mathbf{x} = (\alpha D+(1-\alpha)A)^2\mathbf{x} \\ &= \alpha^2 D^2\mathbf{x} + \alpha(1-\alpha)DA\mathbf{x} + \alpha(1-\alpha)AD\mathbf{x} + (1-\alpha)^2A^2\mathbf{x},\end{aligned}$$

we have

$$\lambda^2(A_\alpha(G))x_i = \alpha^2 d_i^2 x_i + \alpha(1-\alpha)d_i \sum_{j:j\sim i} x_j + \alpha(1-\alpha)\sum_{j:j\sim i} d_j x_j + (1-\alpha)^2 \sum_{j:j\sim i}\sum_{k:k\sim j} x_k.$$

Now, we consider a simple quadratic function of $\lambda(A_\alpha(G))$:

$$\left(\lambda^2(A_\alpha(G)) + \beta\lambda(A_\alpha(G))\right)\mathbf{x} = \Big(\alpha^2 D^2\mathbf{x} + \alpha(1-\alpha)DA\mathbf{x} + \alpha(1-\alpha)AD\mathbf{x} + (1-\alpha)^2A^2\mathbf{x}\Big) + \beta(\alpha D\mathbf{x} + (1-\alpha)A\mathbf{x}).$$

Considering the i-th equation, we have

$$\left(\lambda^2(A_\alpha(G)) + \beta\lambda(A_\alpha(G))\right)x_i = \alpha^2 d_i^2 x_i + \alpha(1-\alpha)d_i \sum_{j:j\sim i} x_j + \alpha(1-\alpha)\sum_{j:j\sim i} d_j x_j + (1-\alpha)^2 \sum_{j:j\sim i}\sum_{k:k\sim j} x_k + \beta\Big(\alpha d_i x_i + (1-\alpha)\sum_{j:j\sim i} x_j\Big).$$

One can easily see that

$$\alpha(1-\alpha)d_i \sum_{j:j\sim i} x_j \le \alpha(1-\alpha)d_i^2 x_i, \quad \alpha(1-\alpha)\sum_{j:j\sim i} d_j x_j \le \alpha(1-\alpha)d_i m_i x_i,$$
$$(1-\alpha)^2 \sum_{j:j\sim i}\sum_{k:k\sim j} x_k \le (1-\alpha)^2 d_i m_i x_i, \quad (1-\alpha)\sum_{j:j\sim i} x_j \le (1-\alpha)d_i x_i.$$

Hence, we obtain

$$\left(\lambda^2(A_\alpha(G)) + \beta\lambda(A_\alpha(G))\right)x_i \le d_i(\alpha d_i + (1-\alpha)m_i)x_i + \beta d_i x_i,$$

$$\text{that is,}\quad \lambda^2(A_\alpha(G)) + \beta\lambda(A_\alpha(G)) - d_i(\alpha d_i + (1-\alpha)m_i + \beta) \le 0,$$

$$\text{that is,}\quad \lambda(A_\alpha(G)) \le \frac{-\beta + \sqrt{\beta^2 + 4d_i(\alpha d_i + (1-\alpha)m_i + \beta)}}{2}.$$

From this the inequality (2.3) follows.

Suppose that equality occurs in (2.3). Then all the inequalities in the above argument occur as equalities. Thus we obtain

$$\alpha(1-\alpha)d_i \sum_{j:j\sim i} x_j = \alpha(1-\alpha)d_i^2 x_i, \quad \alpha(1-\alpha)\sum_{j:j\sim i} d_j x_j = \alpha(1-\alpha)d_i m_i x_i,$$
$$(1-\alpha)^2 \sum_{j:j\sim i}\sum_{k:k\sim j} x_k = (1-\alpha)^2 d_i m_i x_i, \quad (1-\alpha)\sum_{j:j\sim i} x_j = (1-\alpha)d_i x_i.$$

Therefore we must have $x_j = x_i$ for any $j : j \sim i$ and $x_k = x_i$ for any $k : k \sim j, j \sim i$. Let $U = \{v_\ell : x_\ell = x_i\}$. Now we have to prove that $U = V(G)$. Assume to the contrary that $U \neq V(G)$. Then there exists a vertex r in U such that $N(r) \subseteq U$ and $t \in V(G)\backslash U$ with $t \sim s$, where $s \in N(r)$. Then $x_t < x_i$. One can easily see that

$$\lambda(A_\alpha(G)) < \frac{-\beta + \sqrt{\beta^2 + 4d_r(\alpha d_r + (1-\alpha)m_r + \beta)}}{2}$$
$$\leq \max_{1\leq i\leq n}\left\{\frac{-\beta + \sqrt{\beta^2 + 4d_i(\alpha d_i + (1-\alpha)m_i + \beta)}}{2}\right\},$$

a contradiction as the equality holds in (2.3). Therefore $U = V(G)$. Then $x_1 = x_2 = \cdots = x_n$ and $\lambda(A_\alpha(G)) = d_i$, $i = 1, 2, \ldots, n$. Hence G is a regular graph.

Conversely, let G be a r-regular graph. Then

$$\lambda(A_\alpha(G)) = r = \max_{1\leq i\leq n}\left\{\frac{-\beta + \sqrt{\beta^2 + 4d_i(\alpha d_i + (1-\alpha)m_i + \beta)}}{2}\right\}.$$

This completes the proof of the theorem. □

The following upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of vertex degrees and average vertex 2-degrees was obtained in [20]:

$$\lambda(A_\alpha(G)) \leq \max_{1\leq i\leq n}\left\{\sqrt{\alpha d_i^2 + (1-\alpha)w_i}\right\}, \tag{2.4}$$

where $w_i = d_i m_i$ for $i = 1, \ldots, n$. Also, equality holds if and only if $\alpha d_i^2 + (1-\alpha)w_i$ is same for all i.

Remark 2.6. For a connected graph G of order n, the upper bound given by Theorem 2.5 reduces to the upper bound given by (2.4) for $\beta = 0$. For $\beta \neq 0$, the upper bound given by Theorem 2.5 is incomparable with the upper bound given by (2.4). For example, consider the graph $G = K_{1,3}$. For this graph, the upper bound (2.4) gives

$$\lambda(A_\alpha(G)) \leq \max\left\{\sqrt{3+6\alpha}, \sqrt{3-3\alpha}\right\} = \sqrt{3+6\alpha}.$$

While as the upper bound given by Theorem 2.5 gives

$$\lambda(A_\alpha(G)) \leq \max\left\{\frac{-\beta + \sqrt{\beta^2 + 12\beta + 12\alpha + 12}}{2}, \frac{-\beta + \sqrt{\beta^2 + 4\beta - 8\alpha + 12}}{2}\right\}$$
$$= \frac{-\beta + \sqrt{\beta^2 + 12\beta + 12\alpha + 12}}{2}.$$

Taking $\beta = 1$, we have $\frac{-\beta + \sqrt{\beta^2 + 12\beta + 12\alpha + 12}}{2} = \frac{-1 + \sqrt{25 + 12\alpha}}{2} < \sqrt{3+6\alpha}$ giving that $3\alpha^2 - 8\alpha + 2 < 0$. This last inequality holds provided that $\alpha > \frac{4-\sqrt{10}}{3} \approx 0.279240$. This shows that for $\beta = 1$, the upper bound given by Theorem 2.5 is better than the upper bound given by (2.4) for $\alpha > \frac{4-\sqrt{10}}{3}$. Taking $\beta = 0.5$, it can be seen that the upper bound given by Theorem 2.5 is better than the upper bound given by (2.4) for $\alpha > 0.177$ and for $\beta = 0.1$, it can be seen that the upper bound given by Theorem 2.5 is better than the upper bound given by (2.4) provided that $\alpha > 0.008$.

Since for $\beta = 0$, the upper bounds given by Theorem 2.5 and inequality (2.4) are same and for the graph $K_{1,3}$, it follows from the above discussion that for small value of β the upper bound given by Theorem 2.5 behaves well for all α, incomparable to the upper bound given by (2.4). This gives that the choice of parameter β in the upper bound given by Theorem 2.5 can be helpful to obtain a better upper bound.

Let $x_i = \min\{x_j, j = 1, \ldots, n\}$ be the minimum among the entries of the generalized distance Perron vector $\mathbf{x} = (x_1, \ldots, x_n)$ of the graph G. Proceeding similar to Theorem 2.5, we obtain the following lower bound for $\lambda(A_\alpha(G))$, in terms of the vertex degrees, the average vertex 2-degrees and the unknown parameter β.

Theorem 2.7. *Let G be a connected graph of order n having vertex degrees d_i, average vertex 2-degrees m_i, $1 \leq i \leq n$, and let $\alpha \in [0, 1)$. Then*

$$\lambda(A_\alpha(G)) \geq \min_{1 \leq i \leq n} \left\{ \frac{-\beta + \sqrt{\beta^2 + 4d_i(\alpha d_i + (1-\alpha)m_i + \beta)}}{2} \right\},$$

where $\beta \geq 0$ is an unknown parameter. Equality occurs if and only if G is a regular graph.

The following lower bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of vertex degrees and average vertex 2-degrees was obtained in [20]:

$$\lambda(A_\alpha(G)) \geq \min_{1 \leq i \leq n} \left\{ \sqrt{\alpha d_i^2 + (1-\alpha)w_i} \right\}, \tag{2.5}$$

where $w_i = d_i m_i$ for $i = 1, \ldots, n$. Equality occurs if and only if $\alpha d_i^2 + (1-\alpha)w_i$ is same for all i.

Remark 2.8. For a connected graph G of order n, the lower bound given by Theorem 2.7 reduces to the lower bound given by (2.5), for $\beta = 0$. For $\beta \neq 0$, the lower bound given by Theorem 2.7 is incomparable with the lower bound given by (2.5). For example, consider the graph $G = K_{1,3}$. For this graph, the lower bound (2.5) gives

$$\lambda(A_\alpha(G)) \geq \min\left\{\sqrt{3+6\alpha}, \sqrt{3-3\alpha}\right\} = \sqrt{3-3\alpha}.$$

While as the lower bound given by Theorem 2.7 gives

$$\begin{aligned}\lambda(A_\alpha(G)) &\geq \min\left\{ \frac{-\beta + \sqrt{\beta^2 + 12\beta + 12\alpha + 12}}{2}, \frac{-\beta + \sqrt{\beta^2 + 4\beta - 8\alpha + 12}}{2} \right\} \\ &= \frac{-\beta + \sqrt{\beta^2 + 4\beta - 8\alpha + 12}}{2}.\end{aligned}$$

Taking $\beta = 1$, we have $\dfrac{-\beta + \sqrt{\beta^2 + 4\beta - 8\alpha + 12}}{2} = \dfrac{-1 + \sqrt{17 - 8\alpha}}{2} > \sqrt{3 - 3\alpha}$ giving that $4\alpha^2 + 20\alpha - 8 > 0$. This last inequality holds provided that $\alpha > \frac{\sqrt{33}-5}{2} \approx 0.372281$. This shows that for $\beta = 1$, the lower bound given by Theorem 2.7 is better than the lower bound given by (2.5) for $\alpha > \frac{\sqrt{33}-5}{2}$. Taking $\beta = 0.1$, it can be seen that the lower bound given by Theorem 2.7 is better than the lower bound given by (2.5) for

$\alpha > 0.09$ and for $\beta = 0.01$, it can be seen that the lower bound given by Theorem 2.7 is better than the lower bound given by (2.5) provided that $\alpha > 0.023$.

Again, it follows from the above discussion that for small value of β the lower bound given by Theorem 2.7 behaves well for all α, incomparison to the lower bound given by (2.5) for the graph $K_{1,3}$. This gives that the choice of parameter β in the lower bound given by Theorem 2.7 can be helpful to obtain a better lower bound.

We note that if, in particular we take the parameter β in Theorem 2.5/Theorem 2.7 equal to the vertex covering number, the edge covering number, the clique number, the independence number, the domination number, the generalized adjacency rank, minimum degree, maximum degree, etc., then Theorems 2.5/ Theorem 2.7 gives upper bound/lower bound for $\lambda(A_\alpha(G))$, in terms of the vertex covering number, the edge covering number, the clique number, the independence number, the domination number, the generalized adjacency rank, minimum degree, maximum degree, etc.

Let S_n be the class of graphs of order n with maximum degree $n-1$. Clearly, $K_{1,n-1}$, $K_n \in S_n$. The following result gives an upper bound for $\max_{v_j \in V}\{d_j + m_j\}$ in terms of order n and size m.

Lemma 2.9 ([3]). *Let G be a graph of order n with m edges. Then*

$$\max_{1\le j\le n}\Big\{d_j + m_j\Big\} \le \frac{2m}{n-1} + n - 2, \tag{2.6}$$

with equality if and only if $G \in S_n$ or $G \cong K_{n-1} \cup K_1$.

We now generalize the above result.

Theorem 2.10. *Let G be a graph of order n with m edges and real numbers β, θ with $\beta \ge \theta > 0$. Then*

$$\max_{1\le j\le n}\Big\{\beta d_j + \theta\, m_j\Big\} \le \frac{2m\,\theta}{n-1} + \beta\,(n-1) - \theta, \tag{2.7}$$

with equality if and only if $G \in S_n$ or $G \cong K_{n-1} \cup K_1$ $(\beta = \theta)$.

Proof. If $\beta = \theta > 0$, then by Lemma 2.9, we get the required result in (2.7). Moreover, the equality holds if and only if $G \in S_n$ or $G \cong K_{n-1} \cup K_1$ $(\beta = \theta)$. Otherwise, $\beta > \theta > 0$. Let v_i be the vertex in G such that

$$\max_{1\le j\le n}\Big\{\beta d_j + \theta\, m_j\Big\} = \beta d_i + \theta\, m_i.$$

We have $2m = d_i + d_i m_i + (n - d_i - 1)\, p_i$, where p_i is the average of the degrees of the vertices non-adjacent to vertex v_i in G. We consider the following two cases:

Case 1: $d_i = n-1$. One can easily see that

$$\max_{1\le j\le n}\Big\{\beta d_j + \theta\, m_j\Big\} = \beta d_i + \theta\, m_i = \frac{2m\,\theta}{n-1} + \beta\,(n-1) - \theta.$$

In this case $G \in S_n$.

Case 2: $d_i \le n-2$. Now, to arrive at (2.7), we need to show that

$$\beta d_i + \theta\, m_i \le \frac{d_i + d_i m_i + (n - d_i - 1)p_i}{n-1}\,\theta + \beta\,(n-1) - \theta,$$

that is,

$$(n-d_i-1)\Big((n-1)\,\beta+(p_i-1-m_i)\,\theta\Big)\geq 0,$$

that is,

$$(n-1)\,\beta+(p_i-1-m_i)\,\theta\geq 0,$$

that is,

$$(n-1)\,\beta-(\Delta-\delta+1)\,\theta\geq 0, \tag{2.8}$$

as $m_i\leq\Delta$ and $p_i\geq\delta$. We consider the following two subcases:

Subcase 2.1: G is disconnected. Then $\Delta\leq n-2$. From (2.8), we obtain $(n-1)\,(\beta-\theta)>0$, which is true always as $\beta>\theta>0$. This shows that the inequality (2.8) strictly holds in this case.

Subcase 2.2: G is connected. In this case $\Delta-\delta\leq n-2$, again it follows from (2.8) that $(n-1)\ (\beta-\theta)>0$, which is true always as $\beta>\theta>0$. This shows that the inequality (2.8) strictly holds in this case as well. □

As an immediate consequence of Theorem 2.10, we get the following corollary.

Corollary 2.11. *Let G be a graph of order n with m edges and real number $\alpha\geq\frac{1}{2}$. Then*

$$\max_{1\leq j\leq n}\Big\{\alpha d_j+(1-\alpha)\,m_j\Big\}\leq\frac{2m\,(1-\alpha)}{n-1}+\alpha\,n-1, \tag{2.9}$$

with equality if and only if $G\in S_n$ or $G\cong K_{n-1}\cup K_1$ $(\alpha=1/2)$.

Combining Theorem 2.3 with Corollary 2.11, we get the following result, which gives an upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of the order n, the size m and the parameter α.

Theorem 2.12. *Let G be a graph of order n with m edges, with no isolated vertices and let $\alpha\in\left[\frac{1}{2},1\right]$. Then*

$$\lambda(A_\alpha(G))\leq\frac{2m\,(1-\alpha)}{n-1}+\alpha\,n-1.$$

If $\alpha\in\left(\frac{1}{2},1\right)$ and G is connected, equality holds if and only if $G=K_n$.

Let Γ be the class of graphs $G=(V,E)$ such that the maximum degree vertex (of degree Δ) are adjacent to the vertices of degree Δ and non-adjacent to the vertices of degree δ. If m is the number of edges in G $(\in\Gamma)$, then

$$2m=\Delta\,(\Delta+1)+(n-\Delta-1)\,\delta.$$

The following result gives an upper bound for d_i+m_i in terms of the order n, the size m, the maximum degree Δ and the minimum degree δ.

Lemma 2.13 ([3])**.** *Let G be a graph of order n with m edges having maximum degree Δ and minimum degree δ. Then*

$$d_i+m_i\leq\frac{2m}{n-1}+\Delta-\delta+\frac{\Delta}{n-1}\Big[n-2-(\Delta-\delta)\Big],$$

with equality if and only if $G\in S_n$ or $G\in\Gamma$.

The following result gives an upper bound for $\max_{v_j \in V}\{\beta\, d_j + \theta\, m_j\}$ in terms of the order n, the size m, the maximum degree Δ, the minimum degree δ and the parameters β, θ.

Theorem 2.14. *Let G be a graph of order n with m edges and real numbers β, θ with $\beta \geq \theta > 0$. Then*

$$\max_{v_j \in V}\{\beta d_j + \theta m_j\} \leq \frac{2m\theta}{n-1} + \theta\,(\Delta - \delta) + \frac{\Delta}{n-1}\Big[\beta\,(n-1) - \theta(\Delta - \delta + 1)\Big] \quad (2.10)$$

with equality if and only if $G \in S_n$ or $G \in \Gamma$.

Proof. Let v_i be a vertex in G such that

$$\max_{v_j \in V}\{\beta\, d_j + \theta\, m_j\} = \beta\, d_i + \theta\, m_i.$$

First we assume that $\beta = \theta$. Then by Lemma 2.13, we obtain

$$\begin{aligned}\max_{v_j \in V}\{\beta d_j + \theta m_j\} = \beta\,(d_i + m_i) &\leq \beta\left[\frac{2m}{n-1} + \Delta - \delta + \frac{\Delta}{n-1}\Big(n - 2 - (\Delta - \delta)\Big)\right]\\ &= \frac{2m\theta}{n-1} + \theta\,(\Delta - \delta) + \frac{\Delta}{n-1}\Big[\beta\,(n-1) - \theta(\Delta - \delta + 1)\Big],\end{aligned}$$

as $\beta > 0$. Moreover, the equality holds in (2.10) if and only if $G \in S_n$ or $G \in \Gamma$.
Next, we assume that $\beta > \theta$. We consider the following two cases:
Case 1: $d_i = n - 1$. In this case

$$\beta\, d_i + \theta\, m_i = \beta\,(n-1) + \theta\,\frac{2m - (n-1)}{n-1} = \frac{2m\,\theta}{n-1} + \beta\,(n-1) - \theta,$$

and so it is clear that the equality holds in (2.10) as $\Delta = n - 1$.

Case 2: $d_i \leq n - 2$. Then there is at least one vertex non-adjacent to v_i in G. Let G' be the graph obtained from the graph G by adding edges between v_i and the vertices non-adjacent to v_i in G. Let d_i' and m_i' be the degree of the vertex v_i and the average degree of the vertices adjacent to the vertex v_i in G', respectively. Then $d_i' = n - 1$ and hence $G' \in S_n$. Now,

$$\begin{aligned}\beta d_i' + \theta\, m_i' &= \beta(n-1) + \theta\left(\frac{2m + 2(n - d_i - 1) - (n-1)}{n-1}\right)\\ &= \beta\,(n-1) - \theta + \frac{2\theta\,(m + n - d_i - 1)}{n-1}.\end{aligned} \quad (2.11)$$

Let p_i be the average degree of the vertices non-adjacent to vertex v_i in the graph G. Hence

$$\begin{aligned}&\beta\, d_i' + \theta\, m_i' - (\beta\, d_i + \theta\, m_i)\\ &= \beta\,(d_i' - d_i) + \theta\,(m_i' - m_i)\\ &= \beta\,(n - d_i - 1) + \theta\,\left(\frac{2m + (n - d_i - 1) - (n-1)}{n-1} - m_i\right)\\ &= \beta(n - d_i - 1) + \theta\,\left(\frac{d_i m_i + (n - d_i - 1)(p_i + 1)}{n-1} - m_i\right).\end{aligned}$$

Since $\beta \geq \theta > 0$ and $\Delta - \delta \leq n-2$, we have $\beta\,(n-1) \geq \theta\,(\Delta - \delta + 1)$. Moreover, we have $m_i \leq \Delta$ and $p_i \geq \delta$ for any vertex $v_i \in V(G)$. Using these results, we obtain

$$\begin{aligned}
&\beta d_i + \theta\, m_i \\
&= \beta\, d_i - \theta + \frac{2\theta\,(m+n-d_i-1)}{n-1} + \theta\,\left(m_i - \frac{d_i m_i + (n-d_i-1)(p_i+1)}{n-1}\right) \\
&= \frac{2m\,\theta}{n-1} + \frac{d_i}{n-1}\Big(\beta\,(n-1) - \theta\Big) + \theta\Big(1 - \frac{d_i}{n-1}\Big)\,(m_i - p_i) \\
&\leq \frac{2m\,\theta}{n-1} + \frac{d_i}{n-1}\Big(\beta\,(n-1) - \theta\Big) + \theta\Big(1 - \frac{d_i}{n-1}\Big)\,(\Delta - \delta) \qquad (2.12) \\
&= \frac{2m\,\theta}{n-1} + \theta\,(\Delta-\delta) + \frac{d_i}{n-1}\Big(\beta\,(n-1) - \theta - \theta\,(\Delta-\delta)\Big) \\
&\leq \frac{2m\,\theta}{n-1} + \theta\,(\Delta-\delta) + \frac{\Delta}{n-1}\Big(\beta\,(n-1) - \theta\,(\Delta-\delta+1)\Big) \qquad (2.13)
\end{aligned}$$

as $d_i \leq \Delta$. The first part of the proof is done.

Now, suppose that equality in (2.10) holds with $\beta > \theta$. Then all the above inequalities must be equalities. If $d_i = n-1$, then $G \in S_n$. Otherwise, $d_i \leq n-2$. From the equality in (2.12), we have $m_i = \Delta$ and $p_i = \delta$. Since $\beta > \theta$, we have $\beta\,(n-1) > \theta\,(\Delta-\delta+1)$. From the equality in (2.13), we have $d_i = \Delta$. Therefore all the vertices those are adjacent to the vertex v_i are of degree Δ and those are non-adjacent to the vertex v_i are of degree δ. Hence $G \in \Gamma$.

Conversely, let $G \in S_n$. Then $\Delta = n-1$ and hence

$$\begin{aligned}
\max_{v_j \in V}\{\beta d_j + \theta m_j\} &= \frac{2m\theta}{n-1} + \beta\,(n-1) - \theta \\
&= \frac{2m\theta}{n-1} + \theta\,(\Delta-\delta) + \frac{\Delta}{n-1}\Big[\beta\,(n-1) - \theta(\Delta-\delta+1)\Big].
\end{aligned}$$

Let $G \in \Gamma$. Then $2m = \Delta\,(\Delta+1) + (n-\Delta-1)\,\delta$ and hence

$$\max_{v_j \in V}\{\beta d_j + \theta m_j\} = (\beta+\theta)\,\Delta = \frac{2m\theta}{n-1} + \theta\,(\Delta-\delta) + \frac{\Delta}{n-1}\Big[\beta\,(n-1) - \theta(\Delta-\delta+1)\Big].$$

This completes the proof. □

Corollary 2.15. *Let G be a graph of order n with m edges and let $\alpha \geq \frac{1}{2}$. Let Δ and δ are respectively, the maximum degree and the minimum degree of G. Then*

$$\max_{1\leq j\leq n}\Big\{\alpha\, d_j + (1-\alpha)\, m_j\Big\} \leq \frac{2m\,(1-\alpha)}{n-1} + \frac{\alpha n - 1}{n-1}\Delta + (1-\alpha)\left(1 - \frac{\Delta}{n-1}\right)(\Delta-\delta) \qquad (2.14)$$

with equality if and only if $G \in S_n$ or $G \in \Gamma$.

Combining Theorem 2.3 with Corollary 2.15, we get the following result, which gives an upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of the order n, the size m, the maximum degree Δ, the minimum degree δ and the parameter α.

Theorem 2.16. *Let G be a graph of order n, with m edges and let $\alpha \geq \frac{1}{2}$. Let Δ and δ are respectively, the maximum degree and the minimum degree of G. Then*

$$\lambda(A_\alpha(G)) \leq \frac{2m\,(1-\alpha)}{n-1} + \frac{\alpha n - 1}{n-1}\Delta + (1-\alpha)\left(1 - \frac{\Delta}{n-1}\right)(\Delta - \delta).$$

If $\alpha \in \left(\frac{1}{2}, 1\right)$ and G is connected, equality holds if and only if $G \cong K_n$.

The following result gives a Nordhaus–Gaddum type upper bound for the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, in terms of the order n, the size m, the minimum degree δ, the maximum degree Δ and the parameter α.

Theorem 2.17. *Let G be a graph of order n, with m edges and let $\alpha \geq \frac{1}{2}$. Let Δ and δ are respectively, the maximum degree and the minimum degree of G. Then*

$$\lambda(A_\alpha(G)) + \lambda(A_\alpha(\bar{G})) \leq n - 1 + \frac{(1-\alpha)(\Delta-\delta)}{n-1}\left(n + \delta - \Delta - 1 + \frac{\alpha n - 1}{1-\alpha}\right) \quad (2.15)$$

If $\alpha \in \left(\frac{1}{2}, 1\right)$ and G is connected, equality holds if and only if $G = K_n$.

Proof. Following Theorem 2.16, we have

$$\begin{aligned}
\lambda(A_\alpha(G)) + \lambda(A_\alpha(\bar{G})) &\leq (1-\alpha)\frac{2m + 2\bar{m}}{n-1} + \frac{\alpha n - 1}{n-1}(\Delta + \bar{\Delta}) \\
&\quad + (1-\alpha)\left(1 - \frac{\Delta}{n-1}\right)(\Delta - \delta) + (1-\alpha)\left(1 - \frac{\bar{\Delta}}{n-1}\right)(\bar{\Delta} - \bar{\delta}) \\
&= (1-\alpha)n + \frac{\alpha n - 1}{n-1}(\Delta - \delta + n - 1) \\
&\quad + (1-\alpha)(\Delta - \delta)\left(1 - \frac{\Delta}{n-1} + \frac{\delta}{n-1}\right) \\
&= n - 1 + \frac{(1-\alpha)(\Delta-\delta)}{n-1}\left(n + \delta - \Delta - 1 + \frac{\alpha n - 1}{1-\alpha}\right),
\end{aligned}$$

since $m + \bar{m} = \frac{n(n-1)}{2}$, $\bar{\Delta} = n - 1 - \delta$ and $\bar{\delta} = n - 1 - \Delta$.

Now, we consider the equality case in (2.15). If G is regular, then both sides of (2.15) are equal to $n-1$. Now, assume that equality occurs in (2.15) for G. Then the equalities must hold in (2.15) for both G and $\bar{G}$. Hence $G \cong K_n$. □

3 A general upper bound for the generalized adjacency spectral radius

In this section, we obtain a general upper bound for the generalized adjacency spectral radius in terms of vertex degrees and arbitrary positive real numbers b_i. If we replace b_i by some graph parameters, then we can derive some upper bounds for $\lambda(A_\alpha(G))$, in terms of vertex degrees. For this we need the following result:

Lemma 3.1 ([7])**.** *Let $D = (d_{i,j})$ be an $n \times n$ irreducible non-negative matrix with spectral radius σ and let $R_i(D) = \sum\limits_{j=1}^{n} d_{i,j}$ be the i-th row sum of D. Then*

$$\min\{R_i(D) \,:\, 1 \le i \le n\} \le \sigma \le \max\{R_i(D) \,:\, 1 \le i \le n\}\,. \tag{3.1}$$

Moreover, if the row sums of D are not all equal, then the both inequalities in (3.1) *are strict.*

The following result gives an upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and the arbitrary positive real numbers b_i.

Theorem 3.2. *Let G be a connected graph of order n and $0 < \alpha < 1$. Let $d_1 \ge d_2 \ge \cdots \ge d_n$ be the vertex degrees of G. Then*

$$\lambda(A_\alpha(G)) \le \max_{1\le i\le n} \left\{ \frac{\alpha d_i + \sqrt{\alpha^2 d_i^2 + \frac{4}{b_i} \sum\limits_{j:j\sim i} b_j (1-\alpha)(\alpha d_j + (1-\alpha) b_j')}}{2} \right\}, \tag{3.2}$$

where $b_i \in \mathbb{R}^+$ and $b_i' = \frac{1}{b_i} \sum\limits_{j:j\sim i} b_j$. Moreover, the equality holds if and only if $\alpha d_1 + (1-\alpha)b_1' = \alpha d_2 + (1-\alpha)b_2' = \cdots = \alpha d_n + (1-\alpha)b_n'$.

Proof. Let $B = \operatorname{diag}(b_1, b_2, \ldots, b_n)$, where $b_i \in \mathbb{R}^+$ are positive real number. Since the matrices $A_\alpha(G)$ and $B^{-1}A_\alpha(G)B$ are similar and similar matrices have same spectrum, it follows that if $\lambda(A_\alpha(G))$ is the largest eigenvalue of $A_\alpha(G)$, then it is also the largest eigenvalue of $B^{-1}A_\alpha(G)B$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector corresponding to the eigenvalue $\lambda(A_\alpha(G))$ of $B^{-1}A_\alpha(G)B$. We assume that one eigencomponent x_i is equal to 1 and the other eigencomponents are less than or equal to 1. The (i,j)-th entry of $B^{-1}A_\alpha(G)B$ is

$$\begin{cases} \alpha\, d_i & \text{if} \quad i = j, \\ (1-\alpha)\, \dfrac{b_j}{b_i} & \text{if} \quad j \sim i, \\ 0 & \text{otherwise.} \end{cases}$$

We have

$$B^{-1}A_\alpha(G)B\mathbf{x} = \lambda(A_\alpha(G))\mathbf{x}. \tag{3.3}$$

From the i-th equation of (3.3), we have

$$\lambda(A_\alpha(G))x_i = \alpha d_i x_i + (1-\alpha) \sum_{j:j\sim i} \frac{b_j}{b_i} x_j,$$

$$\text{i.e.,}\ \ \lambda(A_\alpha(G)) = \alpha d_i + (1-\alpha) \sum_{j:j\sim i} \frac{b_j}{b_i} x_j. \tag{3.4}$$

Again from the j-th equation of (3.3),

$$\lambda(A_\alpha(G))x_j = \alpha d_j x_j + (1-\alpha) \sum_{k:k\sim j} \frac{b_k}{b_j} x_k.$$

Multiplying both sides of (3.4) by $\lambda(A_\alpha(G))$ and substituting this value $\lambda(A_\alpha(G))x_j$, we get

$$\begin{aligned}\lambda^2(A_\alpha(G)) &= \alpha d_i \lambda(A_\alpha(G)) + (1-\alpha)\sum_{j:j\sim i}\frac{b_j}{b_i}\left[\alpha d_j x_j + (1-\alpha)\sum_{k:k\sim j}\frac{b_k}{b_j}x_k\right]\\ &= \alpha d_i\lambda(A_\alpha(G)) + \alpha(1-\alpha)\sum_{j:j\sim i}\frac{b_j d_j}{b_i}x_j + (1-\alpha)^2\sum_{j:j\sim i}\sum_{k:k\sim j}\frac{b_k}{b_i}x_k\\ &\leq \alpha d_i\lambda(A_\alpha(G)) + \alpha(1-\alpha)\sum_{j:j\sim i}\frac{b_j d_j}{b_i} + (1-\alpha)^2\sum_{j:j\sim i}\frac{b_j b'_j}{b_i} \qquad (3.5)\\ &= \alpha d_i\lambda(A_\alpha(G)) + \sum_{j:j\sim i}\frac{b_j(1-\alpha)(\alpha d_j + (1-\alpha)b'_j)}{b_i},\end{aligned}$$

as $b_i\, b'_i = \sum_{j:j\sim i} b_j$. Hence we get the upper bound.

Suppose that the equality holds in (3.2). Then all inequalities in the above argument must be equalities. Since $0 < \alpha < 1$, from equality in (3.5), we get $x_j = 1$ for all j such that $j \sim i$, and $x_k = 1$ for all k such that $k \sim j$ and $j \sim i$. From the above, one can easily prove that $x_i = 1$ for all $i \in V(G)$, that is, $\alpha d_1 + (1-\alpha)b'_1 = \alpha d_2 + (1-\alpha)b'_2 = \cdots = \alpha d_n + (1-\alpha)b'_n$.

Conversely, let G be a connected graph such that $\alpha d_1 + (1-\alpha)b'_1 = \alpha d_2 + (1-\alpha)b'_2 = \cdots = \alpha d_n + (1-\alpha)b'_n$ ($b_i \in \mathbb{R}^+$). Since $\lambda(A_\alpha(G)) = \lambda(B^{-1}A_\alpha(G)B)$, then by Lemma 3.1, we obtain

$$\begin{aligned}\lambda(A_\alpha(G)) &= \alpha\, d_\ell + (1-\alpha)\, b'_\ell\\ &= \max_{1\leq i\leq n}\left\{\frac{\alpha d_i + \sqrt{\alpha^2 d_i^2 + \frac{4}{b_i}\sum_{j:j\sim i} b_j(1-\alpha)(\alpha d_j + (1-\alpha)b'_j)}}{2}\right\}\end{aligned}$$

for $1 \leq \ell \leq n$. □

Taking $b_i = d_i$ in (3.2), and noting that $b'_i = \frac{1}{b_i}\sum_{j:j\sim i} b_j = \frac{1}{d_i}\sum_{j:j\sim i} d_j = m_i$, we obtain the following upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and average vertex 2-degrees.

Corollary 3.3. *Let G be a connected graph of order n having vertex degrees d_i, average vertex 2-degrees m_i $(1 \leq i \leq n)$ and $0 < \alpha < 1$. Then*

$$\lambda(A_\alpha(G)) \leq \max_{1\leq i\leq n}\left\{\frac{\alpha d_i + \sqrt{\alpha^2 d_i^2 + \frac{4(1-\alpha)}{d_i}\sum_{j:j\sim i} d_j[\alpha d_j + (1-\alpha)m_j]}}{2}\right\}.$$

Equality holds if and only if $\alpha d_1 + (1-\alpha)m_1 = \alpha d_2 + (1-\alpha)m_2 = \cdots = \alpha d_n + (1-\alpha)m_n$.

Taking $b_i = \sqrt{d_i}$ in (3.2), and noting that $b'_i = \frac{1}{b_i}\sum_{j:j\sim i} b_j = \frac{1}{\sqrt{d_i}}\sum_{j:j\sim i}\sqrt{d_j} = m'_i$ (say), we obtain the following upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and m'_i.

Corollary 3.4. *Let G be a connected graph of order n having vertex degrees d_i and let $m_i^{'} = \frac{1}{\sqrt{d_i}} \sum_{j:j\sim i} \sqrt{d_j},\ \ 1 \le i \le n$ and $0 < \alpha < 1$. Then*

$$\lambda(A_\alpha(G)) \le \max_{1\le i\le n} \left\{ \frac{\alpha d_i + \sqrt{\alpha^2 d_i^2 + \frac{4(1-\alpha)}{\sqrt{d_i}} \sum_{j:j\sim i} \sqrt{d_j}[\alpha d_j + (1-\alpha) m_j^{'}]}}{2} \right\}.$$

Equality holds if and only if $\alpha d_1 + (1-\alpha) m_1^{'} = \alpha d_2 + (1-\alpha) m_2^{'} = \cdots = \alpha d_n + (1-\alpha) m_n^{'}$.

Taking $b_i = 1$ in (3.2), and noting that $b_i' = \frac{1}{b_i} \sum_{j:j\sim i} b_j = \sum_{j:j\sim i} 1 = d_i$, we obtain the following upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and average vertex 2-degrees. We note that this upper bound was recently obtained in [15].

Corollary 3.5 ([15]). *Let G be a connected graph of order n having vertex degrees d_i, average vertex 2-degrees m_i $(1 \le i \le n)$ and $0 < \alpha < 1$. Then*

$$\lambda(A_\alpha(G)) \le \max_{1\le i\le n} \left\{ \frac{\alpha d_i + \sqrt{\alpha^2 d_i^2 + 4(1-\alpha) d_i m_i}}{2} \right\}.$$

Equality holds if and only if $d_1 = d_2 = \cdots = d_n$.

Taking $b_i = m_i$ in (3.2), and noting that $b_i' = \frac{1}{m_i} \sum_{j:j\sim i} m_j = \bar{m}_i$, we obtain the following upper bound for $\lambda(A_\alpha(G))$, in terms of vertex degrees and the quantity $\bar{m}_i$.

Corollary 3.6. *Let G be a connected graph of order n having vertex degrees d_i, average vertex 2-degrees m_i $(1 \le i \le n)$ and $0 < \alpha < 1$. Then*

$$\lambda(A_\alpha(G)) \le \max_{1\le i\le n} \left\{ \frac{\alpha d_i + \sqrt{\alpha^2 d_i^2 + \frac{4(1-\alpha)}{m_i} \sum_{j:j\sim i} m_j[\alpha d_j + (1-\alpha)\bar{m}_j]}}{2} \right\},$$

where $\bar{m}_i = \frac{1}{m_i} \sum_{j:j\sim i} m_j$. Equality holds if and only if $\alpha d_1 + (1-\alpha)\bar{m}_1 = \alpha d_2 + (1-\alpha)\bar{m}_2 = \cdots = \alpha d_n + (1-\alpha)\bar{m}_n$.

Taking $b_i = d_i + m_i$, $b_i = d_i + \sqrt{m_i}$, $b_i = \sqrt{d_i} + m_i$, $b_i = \sqrt{d_i} + \sqrt{m_i}$, $b_i = \frac{1}{\sqrt{d_i}}$, $b_i = \frac{1}{\sqrt{m_i}}$, $b_i = \frac{1}{d_i^2}$, $b_i = d_i^2$, etc, and proceeding similarly as above we can obtain some other new upper bounds for $\lambda(A_\alpha(G))$.

4 Relation between $\omega(G)$, $\gamma(G)$ and the generalized adjacency eigenvalues

For a graph G, define $\omega(G)$ and $\gamma(G)$, the *clique number* and the *independence number* of G to be the numbers of vertices of the largest clique and the largest independent set in G, respectively. In this section, we give bounds for clique number and independence number of (regular) graph G involving generalized adjacency eigenvalues.

The following lemma, due to Motzkin and Straus [19], links the spectrum of graphs to its structure.

Lemma 4.1 ([19]). *Let $F = \big\{x = (x_1, x_2, \ldots, x_n)^T \,|\, x_i \ge 0,\ \sum\limits_{i=1}^{n} x_i = 1\big\}$. Then*

$$1 - \frac{1}{\omega(G)} = \max_{x\in F} \langle x, Ax \rangle.$$

The following result gives a lower bound for $\omega(G)$, in terms of the size m, the generalized adjacency spectral radius $\lambda(A_\alpha(G))$, the maximum degree Δ and the parameter α.

Theorem 4.2. *Let G be a graph of order n, with m edges and maximum degree Δ. Then*

$$\omega(G) \geq \frac{2(1-\alpha)^2 m}{2(1-\alpha)^2 m - (\lambda(A_\alpha(G)) - \alpha\Delta)^2}.$$

Proof. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the normalized eigenvector corresponding to $\lambda(A_\alpha(G))$. Then

$$\begin{aligned}\lambda(A_\alpha(G)) &= \alpha \sum_{i=1}^{n} d_i x_i^2 + 2(1-\alpha) \sum_{j:j\sim i} x_i x_j \\ &\leq \alpha\Delta \sum_{i=1}^{n} x_i^2 + 2(1-\alpha) \sum_{j:j\sim i} x_i x_j \\ &= \alpha\Delta + 2(1-\alpha) \sum_{j:j\sim i} x_i x_j.\end{aligned}$$

Since $\lambda(A_\alpha(G)) \geq \alpha(\Delta+1)$, for $\alpha \in [0, \frac{1}{2}]$, (see [20]), by Cauchy-Schwarz inequality, we obtain

$$(\lambda(A_\alpha(G)) - \alpha\Delta)^2 \leq \left(2(1-\alpha) \sum_{j:j\sim i} x_i x_j\right)^2 \leq 2(1-\alpha)^2 m \left(2 \sum_{j:j\sim i} x_i^2 x_j^2\right).$$

Note that $(x_1^2, x_2^2, \ldots, x_n^2)^T \geq 0$ and $x_1^2 + x_2^2 + \cdots + x_n^2 = 1$. Hence, by Lemma 4.1, we have

$$2 \sum_{j:j\sim i} x_i^2 x_j^2 \leq 1 - \frac{1}{\omega(G)},$$

then

$$\frac{(\lambda(A_\alpha(G)) - \alpha\Delta)^2}{2(1-\alpha)^2 m} \leq 1 - \frac{1}{\omega(G)},$$

that is,

$$\omega(G) \geq \frac{2(1-\alpha)^2 m}{2(1-\alpha)^2 m - (\lambda(A_\alpha(G)) - \alpha\Delta)^2}.$$

This completes the proof. □

Note that Theorem 4.2 extends the Theorem 4.1 proved in [12] for the signless Laplacian spectral radius to generalized adjacency spectral radius.

The following result gives a lower bound for $\omega(G)$, when G is a regular graph, in terms of the order n, the second smallest generalized adjacency eigenvalue $\lambda_{n-1} = \lambda_{n-1}(A_\alpha(G))$ and the parameter α

Theorem 4.3. *Let G be a r-regular graph of order $n \geq 3$. Then*

$$\omega(G) \geq \frac{(1-\alpha)n^2}{(1-\alpha)\left(n^2 - nr\right) + S^2(\alpha r - \lambda_{n-1})},$$

where $S = \min_{y_i \neq 0} \frac{1}{|y_i|}$ and $u_{n-1} = (y_1, y_2, \ldots, y_n)^T$ is the normalized eigenvector corresponding to λ_{n-1}, the second smallest eigenvalue of $A_\alpha(G)$.

Proof. Since G is a r-regular graph, we have $\lambda(A_\alpha(G)) = r$ and the normalized eigenvector corresponding to $\lambda(A_\alpha(G))$ is $u_1 = \frac{e}{\sqrt{n}}$, where $e = (1, 1, \ldots, 1)^T$. Let $\Theta = \frac{S}{n}$ and $\mathbf{x} = \frac{e}{n} + \Theta u_{n-1}$. Then $\Theta y_i \geq -\frac{1}{n}$ $(i = 1, 2, \ldots, n)$. Since $\sum_{i=1}^n \lambda_i(G) = 2\alpha m = \alpha n r$ and $n \geq 3$, we have $\lambda(A_\alpha(G)) \neq \lambda_{n-1}(G)$ and $\langle e, u_{n-1}\rangle = 0$. So, $\mathbf{x} \in \left\{(x_1, x_2, \ldots, x_n)^T; x_i \geq 0,\ \sum_{i=1}^n x_i = 1\right\}$. By Lemma 4.1, we have

$$\begin{aligned}
\langle \mathbf{x}, A_\alpha \mathbf{x}\rangle &= \alpha\langle \mathbf{x}, D\mathbf{x}\rangle + (1-\alpha)\langle \mathbf{x}, A\mathbf{x}\rangle \\
&\leq r\alpha\langle \mathbf{x}, \mathbf{x}\rangle + (1-\alpha)\left(1 - \frac{1}{\omega(G)}\right) \\
&= \alpha r\left(\frac{1}{n} + \Theta^2\right) + (1-\alpha)\left(1 - \frac{1}{\omega(G)}\right).
\end{aligned}$$

On the other hand

$$\begin{aligned}
\langle \mathbf{x}, A_\alpha \mathbf{x}\rangle &= \left\langle \frac{e}{n} + \Theta u_{n-1}, A_\alpha\left(\frac{e}{n} + \Theta u_{n-1}\right)\right\rangle \\
&= \left\langle \frac{e}{n}, A_\alpha \frac{e}{n}\right\rangle + \left\langle \frac{e}{n}, A_\alpha \Theta u_{n-1}\right\rangle + \left\langle \Theta u_{n-1}, A_\alpha \frac{e}{n}\right\rangle + \langle \Theta u_{n-1}, A_\alpha \Theta u_{n-1}\rangle \\
&= \frac{nd}{n^2} + \Theta^2 \lambda_{n-1}.
\end{aligned}$$

Then

$$\frac{d}{n} + \Theta^2\lambda_{n-1} \leq \alpha r\left(\frac{1}{n} + \Theta^2\right) + (1-\alpha)\left(1 - \frac{1}{\omega(G)}\right),$$

that is,

$$\omega(G) \geq \frac{1-\alpha}{(1-\alpha)\left(1 - \frac{r}{n}\right) + \Theta^2(\alpha r - \lambda_{n-1})}.$$

Since $\Theta = \frac{S}{n}$ and $S = \min_{y_i \neq 0} \frac{1}{|y_i|}$, we have

$$\omega(G) \geq \frac{(1-\alpha)n^2}{(1-\alpha)\left(n^2 - nr\right) + S^2(\alpha r - \lambda_{n-1})}.$$

This completes the proof. □

Note that Theorem 4.3 extends the Theorem 4.4 proved in [12] for the signless Laplacian spectral radius to generalized adjacency spectral radius.

Consider two sequences of real numbers $\xi_1 \geq \xi_2 \geq \cdots \geq \xi_n$ and $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_t$ with $t < n$. The second sequence is said to *interlace* the first one whenever

$$\xi_i \geq \eta_i \geq \xi_{n-t+i},$$

for $i = 1, 2, \ldots, t$. The interlacing is called *tight* if there exists an integer $k \in [0, t]$ such that $\xi_i = \eta_i$ for $1 \leq i \leq k$ and $\xi_{n-t+i} = \eta_i$ for $k+1 \leq i \leq t$. Suppose rows and columns of the matrix M are partitioned according to a partitioning of $\{1, 2, \ldots, n\}$. The partition is called *regular* if each block of M has constant row (and column) sum. The following lemma can be found in [6].

Lemma 4.4 ([6]). *Let B be the matrix whose entries are the average row sums of the blocks of a symmetric partitioned matrix of M. Then*

(i) *the eigenvalues of B interlace the eigenvalues of M,*

(ii) *if the interlacing is tight, then the partition is regular.*

Next result gives a lower bound for $\gamma(G)$, in terms of the order n, the sum of first two largest generalized adjacency eigenvalues, the maximum degree Δ, the minimum degree δ and the parameter α.

Theorem 4.5. *Let G be a simple graph of order n with at least one edge, with minimum degree δ and maximum degree Δ. Let $\lambda_1(G)$ and $\lambda_2(G)$ are respectively the first and the second largest eigenvalue of $A_\alpha(G)$. If $\lambda_1(G) + \lambda_2(G) - (1+\alpha)\delta \leq 0$, then*

$$\gamma(G) \geq \frac{\lambda_1(G) + \lambda_2(G) - (1+\alpha)\delta}{\delta} \times \frac{n\Delta}{\lambda_1(G) + \lambda_2(G) - 2\Delta}. \tag{4.1}$$

Proof. Let G be a simple graph with order n and a partition $V(G) = V_1 \cup V_2$. Let G_i $(i = 1, 2)$ be the subgraph of G induced by V_i with $n_i < n$ vertices and average degree r_i $(n_1 + n_2 = n)$. Let $t_i = \frac{\sum_{v \in V_i} d(v)}{n_i}$ for $i = 1, 2$. Note that

$$A_\alpha(G) = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} \alpha D_{11} + (1-\alpha)A(G_1) & (1-\alpha)A_{12} \\ (1-\alpha)A_{21} & \alpha D_{22} + (1-\alpha)A(G_2) \end{pmatrix},$$

where $D_{11} = \text{diag}(d(v_1), \ldots, d(v_{n_1}))$, $D_{22} = \text{diag}(d(v_{n_1+1}), \ldots, d(v_n))$ and $A_{21} = A_{12}^T$. Put $M = \left(\frac{m_{ij}}{n_i}\right)$, where m_{ij} is the sum of the entries in $A_{ij}(G)$. Hence

$$M = \begin{pmatrix} \alpha t_1 + (1-\alpha)r_1 & (1-\alpha)(t_1 - r_1) \\ (1-\alpha)(t_2 - r_2) & \alpha t_2 + (1-\alpha)r_2 \end{pmatrix}$$

and

$$\begin{aligned} |\phi I - M| &= \phi^2 - (\alpha t_1 + (1-\alpha)r_1 + \alpha t_2 + (1-\alpha)r_2)\phi \\ &\quad - (1-\alpha)^2(t_1 - r_1)(t_2 - r_2) + (\alpha t_1 + (1-\alpha)r_1)(\alpha t_2 + (1-\alpha)r_2). \end{aligned}$$

Then by Lemma 4.4, we have $\phi_1(M) \leq \lambda_1(G)$ and $\phi_2(M) \leq \lambda_2(G)$, hence

$$\phi_1(M) + \phi_2(M) = \alpha t_1 + (1-\alpha)r_1 + \alpha t_2 + (1-\alpha)r_2 \leq \lambda_1(G) + \lambda_2(G).$$

Note that $2(n_2 t_2 - n_1 t_1) = n_2(t_2 + r_2) - n_1(t_1 + r_1)$, and hence $n_2 t_2 - n_1 t_1 = n_2 r_2 - n_1 r_1$.

Let V_{G_1} be the largest independent set of G, then $r_1 = 0$ and $\gamma(G) = 0$, we have $r_2 = t_2 - \frac{n_1}{n_2} t_1$, and

$$\alpha t_1 + \alpha t_2 + (1-\alpha)\left(t_2 - \frac{n_1}{n_2} t_1\right) = \alpha t_1 + t_2 - (1-\alpha)\frac{n_1}{n_2} t_1 \leq \lambda_1(G) + \lambda_2(G).$$

By $n = n_1 + n_2$, we get

$$\frac{\lambda_1(G)+\lambda_2(G)-t_2-\alpha t_1}{t_1} n \geq \frac{\lambda_1(G)+\lambda_2(G)-t_2-t_1}{t_1} n_1.$$

Since G has at least one edge, $n_1 < n$. Also we have $\delta \leq t_1, t_2 \leq \Delta$, hence

$$\frac{\lambda_1(G)+\lambda_2(G)-(1+\alpha)\delta}{\delta} n \geq \frac{\lambda_1(G)+\lambda_2(G)-2\Delta}{\Delta} n_1.$$

Thus

$$\gamma(G) = n_1 \geq \frac{\lambda_1(G)+\lambda_2(G)-(1+\alpha)\delta}{\delta} \times \frac{n\Delta}{\lambda_1(G)+\lambda_2(G)-2\Delta}.$$

This completes the proof. □

Again, we note that Theorem 4.5 extends the Theorem 4.5 proved in [12] for the signless Laplacian spectral radius to generalized adjacency spectral radius.

Remark 4.6. Note that if $\lambda_1(G)+\lambda_2(G)-(1+\alpha)\delta > 0$, then $\frac{\lambda_1(G)+\lambda_2(G)-(1+\alpha)\delta}{\delta} \times \frac{n\Delta}{\lambda_1(G)+\lambda_2(G)-2\Delta} < 0$, and the inequality in (4.1) is trivial. Hence, we add the restriction $\lambda_1(G)+\lambda_2(G)-(1+\alpha)\delta \leq 0$, in Theorem 4.5. One can easily see that there exists graphs with the property that $\lambda_1(G)+\lambda_2(G)-(1+\alpha)\delta \leq 0$. For example, we have $spec_{A_\alpha}(K_n) = \{n-1, \alpha n - 1^{[n-1]}\}$. Hence, $\lambda_1(K_3)+\lambda_2(K_3)-(1+\alpha)\delta(K_3) = 2+3\alpha-1-2(1+\alpha) = \alpha - 1 \leq 0$.

If G is an r-regular graph, then $\lambda_1(G) = r$ and $\Delta = \delta = r$. Hence, by Theorem 4.5, we get the following bound.

Corollary 4.7. *Let G be a simple r-regular graph of order n with at least one edge. Then*

$$\gamma(G) \geq \frac{n(\lambda_2(G)-\alpha r)}{\lambda_2(G)-r},$$

where $\lambda_2(G)$ is the second largest eigenvalue of $A_\alpha(G)$.

5 Some conclusions

As mentioned in the introduction, for $\alpha = 0$, the generalized adjacency matrix $A_\alpha(G)$ is same as the adjacency matrix $A(G)$ and for $\alpha = \frac{1}{2}$, twice the generalized adjacency matrix $A_\alpha(G)$ is same as the signless Laplacian matrix $Q(G)$. Therefore, if in particular, we put $\alpha = 0$ and $\alpha = \frac{1}{2}$, in all the results obtained in Sections 2, 3 and 4, we obtain the corresponding bounds for the adjacency spectral radius $\lambda(A(G))$ and the signless Laplacian spectral radius $\lambda(Q(G))$. We note most of these results we obtained in Section 2, 3 and 4 has been already discussed for the adjacency spectral radius $\lambda(A(G))$ or/and for the signless Laplacian spectral radius $\lambda(Q(G))$. Therefore, in this setting our results are the generalization of these known results.

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A note on the neighbour-distinguishing index of digraphs

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Abstract

In this note, we introduce and study a new version of neighbour-distinguishing arc-colourings of digraphs. An arc-colouring γ of a digraph D is proper if no two arcs with the same head or with the same tail are assigned the same colour. For each vertex u of D, we denote by $S^-_\gamma(u)$ and $S^+_\gamma(u)$ the sets of colours that appear on the incoming arcs and on the outgoing arcs of u, respectively. An arc colouring γ of D is *neighbour-distinguishing* if, for every two adjacent vertices u and v of D, the ordered pairs $(S^-_\gamma(u), S^+_\gamma(u))$ and $(S^-_\gamma(v), S^+_\gamma(v))$ are distinct. The neighbour-distinguishing index of D is then the smallest number of colours needed for a neighbour-distinguishing arc-colouring of D.

We prove upper bounds on the neighbour-distinguishing index of various classes of digraphs.

Keywords: Digraph, arc-colouring, neighbour-distinguishing arc-colouring.

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1 Introduction

A proper edge-colouring of a graph G is *vertex-distinguishing* if, for every two vertices u and v of G, the sets of colours that appear on the edges incident with u and v are distinct. Vertex-distinguishing proper edge-colourings of graphs were independently introduced by Burris and Schelp [2], and by Černy, Horňák and Soták [5]. Requiring only adjacent vertices to be distinguished led to the notion of *neighbour-distinguishing* edge-colourings, considered in [1, 3, 7].

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Vertex-distinguishing arc-colourings of digraphs have been recently introduced and studied by Li, Bai, He and Sun [4]. An arc-colouring of a digraph is proper if no two arcs with the same head or with the same tail are assigned the same colour. Such an arc-colouring is *vertex-distinguishing* if, for every two vertices u and v of G,

(i) the sets $S^-(u)$ and $S^-(v)$ of colours that appear on the incoming arcs of u and v, respectively, are distinct, and

(ii) the sets $S^+(u)$ and $S^+(v)$ of colours that appear on the outgoing arcs of u and v, respectively, are distinct.

In this paper, we introduce and study a neighbour-distinguishing version of arc-colourings of digraphs, using a slightly different distinction criteria: two neighbours u and v are distinguished whenever $S^-(u) \neq S^-(v)$ or $S^+(u) \neq S^+(v)$.

Definitions and notation are introduced in the next section. We prove a general upper bound on the neighbour-distinguishing index of a digraph in Section 3, and study various classes of digraphs in Section 4. Concluding remarks are given in Section 5.

2 Definitions and notation

All digraphs we consider are without loops and multiple arcs. For a digraph D, we denote by $V(D)$ and $A(D)$ its sets of vertices and arcs, respectively. The *underlying graph* of D, denoted $\mathrm{und}(D)$, is the simple undirected graph obtained from D by replacing each arc uv (or each pair of arcs uv, vu) by the edge uv.

If uv is an arc of a digraph D, u is the *tail* and v is the *head* of uv. For every vertex u of D, we denote by $N_D^+(u)$ and $N_D^-(u)$ the sets of *out-neighbours* and *in-neighbours* of u, respectively. Moreover, we denote by $d_D^+(u) = |N_D^+(u)|$ and $d_D^-(u) = |N_D^-(u)|$ the *outdegree* and *indegree* of u, respectively, and by $d_D(u) = d_D^+(u) + d_D^-(u)$ the *degree* of u.

For a digraph D, we denote by $\delta^+(D)$, $\delta^-(D)$, $\Delta^+(D)$ and $\Delta^-(D)$ the minimum outdegree, minimum indegree, maximum outdegree and maximum indegree of D, respectively. Moreover, we let

$$\Delta^*(D) = \max\{\Delta^+(D),\ \Delta^-(D)\}.$$

A (proper) *k-arc-colouring* of a digraph D is a mapping γ from $V(D)$ to a set of k colours (usually $\{1, \dots, k\}$) such that, for every vertex u,

(i) any two arcs with head u are assigned distinct colours, and

(ii) any two arcs with tail u are assigned distinct colours.

Note here that two consecutive arcs vu and uw, v and w not necessarily distinct, may be assigned the same colour. The *chromatic index* $\chi'(D)$ of a digraph D is then the smallest number k for which D admits a k-arc-colouring.

The following fact is well-known (see e.g. [4, 6, 8]).

Proposition 2.1. *For every digraph D, $\chi'(D) = \Delta^*(D)$.*

For every vertex u of a digraph D, and every arc-colouring γ of D, we denote by $S_\gamma^+(u)$ and $S_\gamma^-(u)$ the sets of colours assigned by γ to the outgoing and incoming arcs of u, respectively. From the definition of an arc-colouring, we get $d^+_D(u) = |S^+_\gamma(u)|$ and $d^-_D(u) = |S^-_\gamma(u)|$ for every vertex u.

We say that two vertices u and v of a digraph D are *distinguished* by an arc-colouring γ of D, if $(S^+_\gamma(u), S^-_\gamma(u)) \neq (S^+_\gamma(v), S^-_\gamma(v))$. Note that we consider here ordered pairs, so that $(A, B) \neq (B, A)$ whenever $A \neq B$. Note also that if u and v are such that $d^+_D(u) \neq d^+_D(v)$ or $d^-_D(u) \neq d^-_D(v)$, which happens in particular if $d_D(u) \neq d_D(v)$, then they are distinguished by every arc-colouring of D. We will write $u \nsim_\gamma v$ if u and v are distinguished by γ and $u \sim_\gamma v$ otherwise.

A k-arc-colouring γ of a digraph D is *neighbour-distinguishing* if $u \nsim_\gamma v$ for every arc $uv \in A(D)$. Such an arc-colouring will be called an *nd-arc-colouring* for short. The *neighbour-distinguishing index* $\mathrm{ndi}(D)$ of a digraph D is then the smallest number of colours required for an nd-arc-colouring of D.

The following lower bound is easy to establish.

Proposition 2.2. *For every digraph D, $\mathrm{ndi}(D) \geq \chi'(D) = \Delta^*(D)$. Moreover, if there are two vertices u and v in D with $d^+_D(u) = d^+_D(v) = d^-_D(u) = d^-_D(v) = \Delta^*(D)$, then $\mathrm{ndi}(D) \geq \Delta^*(D) + 1$.*

Proof. The first statement follows from the definitions. For the second statement, observe that $S^+_\gamma(u) = S^+_\gamma(v) = S^-_\gamma(u) = S^-_\gamma(v) = \{1, \ldots, \Delta^*(D)\}$ for any two such vertices u and v and any $\Delta^*(D)$-arc-colouring γ of D. □

3 A general upper bound

If D is an *oriented graph*, that is, a digraph with no opposite arcs, then every proper edge-colouring φ of $\mathrm{und}(D)$ is an nd-arc-colouring of D since, for every arc uv in D, $\varphi(uv) \in S^+_\varphi(u)$ and $\varphi(uv) \notin S^+_\varphi(v)$, which implies $u \nsim_\varphi v$. Hence, we get the following upper bound for oriented graphs, thanks to classical Vizing's bound.

Proposition 3.1. *If D is an oriented graph, then*

$$\mathrm{ndi}(D) \leq \chi'(\mathrm{und}(D)) \leq \Delta(\mathrm{und}(D)) + 1 \leq 2\Delta^*(D) + 2.$$

However, a proper edge-colouring of $\mathrm{und}(D)$ may produce an arc-colouring of D which is not neighbour-distinguishing when D contains opposite arcs. Consider for instance the digraph D given by $V(D) = \{a, b, c, d\}$ and $A(D) = \{ab, bc, cb, dc\}$. We then have $\mathrm{und}(D) = P_4$, the path of order 4, and thus $\chi'(\mathrm{und}(D)) = 2$. It is then not difficult to check that for any 2-edge-colouring φ of $\mathrm{und}(D)$, $S^+_\varphi(b) = S^+_\varphi(c)$ and $S^-_\varphi(b) = S^-_\varphi(c)$.

We will prove that the upper bound given in Proposition 3.1 can be decreased to $2\Delta^*(D)$, even when D contains opposite arcs. Recall that a digraph D is *k-regular* if $d^+_D(v) = d^-_D(v) = k$ for every vertex v of D. A *k-factor* in a digraph D is a spanning k-regular subdigraph of D. The following result is folklore.

Theorem 3.2. *Every k-regular digraph can be decomposed into k arc-disjoint 1-factors.*

We first determine the neighbour-distinguishing index of a 1-factor.

Proposition 3.3. *If D is a digraph with $d^+_D(u) = d^-_D(u) = 1$ for every vertex u of D, then* $\mathrm{ndi}(D) = 2$.

Proof. Such a digraph D is a disjoint union of directed cycles and any such cycle needs at least two colours to be neighbour-distinguished. An nd-arc-colouring of D using two colours can be obtained as follows. For a directed cycle of even length, use alternately colours 1 and 2. For a directed cycle of odd length, use the colour 2 on any two consecutive arcs, and then use alternately colours 1 and 2. The so-obtained 2-arc-colouring is clearly neighbour-distinguishing, so that $\mathrm{ndi}(D) = 2$. □

We are now able to prove the following general upper bound on the neighbour-distinguishing index of a digraph.

Theorem 3.4. *For every digraph D,* $\mathrm{ndi}(D) \leq 2\Delta^*(D)$.

Proof. Let D' be any $\Delta^*(D)$-regular digraph containing D as a subdigraph. If D is not already regular, such a digraph can be obtained from D by adding new arcs, and maybe new vertices.

By Theorem 3.2, the digraph D' can be decomposed into $\Delta^*(D') = \Delta^*(D)$ arc-disjoint 1-factors, say $F_1, \dots, F_{\Delta^*(D)}$. By Proposition 3.3, we know that D' admits an nd-arc-colouring γ' using $2\Delta^*(D') = 2\Delta^*(D)$ colours. We claim that the restriction γ of γ' to $A(D)$ is also neighbour-distinguishing.

To see that, let uv be any arc of D, and let t and w be the two vertices such that the directed walk $tuvw$ belongs to a 1-factor F_i of D' for some i, $1 \leq i \leq \Delta^*(D)$. Note here that we may have $t = w$, or $w = u$ and $t = v$. If $\gamma(uv) \neq \gamma'(vw)$, then $\gamma(uv) \in S^+_\gamma(u)$ and $\gamma(uv) \notin S^+_\gamma(v)$. Similarly, if $\gamma'(tu) \neq \gamma(uv)$, then $\gamma(uv) \in S^-_\gamma(v)$ and $\gamma(uv) \notin S^-_\gamma(u)$. Since neither three consecutive arcs nor two opposite arcs in a walk of a 1-factor of D' are assigned the same colour by γ', we get that $u \nsim_\gamma v$ for every arc uv of D, as required.

This completes the proof. □

4 Neighbour-distinguishing index of some classes of digraphs

We study in this section the neighbour-distinguishing index of several classes of digraphs, namely complete symmetric digraphs, bipartite digraphs and digraphs whose underlying graph is k-chromatic, $k \geq 3$.

4.1 Complete symmetric digraphs

We denote by K_n^* the complete symmetric digraph of order n. Observe first that any proper edge-colouring ϵ of K_n induces an arc-colouring γ of K_n^* defined by $\gamma(uv) = \gamma(vu) = \epsilon(uv)$ for every edge uv of K_n. Moreover, since $S^+_\gamma(u) = S^-_\gamma(u) = S_\epsilon(u)$ for every vertex u, γ is neighbour-distinguishing whenever ϵ is neighbour-distinguishing. Using a result of Zhang, Liu and Wang (see Theorem 6 in [7]), we get that $\mathrm{ndi}(K_n^*) = \Delta^*(K_n^*) + 1 = n$ if n is odd, and $\mathrm{ndi}(K_n^*) \leq \Delta^*(K_n^*) + 2 = n + 1$ if n is even.

We prove that the bound in the even case can be decreased by one (we recall the proof of the odd case to be complete).

Theorem 4.1. *For every integer* $n \geq 2$, $\mathrm{ndi}(K_n^*) = \Delta^*(K_n^*) + 1 = n$.

Proof. Note first that we necessarily have $\mathrm{ndi}(K_n^*) \geq n$ for every $n \geq 2$ by Proposition 2.2. Let $V(K_n^*) = \{v_0, \dots, v_{n-1}\}$. If $n = 2$, we obviously have $\mathrm{ndi}(K_2^*) = |A(K_2^*)| = 2$ and the result follows. We can thus assume $n \geq 3$. We consider two cases, depending on the parity of n.

Suppose first that n is odd, and consider a partition of the set of edges of K_n into n disjoint maximal matchings, say $M_0, \ldots, M_{n-1}$, such that for each i, $0 \le i \le n-1$, the matching M_i does not cover the vertex v_i. We define an n-arc-colouring γ of K_n^* (using the set of colours $\{0, \ldots, n-1\}$) as follows. For every i and j, $0 \le i < j \le n-1$, we set $\gamma(v_iv_j) = \gamma(v_jv_i) = k$ if and only if the edge v_iv_j belongs to M_k. Observe now that for every vertex v_i, $0 \le i \le n-1$, the colour i is the unique colour that does not belong to $S_\gamma^+(v_i) \cup S_\gamma^-(v_i)$, since v_i is not covered by the matching M_i. This implies that γ is an nd-arc-colouring of K_n^*, and thus $\mathrm{ndi}(K_n^*) = n$, as required.

Suppose now that n is even. Let K' be the subgraph of K_n^* induced by the set of vertices $\{v_0, \ldots, v_{n-2}\}$ and γ' be the $(n-1)$-arc-colouring of K' defined as above. We define an n-arc-colouring γ of K_n^* (using the set of colours $\{0, \ldots, n-1\}$) as follows:

1. for every i and j, $0 \le i < j \le n-2$, $j \not\equiv i+1 \pmod{n-1}$, we set $\gamma(v_iv_j) = \gamma'(v_iv_j)$,
2. for every i, $0 \le i \le n-2$, we set $\gamma(v_iv_{i+1}) = n-1$ and $\gamma(v_{i+1}v_i) = \gamma'(v_{i+1}v_i)$ (subscripts are taken modulo $n-1$),
3. for every i, $0 \le i \le n-2$, we set $\gamma(v_{n-1}v_i) = \gamma'(v_{i-1}v_i)$ and $\gamma(v_iv_{n-1}) = \gamma'(v_{i+1}v_i)$.

Since the colour $n-1$ belongs to $S_\gamma^+(v_i) \cap S_\gamma^-(v_i)$ for every i, $0 \le i \le n-2$, and does not belong to $S_\gamma^+(v_{n-1}) \cup S_\gamma^-(v_{n-1})$, the vertex v_{n-1} is distinguished from every other vertex in K_n^*. Moreover, for every vertex v_i, $0 \le i \le n-2$,

$$S_\gamma^+(v_i) = S_{\gamma'}^+(v_i) \cup \{n-1\} \text{ and } S_\gamma^-(v_i) = S_{\gamma'}^-(v_i) \cup \{n-1\},$$

which implies that any two vertices v_i and v_j, $0 \le i < j \le n-2$, are distinguished since γ' is an nd-arc-colouring of K'. We thus get that γ is an nd-arc-colouring of K_n^*, and thus $\mathrm{ndi}(K_n^*) \le n$, as required.

This completes the proof. □

4.2 Bipartite digraphs

A digraph D is *bipartite* if its underlying graph is bipartite. In that case, $V(D) = X \cup Y$ with $X \cap Y = \emptyset$ and $A(D) \subseteq X \times Y \cup Y \times X$. We then have the following result.

Theorem 4.2. *If D is a bipartite digraph, then* $\mathrm{ndi}(D) \le \Delta^*(D) + 2$.

Proof. Let $V(D) = X \cup Y$ be the bipartition of $V(D)$ and γ be any (not necessarily neighbour-distinguishing) optimal arc-colouring of D using $\Delta^*(D)$ colours (such an arc-colouring exists by Proposition 2.1).

If γ is an nd-arc-colouring we are done. Otherwise, let $M_1 \subseteq A(D) \cap (X \times Y)$ be a maximal matching from X to Y. We define the arc-colouring γ_1 as follows:

$$\gamma_1(uv) = \Delta^*(D) + 1 \text{ if } uv \in M_1,\ \gamma_1(uv) = \gamma(uv) \text{ otherwise.}$$

Note that if uv is an arc such that u or v is (or both are) covered by M_1, then $u \nsim_{\gamma_1} v$ since the colour $\Delta^*(D) + 1$ appears in exactly one of the sets $S_{\gamma_1}^+(u)$ and $S_{\gamma_1}^+(v)$, or in exactly one of the sets $S_{\gamma_1}^-(u)$ and $S_{\gamma_1}^-(v)$.

If γ_1 is an nd-arc-colouring we are done. Otherwise, let $A^\sim$ be the set of arcs $uv \in A(D)$ with $u \sim_{\gamma_1} v$ and $M_2 \subseteq A^\sim \cap (Y \times X)$ be a maximal matching from Y to X of $A^\sim$. We define the arc-colouring γ_2 as follows:

$$\gamma_2(uv) = \Delta^*(D) + 2 \text{ if } uv \in M_2,\ \gamma_2(uv) = \gamma_1(uv) \text{ otherwise.}$$

Again, note that if uv is an arc such that u or v is (or both are) covered by M_2, then $u \not\sim_{\gamma_2} v$. Moreover, since M_2 is a matching of $A^{\sim}$, pairs of vertices that were distinguished by γ_1 are still distinguished by γ_2.

Hence, every arc uv such that u and v were not distinguished by γ_1 are now distinguished by γ_2 which is thus an nd-arc-colouring of D using $\Delta^*(D) + 2$ colours. This concludes the proof. □

The upper bound given in Theorem 4.2 can be decreased when the underlying graph of D is a tree.

Theorem 4.3. *If D is a digraph whose underlying graph is a tree, then* $\mathrm{ndi}(D) \leq \Delta^*(D)+1$.

Proof. The proof is by induction on the order n of D. The result clearly holds if $n \leq 2$. Let now D be a digraph of order $n \geq 3$, such that the underlying graph $\mathrm{und}(D)$ of D is a tree, and $P = v_1 \dots v_k$, $k \leq n$, be a path in $\mathrm{und}(D)$ with maximal length. By the induction hypothesis, there exists an nd-arc-colouring γ of $D - v_k$ using at most $\Delta^*(D - v_k) + 1$ colours. We will extend γ to an nd-arc-colouring of D using at most $\Delta^*(D) + 1$ colours.

If $\Delta^*(D) = \Delta^*(D - v_k) + 1$, we assign the new colour $\Delta^*(D) + 1$ to the at most two arcs incident with v_k so that the so-obtained arc-colouring is clearly neighbour-distinguishing.

Suppose now that $\Delta^*(D) = \Delta^*(D - v_k)$. If all neighbours of v_{k-1} are leaves, the underlying graph of D is a star. In that case, there is at most one arc linking v_{k-1} and v_k, and colouring this arc with any admissible colour produces an nd-arc-colouring of D. If the underlying graph of D is not a star, then, by the maximality of P, we get that v_{k-1} has exactly one neighbour which is not a leaf, namely v_{k-2}. This implies that the only conflict that might appear when colouring the arcs linking v_k and v_{k-1} is between v_{k-2} and v_{k-1} (recall that two neighbours with distinct indegree or outdegree are necessarily distinguished).

Since $d_D^+(v_{k-2}) \leq \Delta^*(D)$ and $d_D^-(v_{k-2}) \leq \Delta^*(D)$, there necessarily exist a colour a such that $S_\gamma^+(v_{k-2}) \neq S_\gamma^+(v_{k-1}) \cup \{a\}$, and a colour b such that $S_\gamma^-(v_{k-2}) \neq S_\gamma^-(v_{k-1}) \cup \{b\}$. Therefore, the at most two arcs incident with v_k can be coloured, using a and/or b, in such a way that the so-obtained arc-colouring is neighbour-distinguishing.

This completes the proof. □

4.3 Digraphs whose underlying graph is k-chromatic

Since the set of edges of every k-colourable graph can be partitionned in $\lceil \log k \rceil$ parts each inducing a bipartite graph (see e.g. Lemma 4.1 in [1]), Theorem 4.2 leads to the following general upper bound:

Corollary 4.4. *If D is a digraph whose underlying graph has chromatic number $k \geq 3$, then* $\mathrm{ndi}(D) \leq \Delta^*(D) + 2\lceil \log k \rceil$.

Proof. Starting from an optimal arc-colouring of D with $\Delta^*(D)$ colours, it suffices to use two new colours for each of the $\lceil \log k \rceil$ bipartite parts (obtained from any optimal vertex-colouring of the underlying graph of D), as shown in the proof of Theorem 4.2, in order to get an nd-arc-colouring of D. □

5 Discussion

In this note, we have introduced and studied a new version of neighbour-distinguishing arc-colourings of digraphs. Pursuing this line of research, we propose the following questions.

1. Is there any general upper bound on the neighbour-distinguishing index of symmetric digraphs?

2. Is there any general upper bound on the neighbour-distinguishing index of not necessarily symmetric complete digraphs?

3. Is there any general upper bound on the neighbour-distinguishing index of directed acyclic graphs?

4. The general bound given in Corollary 4.4 is certainly not optimal. In particular, is it possible to improve this bound for digraphs whose underlying graph is 3-colourable?

We finally propose the following conjecture.

Conjecture 5.1. *For every digraph D,* $\mathrm{ndi}(D) \leq \Delta^*(D) + 1$.

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Complexity of circulant graphs with non-fixed jumps, its arithmetic properties and asymptotics*

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Abstract

In the present paper, we investigate a family of circulant graphs with non-fixed jumps

$$G_n = C_{\beta n}(s_1, \ldots, s_k, \alpha_1 n, \ldots, \alpha_\ell n),$$
$$1 \le s_1 < \ldots < s_k < [\frac{\beta n}{2}],\ 1 \le \alpha_1 < \ldots < \alpha_\ell \le [\frac{\beta}{2}].$$

Here n is an arbitrary large natural number and integers $s_1, \ldots, s_k, \alpha_1, \ldots, \alpha_\ell, \beta$ are supposed to be fixed.

First, we present an explicit formula for the number of spanning trees in the graph G_n. This formula is a product of $\beta s_k - 1$ factors, each given by the n-th Chebyshev polynomial of the first kind evaluated at the roots of some prescribed polynomial of degree s_k. Next, we provide some arithmetic properties of the complexity function. We show that the number of spanning trees in G_n can be represented in the form $\tau(n) = p\, n\, a(n)^2$, where $a(n)$ is an integer sequence and p is a given natural number depending on parity of β and n. Finally, we find an asymptotic formula for $\tau(n)$ through the Mahler measure of the Laurent polynomials differing by a constant from $2k - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i})$.

Keywords: Spanning tree, circulant graph, Laplacian matrix, Chebyshev polynomial, Mahler measure.

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1 Introduction

The *complexity* of a finite connected graph G, denoted by $\tau(G)$, is the number of spanning trees of G. The famous Kirchhoff's Matrix Tree Theorem [13] states that $\tau(G)$ can be expressed as the product of non-zero Laplacian eigenvalues of G divided by the number of its vertices. Since then, a lot of papers devoted to the complexity of various classes of graphs were published. In particular, explicit formulae were derived for complete multipartite graphs [16], wheels [2], fans [10], prisms [1], anti-prisms [32], ladders [26], Möbius ladders [27], lattices [28] and other families. The complexity of circulant graphs has been the subject of study by many authors [4, 5, 17, 34, 35, 36, 37, 38].

Starting with Boesch and Prodinger [2] the idea to calculate the complexity of graphs by making use of Chebyshev polynomials was implemented. This idea provided a way to find complexity of circulant graphs and their natural generalisations in [4, 14, 19, 25, 36, 38].

Recently, asymptotical behavior of complexity for some families of graphs was investigated from the point of view of so called Malher measure [9, 29, 30]. For general properties of the Mahler measure see, for example [31] and [7]. It worth mentioning that the Mahler measure is related to the growth of groups, values of some hypergeometric functions and volumes of hyperbolic manifolds [3].

For a sequence of graphs G_n, one can consider the number of vertices $v(G_n)$ and the number of spanning trees $\tau(G_n)$ as functions of n. Assuming that $\lim_{n\to\infty} \frac{\log \tau(G_n)}{v(G_n)}$ exists, it is called the thermodynamic limit of the family G_n [20]. This number plays an important role in statistical physics and was investigated by many authors [12, 28, 29, 30, 33].

The purpose of this paper is to present new formulas for the number of spanning trees in circulant graphs with non-fixed jumps and investigate their arithmetical properties and asymptotics. We mention that the number of spanning trees for such graphs was found earlier in [5, 8, 17, 19, 37, 38]. Our results are different from those obtained in the cited papers. Moreover, by the authors opinion, the obtained formulas are more convenient for analytical investigation.

The content of the paper is lined up as follows. Basic definitions and preliminary results are given in Sections 2 and 3. Then, in the Section 4, we present an explicit formula for the number of spanning trees in the undirected circulant graph

$$C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n),$$
$$1 \le s_1 < \ldots < s_k < [\frac{\beta n}{2}],\ 1 \le \alpha_1 < \ldots < \alpha_\ell \le [\frac{\beta}{2}].$$

This formula is a product of $\beta s_k - 1$ factors, each given by the n-th Chebyshev polynomial of the first kind evaluated at the roots of a prescribed polynomial of degree s_k. Through the paper, we will assume that $\beta > 1$ and $\ell > 0$. The case $\beta = 1$ and $\ell = 0$ of the circulant graphs with bounded jumps has been investigated in our previous papers [22, 23].

Next, in the Section 5, we provide some arithmetic properties of the complexity function. More precisely, we show that the number of spanning trees of the circulant graph can be represented in the form $\tau(n) = \beta\, p\, n\, a(n)^2$, where $a(n)$ is an integer sequence and p is a prescribed natural number depending only on parity of n and β. Later, in the Section 6, we use explicit formulas for the number of spanning trees to produce its asymptotics through the Mahler measures of the finite set of Laurent polynomials

$$P_u(z) = 2k - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i}) + 4\sum_{m=1}^{\ell} \sin^2(\frac{\pi\, u\, \alpha_m}{\beta}),\ u = 0, 1, \ldots, \beta - 1.$$

As a consequence (Corollary 6.2), we prove that the thermodynamic limit of sequence $C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$ as $n \to \infty$ is the arithmetic mean of small Mahler measures of Laurent polynomials $P_u(z),\ u = 0, 1, \ldots, \beta - 1$. In the Section 7, we illustrate the obtained results by a series of examples.

2 Basic definitions and preliminary facts

Consider a connected finite graph G, allowed to have multiple edges but without loops. We denote the vertex and edge set of G by $V(G)$ and $E(G)$, respectively. Given $u, v \in V(G)$, we set a_{uv} to be equal to the number of edges between vertices u and v. The matrix $A = A(G) = \{a_{uv}\}_{u,v \in V(G)}$ is called *the adjacency matrix* of the graph G. The degree $d(v)$ of a vertex $v \in V(G)$ is defined by $d(v) = \sum_{u \in V(G)} a_{uv}$. Let $D = D(G)$ be the diagonal matrix indexed by the elements of $V(G)$ with $d_{vv} = d(v)$. The matrix $L = L(G) = D(G) - A(G)$ is called *the Laplacian matrix*, or simply *Laplacian*, of the graph G.

In what follows, by I_n we denote the identity matrix of order n.

Let $s_1, s_2, \ldots, s_k$ be integers such that $1 \leq s_1, s_2, \ldots, s_k \leq \frac{n}{2}$. The graph $G = C_n(s_1, s_2, \ldots, s_k)$ with n vertices $0, 1, 2, \ldots,\ n-1$ is called *circulant graph* if the vertex $i,\ 0 \leq i \leq n-1$ is adjacent to the vertices $i \pm s_1, i \pm s_2, \ldots, i \pm s_k \pmod n$. All vertices of the graph G have even degree $2k$. If there is i such that $s_i = \frac{n}{2}$ then graph G has multiple edges.

We call an $n \times n$ matrix *circulant,* and denote it by $circ(a_0, a_1, \ldots, a_{n-1})$ if it is of the form

$$circ(a_0, a_1, \ldots, a_{n-1}) = \begin{pmatrix} a_0 & a_1 & a_2 & \ldots & a_{n-1} \\ a_{n-1} & a_0 & a_1 & \ldots & a_{n-2} \\ & \vdots & & \ddots & \vdots \\ a_1 & a_2 & a_3 & \ldots & a_0 \end{pmatrix}.$$

It easy to chose enumeration of vertices such that adjacency and Laplacian matrices for the circulant graph are circulant matrices. The converse is also true. If the Laplacian matrix of a graph is circulant then the graph is also circulant.

In this paper, we consider a particular class of circulant graphs, namely circulant graphs with *non-fixed jumps.* They are defined as before, with special restrictions on the number of vertices and structure of jumps.

More precisely, we will deal with circulant graphs

$$G_n = C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$$

on βn vertices and jumps $s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n$ satisfying the inequalities $1 \leq s_1 < \ldots < s_k < [\frac{\beta n}{2}],\ 1 \leq \alpha_1 < \ldots < \alpha_\ell \leq [\frac{\beta}{2}]$. Mostly, we are interesting in investigation of such graphs for sufficiently large n. In what follows, the numbers $s_1, s_2, \ldots, s_k, \alpha_1, \alpha_2, \ldots, \alpha_\ell, \beta$ are supposed to be fixed positive integers.

In particular, graph G_n has no multiple edges if $\alpha_\ell < \frac{\beta}{2}$. If $\alpha_\ell = \frac{\beta}{2}$, it has exactly two edges between vertices v_i and $v_{i + \frac{\beta n}{2}}$, where indices are taken $\mod \beta n$. In the latter case, β is certainly an even positive integer. A typical example is graph $C_{2n}(1, n)$ which, under the above agreement, represents a Moebius ladder graph on $2n$ vertices with *double* steps. Circulant graphs with non-fixed jumps have been the subject of investigation in many papers [8, 17, 24, 38].

Warning. In series of papers [5, 22, 23, 37] devoted to circulant graphs with odd degree of vertices the notation $C_{2n}(1, n)$ stands for the Moebius ladder with ordinary steps. The degree of vertices of such graph is three. These families of graphs are outside of consideration in the present paper.

Recall [6] that the eigenvalues of matrix $C = circ(a_0, a_1, \ldots, a_{n-1})$ are given by the following simple formulas $\lambda_j = L(\zeta_n^j)$, $j = 0, 1, \ldots, n-1$, where $L(x) = a_0 + a_1 x + \ldots + a_{n-1}x^{n-1}$ and ζ_n is a primitive n-th root of unity. Moreover, the circulant matrix $C = L(T)$, where $T = circ(0, 1, 0, \ldots, 0)$ is the matrix representation of the shift operator $T\colon (x_0, x_1, \ldots, x_{n-2}, x_{n-1}) \to (x_1, x_2, \ldots, x_{n-1}, x_0)$.

Let $P(z) = a_0 + a_1 z + \ldots + a_d z^d = a_d \prod_{k=1}^{d}(z - \alpha_k)$ be a non-constant polynomial with complex coefficients. Then, following Mahler [21] its *Mahler measure* is defined to be

$$M(P) := \exp(\int_0^1 \log |P(e^{2\pi i t})| dt), \tag{2.1}$$

the geometric mean of $|P(z)|$ for z on the unit circle. However, $M(P)$ had appeared earlier in a paper by Lehmer [15], in an alternative form

$$M(P) = |a_d| \prod_{|\alpha_k|>1} |\alpha_k|. \tag{2.2}$$

The equivalence of the two definitions follows immediately from Jensen's formula [11]

$$\int_0^1 \log |e^{2\pi i t} - \alpha| dt = \log_+ |\alpha|,$$

where $\log_+ x$ denotes $\max(0, \log x)$. We will also deal with the *small Mahler measure* which is defined as

$$m(P) := \log M(P) = \int_0^1 \log |P(e^{2\pi i t})| dt.$$

The concept of Mahler measure can be naturally extended to the class of Laurent polynomials $P(z) = a_0 z^p + a_1 z^{p+1} + \ldots + a_{d-1} z^{p+d-1} + a_d z^{p+d} = a_d z^p \prod_{k=1}^{d}(z - \alpha_k)$, where $a_0, a_d \neq 0$ and p is an arbitrary and not necessarily positive integer.

3 Associated polynomials and their properties

The aim of this section is to introduce a few polynomials naturally associated with the circulant graph

$$G_n = C_{\beta n}(s_1, \ldots, s_k, \alpha_1 n, \ldots, \alpha_\ell n),$$
$$1 \le s_1 < \ldots < s_k < [\frac{\beta n}{2}],\ 1 \le \alpha_1 < \ldots < \alpha_\ell \le [\frac{\beta}{2}].$$

We start with the Laurent polynomial

$$L(z) = 2(k + \ell) - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i}) - \sum_{m=1}^{\ell}(z^{\alpha_m n} + z^{-\alpha_m n})$$

responsible for the structure of Laplacian of graph G_n. More precisely, the Laplacian of G_n is given by the matrix

$$\mathbb{L} = L(T) = 2(k+\ell)I_{\beta n} - \sum_{i=1}^{k}(T^{s_i} + T^{-s_i}) - \sum_{m=1}^{\ell}(T^{\alpha_m n} + T^{-\alpha_m n}),$$

where T the circulant matrix $circ(\underbrace{0, 1, \ldots, 0}_{\beta n})$. We decompose $L(z)$ into the sum of two polynomials $L(z) = P(z) + p(z^n)$, where $P(z) = 2k - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i})$ and $p(z) = 2\ell - \sum_{m=1}^{\ell}(z^{\alpha_m} + z^{-\alpha_m})$. Now, we have to introduce a family of Laurent polynomials differing by a constant from $P(z)$. They are $P_u(z) = P(z) + p(e^{\frac{2\pi\, i\, u}{\beta}})$, $u = 0, 1, \ldots, \beta-1$. One can check that $P_u(z) = 2k - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i}) + 4\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_m}{\beta})$. In particular, $P_0(z) = P(z)$.

We note that all the above Laurent polynomials are *palindromic*, that is they are invariant under replacement z by $1/z$. Any non-trivial palindromic Laurent polynomial can be represented in the form $\mathcal{P}(z) = a_s z^{-s} + a_{s-1}z^{-(s-1)} + \ldots + a_0 + \ldots + a_{s-1}z^{s-1} + a_s z^s$, where $a_s \neq 0$. We will refer to $2s$ as a *degree* of the polynomial $\mathcal{P}(z)$. Since $\mathcal{P}(z) = \mathcal{P}(\frac{1}{z})$, the following polynomial of degree s is well defined

$$\mathcal{Q}(w) = \mathcal{P}(w + \sqrt{w^2 - 1}).$$

We will call it a *Chebyshev trasform* of $\mathcal{P}(z)$. Since $T_k(w) = \frac{(w+\sqrt{w^2-1})^k + (w+\sqrt{w^2-1})^{-k}}{2}$ is the k-th Chebyshev polynomial of the first kind, one can easy deduce that

$$\mathcal{Q}(w) = a_0 + 2a_1T_1(w) + \ldots + 2a_{s-1}T_{s-1}(w) + 2a_sT_s(w).$$

Also, we have $\mathcal{P}(z) = \mathcal{Q}(\frac{1}{2}(z + \frac{1}{z}))$.

Throughout the paper, we will use the following observation. If $z_1, 1/z_1, \ldots, z_s, 1/z_s$ is the list of all the roots of $\mathcal{P}(z)$, then $w_k = \frac{1}{2}(z_k + \frac{1}{z_k})$, $k = 1, 2, \ldots, s$ are all the roots of the polynomial $\mathcal{Q}(w)$.

By direct calculation, we obtain that the Chebyshev transform of polynomial $P_u(z)$ is

$$Q_u(w) = 2k - 2\sum_{i=1}^{k}T_{s_i}(w) + 4\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_m}{\beta}).$$

In particular, if $z_s(u), 1/z_s(u)$, $s = 1, 2, \ldots, s_k$ are the roots of $P_u(z)$, then $w_s(u) = \frac{1}{2}(z_s(u) + z_s(u)^{-1})$, $s = 1, 2, \ldots, s_k$ are all roots of the algebraic equation $\sum_{i=1}^{k}T_{s_i}(w) = k + 2\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_m}{\beta})$. We also need the following lemma.

Lemma 3.1. *Let* $\gcd(\alpha_1, \alpha_2, \ldots, \alpha_\ell, \beta) = 1$. *Suppose that* $P_u(z) = 0$, *where* $0 < u < \beta$. *Then* $|z| \neq 1$.

Proof. Recall that $P_u(z) = P(z) + p(e^{\frac{2\pi\, i\, u}{\beta}})$, where $P(z) = 2k - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i})$ and $p(z) = 2\ell - \sum_{m=1}^{\ell}(z^{\alpha_m} + z^{-\alpha_m})$. We show that $p(e^{\frac{2\pi\, i\, u}{\beta}}) = 4\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_m}{\beta}) > 0$. Indeed, suppose that $p(e^{\frac{2\pi\, i\, u}{\beta}}) = 0$. Then there are integers m_j such that $u\,\alpha_j = m_j\beta$, $j = 1, 2, \ldots, \ell$. Hence

$$B = \gcd(u\,\alpha_1, \ldots, u\,\alpha_\ell, u\,\beta) = u\gcd(\alpha_1, \ldots, \alpha_\ell, \beta) = u < \beta.$$

From the other side

$$B = \gcd(m_1\beta, \ldots, m_\ell\beta, u\,\beta) = \beta\gcd(m_1, \ldots, m_\ell, u) \geq \beta.$$

Contradiction. Now, let $|z| = 1$. Then $z = e^{i\varphi},$ for some $\varphi \in \mathbb{R}$. We have

$$\begin{aligned} P_u(e^{i\varphi}) = P(e^{i\varphi}) + p(e^{\frac{2\pi\, i\, u}{\beta}}) &= 2k - \sum_{j=1}^{k}(e^{is_j\varphi} + e^{-is_j\varphi}) + 4\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\,\alpha_m}{\beta}) \\ &= 2\sum_{j=1}^{k}(1-\cos(s_j\varphi)) + 4\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\,\alpha_m}{\beta}) > 0. \end{aligned}$$

Hence, $P_u(z) > 0$ and lemma is proved. □

4 Complexity of circulant graphs with non-fixed jumps

The aim of this section is to find new formulas for the numbers of spanning trees of circulant graph $C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$ in terms of Chebyshev polynomials. It should be noted that nearby results were obtained earlier by different methods in the papers [5, 8, 17, 19, 37, 38].

Theorem 4.1. *The number of spanning trees in the circulant graph with non-fixed jumps*

$$C_{\beta n}(s_1, \ldots, s_k, \alpha_1 n, \ldots, \alpha_\ell n),\ 1 \leq s_1 < \ldots < s_k < [\frac{\beta n}{2}],\ 1 \leq \alpha_1 < \ldots < \alpha_\ell \leq [\frac{\beta}{2}]$$

is given by the formula

$$\tau(n) = \frac{n}{\beta\, q}\prod_{u=0}^{\beta-1}\prod_{\substack{j=1,\\ w_j(0)\neq 1}}^{s_k}|2T_n(w_j(u)) - 2\cos(\frac{2\pi u}{\beta})|,$$

where for each $u = 0, 1, \ldots, \beta - 1$ the numbers $w_j(u)$, $j = 1, 2, \ldots, s_k$, are all the roots of the equation $\sum_{i=1}^{k} T_{s_i}(w) = k + 2\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\,\alpha_m}{\beta})$, $T_s(w)$ is the Chebyshev polynomial of the first kind and $q = s_1^2 + s_2^2 + \ldots + s_k^2$.

Proof. Let $G = C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$. By the celebrated Kirchhoff theorem, the number of spanning trees $\tau(n)$ in G_n is equal to the product of non-zero eigenvalues of the Laplacian of the graph G_n divided by the number of its vertices βn. To investigate the spectrum of Laplacian matrix, we denote by T the $\beta n \times \beta n$ circulant matrix $circ(0, 1, \ldots, 0)$. Consider the Laurent polynomial

$$L(z) = 2(k+\ell) - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i}) - \sum_{m=1}^{\ell}(z^{\alpha_m n} + z^{-\alpha_m n}).$$

Then the Laplacian of G_n is given by the matrix

$$\mathbb{L} = L(T) = 2(k+\ell)I_{\beta n} - \sum_{i=1}^{k}(T^{s_i} + T^{-s_i}) - \sum_{m=1}^{\ell}(T^{\alpha_m n} + T^{-\alpha_m n}).$$

The eigenvalues of the circulant matrix T are $\zeta_{\beta n}^{j}$, $j = 0, 1, \ldots, \beta n - 1$, where $\zeta_\ell = e^{\frac{2\pi i}{\ell}}$. Since all of them are distinct, the matrix T is similar to the diagonal matrix $\mathbb{T} = diag(1, \zeta_{\beta n}, \ldots, \zeta_{\beta n}^{\beta n-1})$. To find spectrum of $\mathbb{L}$, without loss of generality, one can assume that $T = \mathbb{T}$. Then $\mathbb{L}$ is a diagonal matrix. This essentially simplifies the problem of finding eigenvalues of $\mathbb{L}$. Indeed, let λ be an eigenvalue of $\mathbb{L}$ and x be the respective eigenvector. Then we have the following system of linear equations

$$((2(k+\ell)-\lambda)I_{\beta n} - \sum_{i=1}^{k}(T^{s_i}+T^{-s_i}) - \sum_{m=1}^{\ell}(T^{\alpha_m n}+T^{-\alpha_m n}))x = 0.$$

Let $\mathbf{e}_j = (0, \ldots, \underbrace{1}_{j-th}, \ldots, 0)$, $j = 1, \ldots, \beta n$. The (j,j)-th entry of $\mathbb{T}$ is equal to $\zeta_{\beta n}^{j-1}$. Then, for $j = 0, \ldots, \beta n - 1$, the matrix $\mathbb{L}$ has an eigenvalue

$$\lambda_j = L(\zeta_{\beta n}^{j}) = 2(k+\ell) - \sum_{i=1}^{k}(\zeta_{\beta n}^{js_i}+\zeta_{\beta n}^{-js_i}) - \sum_{m=1}^{\ell}(\zeta_{\beta}^{j\alpha_m}+\zeta_{\beta}^{-j\alpha_m}), \tag{4.1}$$

with eigenvector $\mathbf{e}_{j+1}$. Since all graphs under consideration are supposed to be connected, we have $\lambda_0 = 0$ and $\lambda_j > 0$, $j = 1, 2, \ldots, \beta n - 1$. Hence

$$\tau(n) = \frac{1}{\beta n}\prod_{j=1}^{\beta n-1} L(\zeta_{\beta n}^{j}). \tag{4.2}$$

By setting $j = \beta t + u$, where $0 \le t \le n-1$, $0 \le u \le \beta - 1$, we rewrite the formula (4.2) in the form

$$\tau(n) = (\frac{1}{n}\prod_{t=1}^{n-1} L(\zeta_{\beta n}^{\beta t}))(\frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{t=0}^{n-1} L(\zeta_{\beta n}^{t\beta+u})). \tag{4.3}$$

It is easy to see that $\tau(n)$ is the product of two numbers $\tau_1(n) = \frac{1}{n}\prod_{t=1}^{n-1} L(\zeta_{\beta n}^{\beta t})$ and $\tau_2(n) = \frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{t=0}^{n-1} L(\zeta_{\beta n}^{t\beta+u})$.

We note that

$$L(\zeta_{\beta n}^{\beta t}) = 2k - \sum_{i=1}^{k}(\zeta_{\beta n}^{\beta t s_i}+\zeta_{\beta n}^{-\beta t s_i}) = 2k - \sum_{i=1}^{k}(\zeta_{n}^{t s_i}+\zeta_{n}^{-t s_i}) = P(\zeta_n^t),\ 1 \le t \le n-1.$$

The numbers $\mu_t = P(\zeta_n^t)$, $1 \le t \le n-1$ run through all non-zero Laplacian eigenvalues of circulant graph $C_n(s_1, s_2, \ldots, s_k)$ with fixed jumps $s_1, s_2, \ldots, s_k$ and n vertices. So $\tau_1(n)$ coincide with the number of spanning trees in $C_n(s_1, s_2, \ldots, s_k)$. By ([23], Corollary 1) we get

$$\tau_1(n) = \frac{n}{q}\prod_{\substack{j=1,\\ w_j(0)\neq 1}}^{s_k} |2T_n(w_j(0)) - 2|, \tag{4.4}$$

where $w_j(0)$, $j = 1, 2, \ldots, s_k$, are all the roots of the equation $\sum_{i=1}^{k} T_{s_i}(w) = k$.

In order to continue the calculation of $\tau(n)$ we have to find the product

$$\tau_2(n) = \frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{t=0}^{n-1} L(\zeta_{\beta n}^{t\beta+u}).$$

Recall that $L(z) = P(z) + p(z^n)$. Since $(\zeta_{\beta n}^{\beta t+u})^n = \zeta_\beta^{\beta t+u} = \zeta_\beta^u$, we obtain

$$L(\zeta_{\beta n}^{\beta t+u}) = P(\zeta_{\beta n}^{\beta t+u}) + p(\zeta_\beta^{\beta t+u}) = P(\zeta_{\beta n}^{\beta t+u}) + p(\zeta_\beta^u) = P_u(\zeta_{\beta n}^{\beta t+u}),$$

where $P_u(z) = P(z) + p(\zeta_\beta^u)$. By Section 3, we already know that

$$P_u(z) = -\prod_{j=1}^{s_k}(z - z_j(u))(z - z_j(u)^{-1}),$$

where $w_j(u) = \frac{1}{2}(z_j(u) + z_j(u)^{-1})$, $j = 1, 2, \ldots, s_k$ are all roots of the equation $\sum_{i=1}^k T_{s_i}(w) = k + 2\sum_{d=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_d}{\beta})$.

We note that $\zeta_{\beta n}^{t\beta+u} = e^{\frac{i(2\pi t+\omega_u)}{n}}$, where $\omega_u = \frac{2\pi u}{\beta}$. Then $\prod_{t=0}^{n-1} L(\zeta_{\beta n}^{t\beta+u}) = \prod_{t=0}^{n-1} P_u(e^{\frac{i(2\pi t+\omega_u)}{n}})$. To evaluate the latter product, we need following lemma.

Lemma 4.2. *Let $H(z) = \prod_{s=1}^m (z - z_s)(z - z_s^{-1})$ and ω be a real number. Then*

$$\prod_{t=0}^{n-1} H(e^{\frac{i(2\pi t+\omega)}{n}}) = (-e^{i\omega})^m \prod_{s=1}^m (2T_n(w_s) - 2\cos(\omega)),$$

where $w_s = \frac{1}{2}(z_s + z_s^{-1})$, $s = 1, \ldots, m$ and $T_n(w)$ is the n-th Chebyshev polynomial of the first kind.

Proof of Lemma 4.2. We note that $\frac{1}{2}(z^n + z^{-n}) = T_n(\frac{1}{2}(z + z^{-1}))$. By the substitution $z = e^{i\,\varphi}$, this follows from the evident identity $\cos(n\varphi) = T_n(\cos\varphi)$. Then we have

$$\begin{aligned}
\prod_{t=0}^{n-1} H(e^{\frac{i(2\pi t+\omega)}{n}}) &= \prod_{t=0}^{n-1}\prod_{s=1}^{m}(e^{\frac{i(2\pi t+\omega)}{n}} - z_s)(e^{\frac{i(2\pi t+\omega)}{n}} - z_s^{-1}) \\
&= \prod_{s=1}^{m}\prod_{t=0}^{n-1}(-e^{\frac{i(2\pi t+\omega)}{n}} z_s^{-1})(z_s - e^{\frac{i(2\pi t+\omega)}{n}})(z_s - e^{-\frac{i(2\pi t+\omega)}{n}}) \\
&= \prod_{s=1}^{m}(-e^{i\omega} {z_s}^{-n}) \prod_{t=0}^{n-1}(z_s - e^{\frac{i(2\pi t+\omega)}{n}})(z_s - e^{-\frac{i(2\pi t+\omega)}{n}}) \\
&= \prod_{s=1}^{m}(-e^{i\omega} {z_s}^{-n})(z_s^{2n} - 2\cos(\omega) z_s^n + 1) \\
&= \prod_{s=1}^{m}(-e^{i\omega})(2\,\frac{z_s^n + z_s^{-n}}{2} - 2\cos(\omega)) \\
&= (-e^{i\omega})^m \prod_{s=1}^{m}(2T_n(w_s) - 2\cos(\omega)).
\end{aligned}$$

□

Since $P_u(z) = -H_u(z)$, where $H_u(z) = \prod_{j=1}^{s_k}(z - z_j(u))(z - z_j(u)^{-1})$, by Lemma 4.2 we get

$$\prod_{t=0}^{n-1} P_u(e^{\frac{i(2\pi t+\omega_u)}{n}}) = (-1)^n(-e^{\frac{2\pi\, i\, u}{\beta}})^{s_k}\prod_{j=1}^{s_k}(2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})).$$

Then,

$$\begin{aligned}\tau_2(n) &= \frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{t=0}^{n-1} L(\zeta_{\beta n}^{\beta t+u}) = \frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{t=0}^{n-1} P_u(e^{\frac{i(2\pi j+\omega_u)}{n}})\\ &= \frac{(-1)^{n(\beta-1)}}{\beta}\prod_{u=1}^{\beta-1}(-e^{\frac{2\pi\, i\, u}{\beta}})^{s_k}\prod_{j=1}^{s_k}(2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})) \qquad (4.5)\\ &= \frac{(-1)^{n(\beta-1)}}{\beta}\prod_{u=1}^{\beta-1}\prod_{j=1}^{s_k}(2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})).\end{aligned}$$

Since the number $\tau_2(n)$ is a product of positive eigenvalues of G_n divided by β, from (4.5) we have

$$\tau_2(n) = \frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{j=1}^{s_k}|2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})|. \qquad (4.6)$$

Combining Equations (4.4) and (4.6) we finish the proof of the theorem. □

As the first consequence from Theorem 4.1 we have the following result obtained earlier by Justine Louis [19] in a slightly different form.

Corollary 4.3. *The number of spanning trees in the circulant graphs with non-fixed jumps* $C_{\beta n}(1, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$, *where* $1 \le \alpha_1 < \alpha_2 < \ldots < \alpha_\ell \le [\frac{\beta}{2}]$ *is given by the formula*

$$\tau(n) = \frac{n\, 2^{\beta-1}}{\beta}\prod_{u=1}^{\beta-1}(T_n(1 + 2\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_m}{\beta})) - \cos(\frac{2\pi\, u}{\beta})),$$

where $T_n(w)$ *is the Chebyshev polynomial of the first kind.*

Proof. Follows directly from the theorem. □

The next corollary is new.

Corollary 4.4. *The number of spanning trees in the circulant graphs with non-fixed jumps* $C_{\beta n}(1, 2, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$, *where* $1 \le \alpha_1 < \alpha_2 < \ldots < \alpha_\ell \le [\frac{\beta}{2}]$ *is given by the formula*

$$\tau(n) = \frac{nF_n^2}{\beta}\prod_{u=1}^{\beta-1}\prod_{j=1}^{2}|2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})|,$$

where F_n *is the* n*-th Fibonacci number,* $T_n(w)$ *is the Chebyshev polynomial of the first kind and* $w_{1,2}(u) = \left(-1 \pm \sqrt{25 + 16\sum_{m=1}^{\ell}\sin^2(\frac{\pi\, u\, \alpha_m}{\beta})}\right)/4.$

We note that nF_n^2 is the number of spanning trees in the graph $C_n(1,2)$.

Proof. In this case, $k = 2$, $s_1 = 1$, $s_2 = 2$ and $q = s_1^2 + s_2^2 = 5$. Given u we find $w_j(u)$, $j = 1,2$ as the roots of the algebraic equation

$$T_1(w) + T_2(w) = 2 + 2\sum_{m=1}^{\ell} \sin^2(\frac{\pi\, u\, \alpha_m}{\beta}),$$

where $T_1(w) = w$ and $T_2(w) = 2w^2 - 1$. For $u = 0$ the roots are $w_1(0) = 1$ and $w_2(0) = -3/2$. Hence, by (4.4), $\tau_1(n) = \frac{n}{5}|2T_n(-\frac{3}{2}) - 2| = \frac{n}{5}|(\frac{-3+\sqrt{5}}{2})^n + (\frac{-3-\sqrt{5}}{2})^n - 2| = nF_n^2$ gives the well-known formula for the number of spanning trees in the graph $C_n(1,2)$. (See, for example, [2], Theorem 4). For $u > 0$ the numbers $w_1(u)$ and $w_2(u)$ are roots of the quadratic equation

$$2w^2 + w - 3 - 2\sum_{m=1}^{\ell} \sin^2(\frac{\pi\, u\, \alpha_m}{\beta}) = 0.$$

By (4.6) we get $\tau_2(n) = \frac{1}{\beta}\prod_{u=1}^{\beta-1}\prod_{j=1}^{2}|2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})|$. Since $\tau(n) = \tau_1(n)\tau_2(n)$, the result follows. □

5 Arithmetic properties of the complexity for circulant graphs

It was noted in the series of paper [14, 22, 23, 25] that in many important cases the complexity of graphs is given by the formula $\tau(n) = p\, n\, a(n)^2$, where $a(n)$ is an integer sequence and p is a prescribed constant depending only on parity of n.

The aim of the next theorem is to explain this phenomena for circulant graphs with non-fixed jumps. Recall that any positive integer p can be uniquely represented in the form $p = q\, r^2$, where p and q are positive integers and q is square-free. We will call q the *square-free part* of p.

Theorem 5.1. *Let $\tau(n)$ be the number of spanning trees of the circulant graph*

$$G_n = C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n),$$

where $1 \le s_1 < s_2 < \ldots < s_k < [\frac{\beta n}{2}]$, $1 \le \alpha_1 < \alpha_2 < \ldots, \alpha_\ell \le [\frac{\beta}{2}]$.

Denote by p and q the number of odd elements in the sequences $s_1, s_2, \ldots, s_k$ and $\alpha_1, \alpha_2, \ldots, \alpha_\ell$, respectively. Let r be the square-free part of p and s be the square-free part of p + q. Then there exists an integer sequence $a(n)$ such that

1^0 $\tau(n) = \beta\, n\, a(n)^2$, *if n and β are odd;*

2^0 $\tau(n) = \beta\, r\, n\, a(n)^2$, *if n is even;*

3^0 $\tau(n) = \beta\, s\, n\, a(n)^2$, *if n is odd and β is even.*

Proof. The number of odd elements in the sequences $s_1, s_2, \ldots, s_k$ and $\alpha_1, \alpha_2, \ldots, \alpha_\ell$, respectively is counted by the formulas $p = \sum_{i=1}^{k} \frac{1-(-1)^{s_i}}{2}$ and $q = \sum_{i=1}^{\ell} \frac{1-(-1)^{\alpha_i}}{2}$. We already know that all non-zero Laplacian eigenvalues of the graph G_n are given by the formulas $\lambda_j = L(\zeta_{\beta n}^j)$, $j = 1, \ldots, \beta n - 1$, where $\zeta_{\beta n} = e^{\frac{2\pi i}{\beta n}}$ and

$$L(z) = 2(k+l) - \sum_{i=1}^{k}(z^{s_i} + z^{-s_i}) - \sum_{m=1}^{\ell}(z^{n\alpha_m} + z^{-n\alpha_m}).$$

We note that $\lambda_{\beta n-j} = L(\zeta_{\beta n}^{\beta n-j}) = L(\zeta_{\beta n}^{j}) = \lambda_j$.

By the Kirchhoff theorem we have $\beta n\,\tau(n) = \prod_{j=1}^{\beta n-1}\lambda_j$. Since $\lambda_{\beta n-j} = \lambda_j$, we obtain $\beta n\,\tau(n) = (\prod_{j=1}^{\frac{\beta n-1}{2}}\lambda_j)^2$ if βn is odd and $\beta n\,\tau(n) = \lambda_{\frac{\beta n}{2}}(\prod_{j=1}^{\frac{\beta n}{2}-1}\lambda_j)^2$ if βn is even. We note that each algebraic number λ_j comes into the above products together with all its Galois conjugate [18]. So, the numbers $c(n) = \prod_{j=1}^{\frac{\beta n-1}{2}}\lambda_j$ and $d(n) = \prod_{j=1}^{\frac{\beta n}{2}-1}\lambda_j$ are integers. Also, for even n we have

$$\lambda_{\frac{\beta n}{2}} = L(-1) = 2(k+l) - \sum_{i=1}^{k}((-1)^{s_i} + (-1)^{-s_i}) - \sum_{m=1}^{\ell}((-1)^{n\alpha_m} + (-1)^{-n\alpha_m})$$
$$= 2k - \sum_{i=1}^{k}((-1)^{s_i} + (-1)^{-s_i}) = 4\sum_{i=1}^{k}\frac{1-(-1)^{s_i}}{2} = 4p.$$

If n is odd and β is even, the number $\frac{\beta n}{2}$ is integer again. Then we obtain

$$\lambda_{\frac{\beta n}{2}} = L(-1) = 2(k+l) - \sum_{i=1}^{k}((-1)^{s_i} + (-1)^{-s_i}) - \sum_{m=1}^{\ell}((-1)^{\alpha_m} + (-1)^{-\alpha_m})$$
$$= 4\sum_{i=1}^{k}\frac{1-(-1)^{s_i}}{2} + 4\sum_{m=1}^{\ell}\frac{1-(-1)^{\alpha_m}}{2} = 4p + 4q.$$

Therefore, $\beta\, n\,\tau(n) = c(n)^2$ if β and n are odd, $\beta\, n\,\tau(n) = 4p\,d(n)^2$ if n is even and $\beta\, n\,\tau(n) = 4(p+q)\,d(n)^2$ if n is odd and β is even. Let r be the square-free part of p and s be the square-free part of $p+q$. Then there are integers u and v such that $p = ru^2$ and $s = (p+q)v^2$. Hence,

1° $\dfrac{\tau(n)}{\beta\, n} = \left(\dfrac{c(n)}{\beta\, n}\right)^2$ if n and β are odd,

2° $\dfrac{\tau(n)}{\beta\, n} = r\left(\dfrac{2\,u\,d(n)}{\beta\, n}\right)^2$ if n is even and

3° $\dfrac{\tau(n)}{\beta\, n} = s\left(\dfrac{2\,v\,d(n)}{\beta\, n}\right)^2$ if n is odd and β is even.

Consider an automorphism group $\mathbb{Z}_{\beta n} = \langle g\rangle$ of the graph G_n generated by the element g circularly permuting vertices $v_0, v_1, \ldots, v_{\beta\, n-1}$ by the rule $v_i \to v_{i+1}$ and the addition in the indices is done modulo βn. The action of such a group is uniquely defined on the set of all edges of G_n, except for those that connect diametrically opposite vertices. Consider separately two cases $\alpha_\ell = \beta/2$ and $\alpha_\ell < \beta/2$.

In the first case, we have two parallel edges between the diametrically opposite vertices v_i and $v_{i+\frac{\beta\, n}{2}}$, where the indices are taken mod $\beta\, n$. To distinguish them, we orient one of this edges by the arrow from v_i and $v_{i+\frac{\beta\, n}{2}}$ and the other one by the arrow from $v_{i+\frac{\beta\, n}{2}}$ to v_i. As a result, we get exactly $\beta\, n$ oriented edges. Denote the edge oriented from $v_{i+\frac{\beta\, n}{2}}$ to v_i by e_i and define the action of g on such edges by the rule $e_i \to e_{i+1}$, where i is taken $\bmod\ \beta\, n$.

In the second case, we have $\alpha_\ell < \frac{\beta}{2}$ and $s_k < \frac{\beta n}{2}$. Therefore, all jumps $\alpha_1 n, \ldots, \alpha_\ell n$ and $s_1, \ldots, s_k$ of the graph G_n are strictly less then $\frac{\beta n}{2}$ and G_n has no edges between the diametrically opposite edges. That is, the action of group $\mathbb{Z}_{\beta n}$ is well defined on its edges.

So, one can conclude that group $\mathbb{Z}_{\beta n}$ acts fixed point free on the set vertices and on the set of edges of G_n.

We are aimed to show that it also acts freely on the set of the spanning trees in the graph. Indeed, suppose that some non-trivial element γ of $\mathbb{Z}_{\beta n}$ leaves a spanning tree A in the graph G_n invariant. Then γ fixes the center of A. The center of a tree is a vertex or an edge. The first case is impossible, since γ acts freely on the set of vertices. In the second case, γ permutes the endpoints of an edge connecting the opposite vertices of G_n. This means that $\beta\, n$ is even, and γ is the unique involution in the group $\mathbb{Z}_{\beta n}$. This is also impossible, since the group is acting without fixed edges.

So, the cyclic group $\mathbb{Z}_{\beta n}$ acts on the set of spanning trees of the graph G_n fixed point free. Therefore $\tau(n)$ is a multiple of $\beta\, n$ and their quotient $\frac{\tau(n)}{\beta\, n}$ is an integer.

Setting $a(n) = \frac{c(n)}{\beta\, n}$ in the case 1°, $a(n) = \frac{2\, u\, d(n)}{\beta\, n}$ in the case 2° and $a(n) = \frac{2\, v\, d(n)}{\beta\, n}$ in the case 3° we conclude that number $a(n)$ is always integer and the statement of the theorem follows. □

6 Asymptotic for the number of spanning trees

In this section, we give asymptotic formulas for the number of spanning trees for circulant graphs. It is interesting to compare these results with those in papers [5, 8, 17, 19, 37], where the similar results were obtained by different methods.

Theorem 6.1. *Let* $\gcd(s_1, s_2, \ldots, s_k) = d$ *and* $\gcd(\alpha_1, \alpha_2, \ldots, \alpha_\ell, \beta) = 1$. *Then the number of spanning trees in the circulant graph*

$$C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n),$$
$$1 \le s_1 < s_2 < \ldots < s_k < [\frac{\beta n}{2}],\ 1 \le \alpha_1 < \alpha_2 < \ldots < \alpha_\ell \le [\frac{\beta}{2}],$$

has the following asymptotic

$$\tau(n) \sim \frac{n\, d^2}{\beta\, q} A^n,\ \textit{as } n \to \infty \textit{ and } (n, d) = 1,$$

where $q = s_1^2 + s_2^2 + \ldots + s_k^2$, $A = \prod_{u=0}^{\beta-1} M(P_u)$ *and* $M(P_u) = \exp(\int_0^1 \log |P_u(e^{2\pi i t})| dt)$ *is the Mahler measure of Laurent polynomial*

$$P_u(z) = 2k - \sum_{i=1}^{k} (z^{s_i} + z^{-s_i}) + 4 \sum_{m=1}^{\ell} \sin^2(\frac{\pi u \alpha_m}{\beta}).$$

Proof. By Theorem 4.1, $\tau(n) = \tau_1(n)\tau_2(n)$, where $\tau_1(n)$ is the number of spanning trees in $C_n(s_1, s_2, \ldots, s_k)$ and $\tau_2(n) = \frac{1}{\beta} \prod_{u=1}^{\beta-1} \prod_{j=1}^{s_k} |2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})|$. By ([23], Theorem 5) we already know that

$$\tau_1(n) \sim \frac{n\, d^2}{q} A_0^n,\ \text{as } n \to \infty \text{ and } (n, d) = 1,$$

where A_0 is the Mahler measure of Laurent polynomial $P_0(z)$. So, we have to find asymptotics for $\tau_2(n)$ only.

By Lemma 3.1, for any integer u, $0 < u < \beta$ we obtain $T_n(w_j(u)) = \frac{1}{2}(z_j(u)^n + z_j(u)^{-n})$, where the $z_j(u)$ and $1/z_j(u)$ are roots of the polynomial $P_u(z)$ satisfying the inequality $|z_j(u)| \neq 1$, $j = 1, 2, \ldots, s_k$. Replacing $z_j(u)$ by $1/z_j(u)$, if necessary, we can assume that $|z_j(u)| > 1$ for all $j = 1, 2, \ldots, s_k$. Then $T_n(w_j(u)) \sim \frac{1}{2} z_j(u)^n$, as n tends to ∞. So $|2T_n(w_j(u)) - 2\cos(\frac{2\pi u}{\beta})| \sim |z_j(u)|^n,\ n \to \infty$. Hence

$$\prod_{j=1}^{s_k} |2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})| \sim \prod_{s=1}^{s_k} |z_j(u)|^n = \prod_{P_u(z)=0,\, |z|>1} |z|^n = A_u^n,$$

where $A_u = \prod_{P_u(z)=0,\, |z|>1} |z|$ coincides with the Mahler measure of $P_u(z)$. As a result,

$$\tau_2(n) = \frac{1}{\beta} \prod_{u=1}^{\beta-1} \prod_{j=1}^{s_k} |2T_n(w_j(u)) - 2\cos(\frac{2\pi\, u}{\beta})| \sim \frac{1}{\beta} \prod_{u=1}^{\beta-1} A_u^n.$$

Finally, $\tau(n) = \tau_1(n)\tau_2(n) \sim \frac{n\, d^2}{\beta\, q} \prod_{u=0}^{\beta-1} A_u^n$, as $n \to \infty$ and $(n, d) = 1$. Since $A_u = M(P_u)$, the result follows. □

As an immediate consequence of above theorem we have the following result obtained earlier in ([8], Theorem 3) by completely different methods.

Corollary 6.2. *The thermodynamic limit of the sequence* $C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n)$ *of circulant graphs is equal to the arithmetic mean of small Mahler measures of Laurent polynomials* $P_u(z)$, $u = 0, 1, \ldots, \beta - 1$. *More precisely,*

$$\lim_{n\to\infty} \frac{\log \tau(C_{\beta n}(s_1, s_2, \ldots, s_k, \alpha_1 n, \alpha_2 n, \ldots, \alpha_\ell n))}{\beta\, n} = \frac{1}{\beta} \sum_{u=0}^{\beta-1} m(P_u),$$

where $m(P_u) = \int_0^1 \log |P_u(e^{2\pi i t})| dt$ *and* $P_u(z) = 2k - \sum_{i=1}^{k} (z^{s_i} + z^{-s_i}) + 4\sum_{m=1}^{\ell} \sin^2(\frac{\pi\, u\, \alpha_m}{\beta})$.

7 Examples

1. **Graph** $C_{2n}(1, n)$. (Möbius ladder with double steps). By Theorem 4.1, we have $\tau(n) = \tau(C_{2n}(1, n)) = n\,(T_n(3) + 1)$. Compare this result with ([38], Theorem 4). Recall [2] that the number of spanninig trees in the Möbius ladder with single steps is given by the formula $n\,(T_n(2) + 1)$.

2. **Graph** $C_{2n}(1, 2, n)$. We have $\tau(n) = 2nF_n^2 |T_n(\frac{-1-\sqrt{41}}{4}) - 1||T_n(\frac{-1+\sqrt{41}}{4}) - 1|$. By Theorem 5.1, one can find an integer sequence $a(n)$ such that $\tau(n) = 2n\, a(n)^2$ if n is even and $\tau(n) = na(n)^2$ if n is odd.

3. **Graph** $C_{2n}(1, 2, 3, n)$. Here $\tau(n) = \frac{8n}{7}(T_n(\theta_1) - 1)(T_n(\theta_2) - 1)\prod_{p=1}^{3}(T_n(\omega_p) + 1)$, where $\theta_1 = \frac{-3+\sqrt{-7}}{4}$, $\theta_2 = \frac{-3-\sqrt{-7}}{4}$ and ω_p, $p = 1, 2, 3$ are roots of the cubic equation $2w^3 + w^2 - w - 3 = 0$. We have $\tau(n) = 6na(n)^2$ is n is odd and $\tau(n) = 4n\, a(n)^2$ is n is even. Also, $\tau(n) \sim \frac{n}{28} A^n$, $n \to \infty$, where $A \approx 42.4038$.

4. **Graph** $C_{3n}(1, n)$. We have

$$\tau(n) = \frac{n}{3}(2\,T_n(\frac{5}{2}) + 1)^2 = \frac{n}{3}((\frac{5+\sqrt{21}}{2})^n + (\frac{5-\sqrt{21}}{2})^n + 1)^2.$$

See also ([38], Theorem 5). We note that $\tau(n) = 3n\,a(n)^2$, where $a(n)$ satisfies the recursive relation $a(n) = 6a(n-1) - 6a(n-2) + a(n-3)$ with initial data $a(1) = 2$, $a(2) = 8$, $a(3) = 37$.

5. **Graph** $C_{3n}(1, 2, n)$. By Theorem 4.1, we obtain

$$\tau(n) = \frac{n}{3}F_n^2(2\,T_n(\omega_1) + 1)^2(2\,T_n(\omega_2) + 1)^2,$$

where $\omega_1 = \frac{-1+\sqrt{37}}{4}$ and $\omega_2 = \frac{-1-\sqrt{37}}{4}$. By Theorem 5.1, $\tau(n) = 3n\,a(n)^2$ for some integer sequence $a(n)$.

6. **Graph** $C_{6n}(1, n, 3n)$. Now, we get

$$\tau(n) = \frac{n}{3}(2\,T_n(\frac{5}{2}) + 1)^2(2\,T_n(\frac{7}{2}) - 1)^2(T_n(5) + 1).$$

For a suitable integer sequence $a(n)$, one has $\tau(n) = 6n\,a(n)^2$ if n is even and $\tau(n) = 18n\,a(n)^2$ if n is odd.

7. **Graph** $C_{12n}(1, 3n, 4n)$. In this case

$$\tau(n) = \frac{2n}{3}T_n(2)^2(2\,T_n(\frac{5}{2}) + 1)^2(T_n(3) + 1)(4\,T_n(\frac{7}{2})^2 - 3)^2(2\,T_n(\frac{9}{2}) - 1)^2.$$

By Theorem 5.1, one can conclude that $\tau(n) = 3n\,a(n)^2$ if n is even and $\tau(n) = 6n\,a(n)^2$ if n is odd, for some sequence $a(n)$ of even numbers.

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On generalized Minkowski arrangements*

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Abstract

The concept of a Minkowski arrangement was introduced by Fejes Tóth in 1965 as a family of centrally symmetric convex bodies with the property that no member of the family contains the center of any other member in its interior. This notion was generalized by Fejes Tóth in 1967, who called a family of centrally symmetric convex bodies a generalized Minkowski arrangement of order μ for some $0 < \mu < 1$ if no member K of the family overlaps the homothetic copy of any other member K' with ratio μ and with the same center as K'. In this note we prove a sharp upper bound on the total area of the elements of a generalized Minkowski arrangement of order μ of finitely many circular disks in the Euclidean plane. This result is a common generalization of a similar result of Fejes Tóth for Minkowski arrangements of circular disks, and a result of Böröczky and Szabó about the maximum density of a generalized Minkowski arrangement of circular disks in the plane. In addition, we give a sharp upper bound on the density of a generalized Minkowski arrangement of homothetic copies of a centrally symmetric convex body.

Keywords: Arrangement, Minkowski arrangement, density, homothetic copy.

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1 Introduction

The notion of a *Minkowski arrangement* of convex bodies was introduced by L. Fejes Tóth in [6], who defined it as a family $\mathcal{F}$ of centrally symmetric convex bodies in the d-dimensional Euclidean space $\mathbb{R}^d$, with the property that no member of $\mathcal{F}$ contains the center of any other member of $\mathcal{F}$ in its interior. He used this concept to show, in particular, that the density of a Minkowski arrangement of homothets of any given plane convex body with positive homogeneity is at most four. Here an arrangement is meant to have positive homogeneity if the set of the homothety ratios is bounded from both directions by positive constants. It is worth mentioning that the above result is a generalization of the planar case of the famous Minkowski Theorem from lattice geometry [11]. Furthermore, Fejes Tóth proved in [6] that the density of a Minkowski arrangement of circular disks in $\mathbb{R}^2$ with positive homogeneity is maximal for a Minkowski arrangement of congruent circular disks whose centers are the points of a hexagonal lattice and each disk contains the centers of six other members on its boundary.

In [7], extending the investigation to finite Minkowski arrangements, Fejes Tóth gave a sharp upper bound on the total area of the members of a Minkowski arrangement of finitely many circular disks, and showed that this result immediately implies the density estimate in [6] for infinite Minkowski circle-arrangements. Following a different direction, in [8] for any $0 < \mu < 1$ Fejes Tóth defined a *generalized Minkowski arrangements of order* μ as a family $\mathcal{F}$ of centrally symmetric convex bodies with the property that for any two distinct members K, K' of $\mathcal{F}$, K does not overlap the μ-*core* of K', defined as the homothetic copy of K' of ratio μ and concentric with K'. In this paper he made the conjecture that for any $0 < \mu \leq \sqrt{3} - 1$, the density of a generalized Minkowski arrangement of circular disks with positive homogeneity is maximal for a generalized Minkowski arrangement of congruent disks whose centers are the points of a hexagonal lattice and each disk touches the μ-core of six other members of the family. According to [8], this conjecture was verified by Böröczky and Szabó in a seminar talk in 1965, though the first written proof seems to be published only in [4] in 2002. It was observed both in [8] and [4] that if $\sqrt{3} - 1 < \mu < 1$, then, since the above hexagonal arrangement does not cover the plane, that arrangement has no maximal density.

In this paper we prove a sharp estimate on the total area of a generalized Minkowski arrangement of finitely many circular disks, with a characterization of the equality case. Our result includes the result in [7] as a special case, and immediately implies the one in [4]. The proof of our statement relies on tools from both [4, 7], but uses also some new ideas. In addition, we also generalize a result from Fejes Tóth [6] to find a sharp upper bound on the density of a generalized Minkowski arrangement of homothetic copies of a centrally symmetric convex body.

For completeness, we mention that similar statements for (generalized) Minkowski arrangements in other geometries and in higher dimensional spaces were examined, e.g. in [5, 9, 13]. Minkowski arrangements consisting of congruent convex bodies were considered in [3]. Estimates for the maximum cardinality of mutually intersecting members in a (generalized) Minkowski arrangement can be found in [10, 14, 15, 17]. The problem investigated in this paper is similar in nature to those dealing with the volume of the convex hull of a family of convex bodies, which has a rich literature. This includes a result of Oler [16] (see also [2]), which is also of lattice geometric origin [20], and the notion of parametric density of Betke, Henk and Wills [1]. In particular, our problem is closely related to the notion of density with respect to outer parallel domains defined in [2]. Applications of (generalized) Minkowski arrangements in other branches of mathematics can be found in [18, 19].

As a preliminary observation, we start with the following generalization of Remark 2 of [6], stating the same property for (not generalized) Minkowski arrangements of plane convex bodies. In Proposition 1.1, by $\mathrm{vol}_d(\cdot)$ we denote d-dimensional volume, and by $\mathbf{B}^d$ we denote the closed Euclidean unit ball centered at the origin.

Proposition 1.1. *Let* $0 < \mu < 1$, *let* $K \subset \mathbb{R}^d$ *be an origin-symmetric convex body and let* $\mathcal{F} = \{x_1 + \lambda_1 K, x_2 + \lambda_2 K, \dots\}$ *be a generalized Minkowski arrangement of order* μ, *where* $x_i \in \mathbb{R}^d, \lambda_i > 0$ *for each* $i = 1, 2, \dots$. *Assume that* $\mathcal{F}$ *is of positive homogeneity, that is, there are constants* $0 < C_1 < C_2$ *satisfying* $C_1 \leq \lambda_i \leq C_2$ *for all values of* i, *and define the (upper) density* $\delta(\mathcal{F})$ *of* $\mathcal{F}$ *in the usual way as*

$$\delta(\mathcal{F}) = \limsup_{R \to \infty} \frac{\sum_{x_i \in R\mathbf{B}^d} \mathrm{vol}_d(x_i + \lambda_i K)}{\mathrm{vol}_d(R\mathbf{B}^d)},$$

if it exists. Then

$$\delta(\mathcal{F}) \leq \frac{2^d}{(1+\mu)^d}, \tag{1.1}$$

where equality is attained, e.g. if $\{x_1, x_2, \dots\}$ *is a lattice with* K *as its fundamental region, and* $\lambda_i = 2/(1+\mu)$ *for all values of* i.

Proof. Note that the equality part of Proposition 1.1 clearly holds, and thus, we prove only the inequality in (1.1). Let $||\cdot||_K : \mathbb{R}^d \to [0, \infty)$ denote the norm with K as its unit ball. Then, by the definition of a generalized Minkowski arrangement, we have

$$\begin{aligned} ||x_i - x_j||_K &\geq \max\{\lambda_i + \mu\lambda_j, \lambda_j + \mu\lambda_i\} \\ &\geq \frac{1}{2}\left((\lambda_i + \mu\lambda_j) + (\lambda_j + \mu\lambda_i)\right) \\ &= \frac{1+\mu}{2}(\lambda_i + \lambda_j), \end{aligned}$$

implying that the homothets $x_i + (\lambda_i/2) \cdot (1+\mu)\, K$ are pairwise non-overlapping. In other words, the family $\mathcal{F}' = \{x_i + (\lambda_i/2) \cdot (1+\mu)\, K : i = 1, 2, \dots\}$ is a packing. Thus, the density of $\mathcal{F}'$ is at most one, from which (1.1) readily follows. Furthermore, if K is the fundamental region of a lattice formed by the x_i's and $\lambda_i = 2/(1+\mu)$ for all values of i, then $\mathcal{F}'$ is a tiling, implying the equality case. □

Following the terminology of Fejes Tóth in [7] and to permit a simpler formulation of our main result, in the remaining part of the paper we consider generalized Minkowski arrangements of *open* circular disks, where we note that generalized Minkowski arrangements can be defined for families of open circular disks in the same way as for families of closed circular disks.

To state our main result, we need some preparation, where we denote the boundary of a set by $\mathrm{bd}(\cdot)$. Consider some generalized Minkowski arrangement $\mathcal{F} = \{B_i = x_i + \rho_i \,\mathrm{int}(\mathbf{B}^2) : i = 1, 2, \dots, n\}$ of open circular disks in $\mathbb{R}^2$ of order μ, where $0 < \mu < 1$. Set $U(\mathcal{F}) = \bigcup_{i=1}^n B_i = \bigcup \mathcal{F}$. Then each circular arc Γ in $\mathrm{bd}(U(\mathcal{F}))$ corresponds to a circular sector, which can be obtained as the union of the segments connecting a point of Γ to the center of the disk in $\mathcal{F}$ whose boundary contains Γ. We call the union of these circular sectors the *outer shell* of $\mathcal{F}$. Now consider a point $p \in \mathrm{bd}(U(\mathcal{F}))$ belonging to at least two members of $\mathcal{F}$, say B_i and B_j, such that x_i, x_j and p are not collinear. Assume that the convex angular region bounded by the two closed half lines starting at p and passing through x_i and x_j, respectively, do not contain the center of another element of $\mathcal{F}$ in its interior which contains p on its boundary. We call the union of the triangles $\mathrm{conv}\{p, x_i, x_j\}$ satisfying these conditions the *inner shell* of $\mathcal{F}$. We denote the inner and the outer shell of $\mathcal{F}$ by $I(\mathcal{F})$ and $O(\mathcal{F})$, respectively. Finally, we call the set $C(\mathcal{F}) = U(\mathcal{F}) \setminus (I(\mathcal{F}) \cup O(\mathcal{F}))$ the *core* of $\mathcal{F}$ (cf. Figure 1). Clearly, the outer shell of any generalized Minkowski arrangement of open circular disks is nonempty, but there are arrangements for which $I(\mathcal{F}) = \emptyset$ or $C(\mathcal{F}) = \emptyset$.

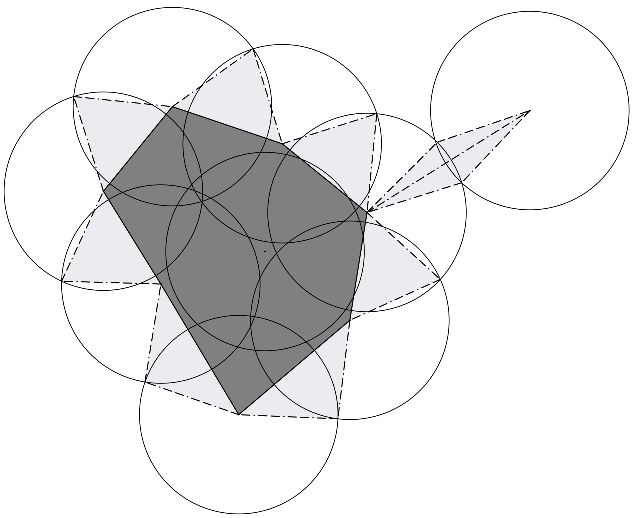

Figure 1: The outer and inner shell, and the core of an arrangement, shown in white, light grey and dark grey, respectively.

If the intersection of two members of $\mathcal{F}$ is nonempty, then we call this intersection a *digon*. If a digon touches the μ-cores of both disks defining it, we call the digon *thick*. A digon which is not contained in a third member of $\mathcal{F}$ is called a *free digon*. Our main theorem is as follows, where $\mathrm{area}(X)$ denotes the area of the set X.

Theorem 1.2. *Let* $0 < \mu \leq \sqrt{3} - 1$*, and let* $\mathcal{F} = \{B_i = x_i + \rho_i \,\mathrm{int}(\mathbf{B}^2) : i = 1, 2, \ldots, n\}$ *be a generalized Minkowski arrangement of finitely many open circular disks of order* μ*. Then*

$$T = \pi \sum_{i=1}^{n} \rho_i^2 \leq \frac{2\pi}{\sqrt{3}(1+\mu)^2} \,\mathrm{area}(C(\mathcal{F})) + \\ + \frac{4 \cdot \arccos(\frac{1+\mu}{2})}{(1+\mu) \cdot \sqrt{(3+\mu)(1-\mu)}} \,\mathrm{area}(I(\mathcal{F})) + \mathrm{area}(O(\mathcal{F})),$$

where T is the total area of the circles, with equality if and only if each free digon in $\mathcal{F}$ is thick.

In the paper, for any points $x, y, z \in \mathbb{R}^2$, we denote by $[x, y]$ the closed segment with endpoints x, y, by $[x, y, z]$ the triangle $\operatorname{conv}\{x, y, z\}$, by $|x|$ the Euclidean norm of x, and if x and z are distinct from y, by $\angle xyz$ we denote the measure of the angle between the closed half lines starting at y and passing through x and z. Note that according to our definition, $\angle xyz$ is at most π for any $x, z \neq y$. For brevity we call an open circular disk a *disk*, and a generalized Minkowski arrangement of disks of order μ a *μ-arrangement*. Throughout Sections 2 and 3 we assume that $0 < \mu \leq \sqrt{3} - 1$.

In Section 2, we prove some preliminary lemmas. In Section 3, we prove Theorem 1.2. Finally, in Section 4, we collect additional remarks and questions.

2 Preliminaries

For any $B_i, B_j \in \mathcal{F}$, if $B_i \cap B_j \neq \emptyset$, we call the two intersection points of $\operatorname{bd}(B_i)$ and $\operatorname{bd}(B_j)$ the *vertices* of the digon $B_i \cap B_j$.

First, we recall the following lemma of Fejes Tóth [7, Lemma 2]. To prove it, we observe that for any $\mu > 0$, a generalized Minkowski arrangement of order μ is a Minkowski arrangement as well.

Lemma 2.1. *Let $B_i, B_j, B_k \in \mathcal{F}$ such that the digon $B_i \cap B_j$ is contained in B_k. Then the digon $B_i \cap B_k$ is free (with respect to $\mathcal{F}$).*

From now on, we call the maximal subfamilies $\mathcal{F}'$ of $\mathcal{F}$ (with respect to containment) with the property that $\bigcup_{B_i \in \mathcal{F}'} B_i$ is connected the *connected components* of $\mathcal{F}$. Our next lemma has been proved by Fejes Tóth in [7] for Minkowski arrangements of order $\mu = 0$. His argument can be applied to prove Lemma 2.2 for an arbitrary value of μ. Here we include this proof for completeness.

Lemma 2.2. *If $\mathcal{F}'$ is a connected component of $\mathcal{F}$ in which each free digon is thick, then the elements of $\mathcal{F}'$ are congruent.*

Proof. We need to show that for any $B_i, B_j \in \mathcal{F}'$, B_i and B_j are congruent. Observe that by connectedness, we may assume that $B_i \cap B_j$ is a digon. If $B_i \cap B_j$ is free, then it is thick, which implies that B_i and B_j are congruent. If $B_i \cap B_j$ is not free, then there is a disk $B_k \in \mathcal{F}'$ containing it. By Lemma 2.1, the digons $B_i \cap B_k$ and $B_j \cap B_k$ are free. Thus B_k is congruent to both B_i and B_j. □

In the remaining part of Section 2, we examine densities of some circular sectors in certain triangles. The computations in the proofs of these lemmas were carried out by a Maple 18.00 software.

Lemma 2.3. *Let $0 < \gamma < \pi$ and $A, B > 0$ be arbitrary. Let $T = [x, y, z]$ be a triangle such that $\angle xzy = \gamma$, and $|x - z| = A$ and $|y - z| = B$. Let $\Delta = \Delta(\gamma, A, B)$, $\alpha = \alpha(\gamma, A, B)$ and $\beta = \beta(\gamma, A, B)$ denote the functions with variables γ, A, B whose values are the area and the angles of T at x and y, respectively, and set $f_{A,B}(\gamma) = \left(\alpha A^2 + \beta B^2\right)/\Delta$. Then, for any $A, B > 0$, the function $f_{A,B}(\gamma)$ is strictly decreasing on the interval $\gamma \in (0, \pi)$.*

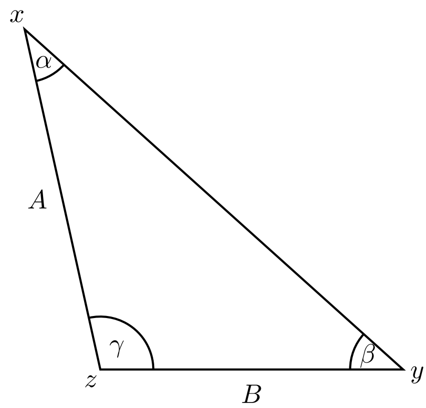

Figure 2: Notation in Lemma 2.3.

Proof. Without loss of generality, assume that $A \leq B$, and let $g = \alpha A^2 + \beta B^2$. Then, by an elementary computation, we have that

$$g = A^2 \operatorname{arccot} \frac{A - B\cos\gamma}{B \sin\gamma} + B^2 \operatorname{arccot} \frac{B - A\cos\gamma}{A\sin\gamma}, \text{ and } \Delta = \frac{1}{2} AB \sin\gamma.$$

We regard g and Δ as functions of γ. We intend to show that $g'\Delta - g\Delta'$ is negative on the interval $(0, \pi)$ for all $A, B > 0$. Let $h = g' \cdot \Delta/\Delta' - g$, and note that this expression is continuous on $(0, \pi/2)$ and $(\pi/2, \pi)$ for all $A, B > 0$. By differentiating and simplifying, we obtain

$$h' = \frac{-2\left(A^2(1+\cos^2(\gamma)) + B^2(1+\cos^2(\gamma)) - 4AB\cos(\gamma)\right) A^2 B^2 \sin^2(\gamma)}{\cos^2(\gamma)(A^2 + B^2 - 2AB\cos(\gamma))^2},$$

which is negative on its domain. This implies that $g'\Delta - g\Delta'$ is strictly decreasing on $(0, \pi/2)$ and strictly increasing on $(\pi/2, \pi)$. On the other hand, we have $\lim_{\gamma\to 0^+}(g'\Delta - g\Delta') = -A^3 B\pi$, and $\lim_{\gamma\to\pi^-}(g'\Delta - g\Delta') = 0$. This yields the assertion. □

Lemma 2.4. *Consider two disks $B_i, B_j \in \mathcal{F}$ such that $|x_i - x_j| < \rho_i + \rho_j$, and let v be a vertex of the digon $B_i \cap B_j$. Let $T = [x_i, x_j, v]$, $\Delta = \operatorname{area}(T)$, and let $\alpha_i = \angle v x_i x_j$ and $\alpha_j = \angle v x_j x_i$. Then*

$$\frac{1}{2}\alpha_i \rho_i^2 + \frac{1}{2}\alpha_j \rho_j^2 \leq \frac{4 \arccos\frac{1+\mu}{2}}{(1+\mu)\sqrt{(1-\mu)(3+\mu)}} \Delta, \tag{2.1}$$

with equality if and only if $\rho_i = \rho_j$ and $|x_i - x_j| = \rho_i(1+\mu)$.

Proof. First, an elementary computation shows that if $\rho_i = \rho_j$ and $|x_i - x_j| = \rho_i(1+\mu)$, then there is equality in (2.1).

Without loss of generality, let $\rho_i = 1$, and $0 < \rho_j = \rho \leq 1$. By Lemma 2.3, we may assume that $|x_i - x_j| = 1 + \mu\rho$. Thus, the side lengths of T are $1, \rho, 1 + \mu\rho$.

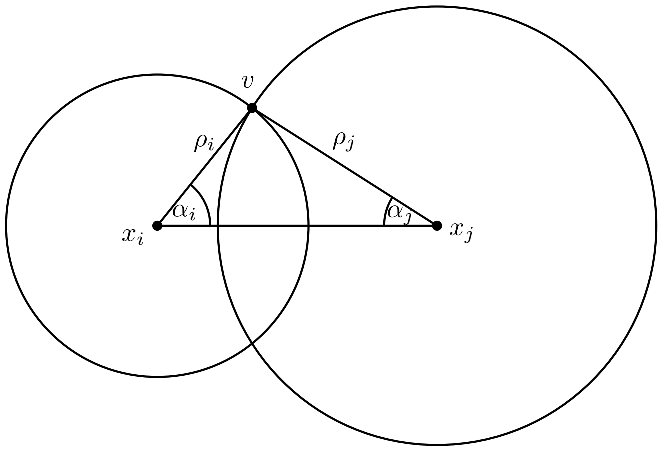

Figure 3: Notation in Lemma 2.4.

Applying the Law of Cosines and Heron's formula to T we obtain that

$$\frac{\frac{1}{2}\alpha_i\rho_i^2 + \frac{1}{2}\alpha_j\rho_j^2}{\Delta} = \frac{f(\rho,\mu)}{g(\rho,\mu)},$$

where

$$f(\rho,\mu) = \frac{1}{2}\arccos\frac{1+(1+\mu\rho)^2-r^2}{2(1+\mu\rho)} + \frac{1}{2}\rho^2\arccos\frac{\rho^2+(1+\mu\rho)^2-1}{2\rho(1+\mu\rho)},$$

and

$$g(\rho,\mu) = \rho\sqrt{2+\rho+\mu\rho)(2-\rho+\mu\rho)(1-\mu^2)}.$$

In the remaining part we show that

$$\frac{f(\rho,\mu)}{g(\rho,\mu)} < \frac{4\arccos\frac{1+\mu}{2}}{(1+\mu)\sqrt{(1-\mu)(3+\mu)}}$$

if $0<\rho<1$ and $0\le\mu\le\sqrt{3}-1$. To do it we distinguish two separate cases.

Case 1: $0<\rho\le 1/5$. In this case we estimate $f(\rho,\mu)/g(\rho,\mu)$ as follows. Let the part of $[x_i,x_j]$ covered by both disks B_i and B_j be denoted by S. Then S is a segment of length $(1-\mu)\rho$. On the other hand, if A_i denotes the convex circular sector of B_i bounded by the radii $[x_i,v]$ and $[x_i,x_j]\cap B_i$, and we define A_j analogously, then the sets $A_i\cap A_j$ and $(A_i\cup A_j)\setminus T$ are covered by the rectangle with S as a side which contains v on the side parallel to S. The area of this rectangle is twice the area of the triangle $\operatorname{conv}(S\cup\{v\})$, implying that

$$\frac{f(\rho,\mu)}{g(\rho,\mu)} \le 1+\frac{2(1-\mu)\rho}{1+\mu\rho}.$$

We show that if $0<\rho\le 1/5$, then the right-hand side quantity in this inequality is strictly less than the right-hand side quantity in (2.1). By differentiating with respect to ρ, we see that as a function of ρ, $1+(2(1-\mu)\rho)/(1+\mu\rho)$ is strictly increasing on its domain and attains its maximum at $\rho = 1/5$. Thus, using the fact that this maximum is equal to $(7-\mu)/(5+\mu)$, we need to show that

$$\frac{4\arccos\frac{1+\mu}{2}}{(1+\mu)\sqrt{(1-\mu)(3+\mu)}} - \frac{7-\mu}{5+\mu} > 0.$$

Clearly, the function

$$\mu \mapsto \frac{\arccos\frac{1+\mu}{2}}{\frac{1+\mu}{2}}$$

is strictly decreasing on the interval $[0, \sqrt{3}-1]$. By differentiation one can easily check that the function

$$\mu \mapsto \frac{7-\mu}{5+\mu}\sqrt{(1-\mu)(3+\mu)}$$

is also strictly increasing on the same interval. Thus, we obtain that the above expression is minimal if $\mu = \sqrt{3}-1$, implying that it is at least $0.11570\ldots$.

Case 2: $1/5 < \rho \le 1$.

We show that in this case the partial derivative $\partial_\rho\left(f(\rho,\mu)/g(\rho,\mu)\right)$, or equivalently, the quantity $h(\rho,\mu) = f'_\rho(\rho,\mu)g(\rho,\mu) - g'_\rho(\rho,\mu)f(\rho,\mu)$ is strictly positive. By plotting the latter quantity on the rectangle $0 \le \mu \le \sqrt{3}-1$, $1/5 \le \rho \le 1$, its minimum seems to be approximately 0.00146046085. To use this fact, we upper bound the two partial derivatives of this function, and compute its values on a grid. In particular, using the monotonicity properties of the functions f, g, we obtain that under our conditions $|f(\rho,\mu)| < 1.25$ and $|g(\rho,\mu)| \le 0.5$. Furthermore, using the inequalities $0 \le \mu \le \sqrt{3}-1$, $1/5 \le \rho \le 1$ and also the triangle inequality to estimate the derivatives of f and g, we obtain that

$$|f'_\rho(\rho,\mu)| < 1.95,\ |f'_\mu(\rho,\mu)| < 2.8,\ |f''_{\rho\rho}(\rho,\mu)| < 2.95,\ |f''_{\rho\mu}(\rho,\mu)| < 9.8,$$

and

$$|g'_\rho(\rho,\mu)| < 0.93,\ |g'_\mu(\rho,\mu)| < 1.08,\ |g''_{\rho\rho}(\rho,\mu)| < 2.64,\ |g''_{\rho\mu}(\rho,\mu)| < 15.1.$$

These inequalities imply that $|h'_\rho(\rho,\mu)| < 4.78$ and $|h'_\mu(\rho,\mu)| < 28.49$, and hence, for any Δ_ρ and Δ_μ, we have $h(\rho+\Delta_\rho, \mu+\Delta_\mu) > h(\rho,\mu) - 4.78|\Delta_\rho| - 28.49|\Delta_\mu|$. Thus, we divided the rectangle $[0.2, 1] \times [0, \sqrt{3}-1]$ into a 8691×8691 grid, and by numerically computing the value of $h(\rho,\mu)$ at the gridpoints, we showed that at any such point the value of h (up to 12 digits) is at least 0.00144. According to our estimates above, this implies that $h(\rho,\mu) \ge 0.00002$ for all values of ρ and μ. □

Before our next lemma, recall that $\mathbf{B}^2$ denotes the *closed* unit disk centered at the origin.

Lemma 2.5. *For some* $0 < \nu < 1$, *let* $x, y, z \in \mathbb{R}^2$ *be non-collinear points, and let* $\{B_u = u + \rho_u \mathbf{B}^2 : u \in \{x,y,z\}\}$ *be a* ν*-arrangement of disks; that is, assume that for any* $\{u,v\} \subset \{x,y,z\}$, *we have* $|u-v| \ge \max\{\rho_u,\rho_v\} + \nu\min\{\rho_u,\rho_v\}$. *Assume that for any* $\{u,v\} \subset \{x,y,z\}$, $B_u \cap B_v \ne \emptyset$, *and that the union of the three disks covers the triangle* $[x,y,z]$. *Then* $\nu \le \sqrt{3}-1$.

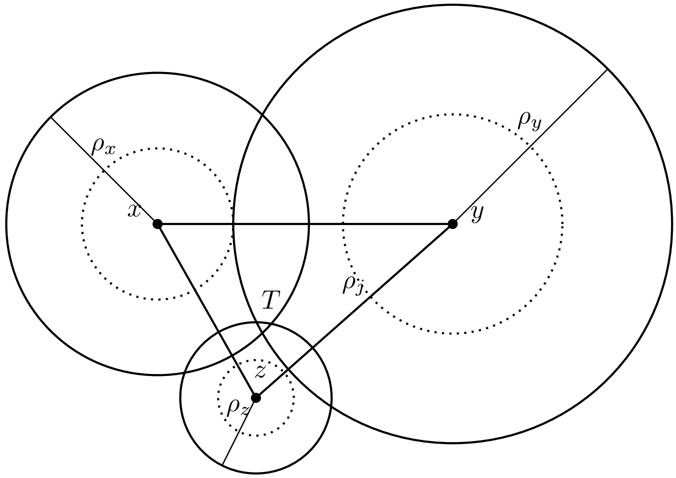

Figure 4: Notation in Lemma 2.5. The circles drawn with dotted lines represent the μ-cores of the disks.

Proof. Without loss of generality, assume that $0 < \rho_z \leq \rho_y \leq \rho_x$. Since the disks are compact sets, by the Knaster-Kuratowski-Mazurkiewicz lemma [12], there is a point q of T belonging to all the disks, or in other words, there is some point $q \in T$ such that $|q-u| \leq \rho_u$ for any $u \in \{x,y,z\}$. Recalling the notation $T=[x,y,z]$ from the introduction, let $T'=[x',y',z']$ be a triangle with edge lengths $|y'-x'| = \rho_x + \nu\rho_y$, $|z'-x'| = \rho_x+\nu\rho_z$ and $|z'-y'| = \rho_y+\nu\rho_z$, and note that these lengths satisfy the triangle inequality.

We show that the disks $x'+\rho_x\mathbf{B}^2$, $y'+\rho_y\mathbf{B}^2$ and $z'+\rho_z\mathbf{B}^2$ and T' satisfy the conditions in the lemma. To do this, we show the following, more general statement, which, together with the trivial observation that any edge of T' is covered by the two disks centered at its endpoints, clearly implies what we want: For any triangles $T=[x,y,z]$ and $T'=[x',y',z']$ satisfying $|u'-v'| \leq |u-v|$ for any $u,v \in \{x,y,z\}$, and for any point $q \in T$ there is a point $q' \in T'$ such that $|q'-u'| \leq |q-u|$ for any $u \in \{x,y,z\}$. The main tool in the proof of this statement is the following straightforward consequence of the Law of Cosines, stating that if the side lengths of a triangle are A,B,C, and the angle of the triangle opposite of the side of length C is γ, then for any fixed values of A and B, C is a strictly increasing function of γ on the interval $(0,\pi)$.

To apply it, observe that if we fix x,y and q, and rotate $[x,z]$ around x towards $[x,q]$, we strictly decrease $|z-y|$ and $|z-q|$ and do not change $|y-x|, |z-x|, |x-q|$ and $|y-q|$. Thus, we may replace z by a point z^* satisfying $|z^*-y| = |z'-y'|$, or the property that z^*, q, x are collinear. Repeating this transformation by x or y playing the role of z we obtain either a triangle congruent to T' in which q satisfies the required conditions, or a triangle in which q is a boundary point. In other words, without loss of generality we may assume that $q \in \operatorname{bd}(T)$. If $q \in \{x,y,z\}$, then the statement is trivial, and so we assume that q is a relative interior point of, say, $[x,y]$. In this case, if $|z-x| > |z'-x'|$ or $|z-y| > |z'-y'|$, then we may rotate $[y,z]$ or $[x,z]$ around y or x, respectively. Finally, if $|y-x| > |y'-x'|$, then one of the angles $\angle yxz$ or $\angle xyz$, say $\angle xyz$, is acute, and then we may rotate $[z,y]$ around z towards $[z,q]$. This implies the statement.

By our argument, it is sufficient to prove Lemma 2.5 under the assumption that $|y-x| = \rho_x+\nu\rho_y$, $|z-x| = \rho_x+\nu\rho_z$ and $|z-y| = \rho_y+\nu\rho_z$. Consider the case that $\rho_x > \rho_y$. Let q be a point of T belonging to each disk, implying that $|q-u| \leq \rho_u$ for all $u \in \{x, y, z\}$. Clearly, from our conditions it follows that $|x-q| > \rho_x - \rho_y$. Let us define a 1-parameter family of configurations, with the parameter $t \in [0, \rho_x - \rho_y]$, by setting $x(t) = x - tw$, where w is the unit vector in the direction of $x - q$, $\rho_x(t) = \rho_x - t$, and keeping q, y, z, ρ_y, ρ_z fixed. Note that in this family $q \in B_{x(t)} = x(t) + \rho_x(t)\mathbf{B}^2$, which implies that $|x(t) - u| \leq \rho_x(t) + \rho_u$ for $u \in \{y, z\}$. Thus, for any $\{u, v\} \subset \{x(t), y, z\}$, there is a point of $[u, v]$ belonging to both B_u and B_v. This, together with the property that q belongs to all three disks and using the convexity of the disks, yields that the triangle $[x(t), y, z]$ is covered by $B_{x(t)} \cup B_y \cup B_z$.

Let the angle between $u - x(t)$ and w be denoted by φ. Then, using the linearity of directional derivatives, we have that for $f(t) = |x(t) - u|$, $f'(t) = -\cos\varphi \geq -1$ for $u \in \{y, z\}$, implying $|x(t) - u| \geq |x - u| - t = \rho_x(t) + \nu\rho_u$ for $u \in \{y, z\}$, and also that the configuration is a ν-arrangement for all values of t. Hence, all configurations in this family, and in particular, the configuration with $t = \rho_x - \rho_y$ satisfies the conditions in the lemma. Thus, repeating again the argument in the first part of the proof, we may assume that $\rho_x = \rho_y \geq \rho_z$, $|y - x| = (1 + \mu)\rho_x$ and $|z - x| = |z - y| = \rho_x + \nu\rho_z$. Finally, if $\rho_x = \rho_y > \rho_z$, then we may assume that q lies on the symmetry axis of T and satisfies $|x - q| = |y - q| > \rho_x - \rho_z$. In this case we apply a similar argument by moving x and y towards q at unit speed and decreasing $\rho_x = \rho_y$ simultaneously till they reach ρ_z, and, again repeating the argument in the first part of the proof, obtain that the family $\{\bar{u} + \rho_z\mathbf{B}^2 : \bar{u} \in \{\bar{x}, \bar{y}, \bar{z}\}\}$, where $\bar{T} = [\bar{x}, \bar{y}, \bar{z}]$ is a regular triangle of side lengths $(1 + \nu)\rho_z$, covers $\bar{T}$. Thus, the inequality $\nu \leq \sqrt{3} - 1$ follows by an elementary computation. □

In our next lemma, for any disk $B_i \in \mathcal{F}$ we denote by $\bar{B}_i$ the closure $x_i + \rho_i\mathbf{B}^2$ of B_i.

Lemma 2.6. *Let $B_i, B_j, B_k \in \mathcal{F}$ such that $\bar{B}_u \cap \bar{B}_v \not\subseteq B_w$ for any $\{u, v, w\} = \{i, j, k\}$. Let $T = [x_i, x_j, x_k]$, $\Delta = \operatorname{area}(T)$, and $\alpha_u = \angle x_v x_u x_w$. If $T \subset \bar{B}_i \cup \bar{B}_j \cup \bar{B}_k$, then*

$$\frac{1}{2}\sum_{u\in\{i,j,k\}} \alpha_u\rho_u^2 \leq \frac{2\pi}{\sqrt{3}(1+\mu)^2}\Delta, \tag{2.2}$$

with equality if and only if $\rho_i = \rho_j = \rho_k$, and T is a regular triangle of side length $(1 + \mu)\rho_i$.

Proof. In the proof we call

$$\delta = \frac{\sum_{u\in\{i,j,k\}} \alpha_u\rho_u^2}{2\Delta}$$

the *density* of the configuration.

Consider the 1-parameter families of disks $B_u(\nu) = x_u + (1 + \mu) / (1 + \nu)\, \rho_u \operatorname{int}(\mathbf{B}^2)$, where $u \in \{i, j, k\}$ and $\nu \in [\mu, 1]$. Observe that the three disks $B_u(\nu)$, where $u \in \{i, j, k\}$, form a ν-arrangement for any $\nu \geq \mu$. Indeed, in this case for any $\{u, v\} \subset \{i, j, k\}$, if $\rho_u \leq \rho_v$, we have

$$\frac{1+\mu}{1+\nu}\rho_v + \nu\left(\frac{1+\mu}{1+\nu}\rho_u\right) = \rho_v + \mu\rho_u - \frac{\nu-\mu}{1+\nu}(\rho_v - \rho_u) \leq \rho_v + \mu\rho_u \leq |x_u - x_v|.$$

Furthermore, for any $\nu \geq \mu$, we have

$$(1+\mu)^2 \sum_{u \in \{i,j,k\}} \alpha_u \rho_u^2 = (1+\nu)^2 \sum_{u \in \{i,j,k\}} \alpha_u \left(\frac{1+\mu}{1+\nu} \right)^2 \rho_u^2.$$

Thus, it is sufficient to prove the assertion for the maximal value $\bar{\nu}$ of ν such that the conditions $T \subset \bar{B}_i(\nu) \cup \bar{B}_j(\nu) \cup \bar{B}_k(\nu)$ and $\bar{B}_u \cap \bar{B}_v \not\subseteq B_w$ are satisfied for any $\{u,v,w\} = \{i,j,k\}$. Since the relation $\bar{B}_u \cap \bar{B}_v \not\subseteq B_w$ implies, in particular, that $\bar{B}_u \cap \bar{B}_v \neq \emptyset$, in this case the conditions of Lemma 2.5 are satisfied, yielding $\bar{\nu} \leq \sqrt{3}-1$. Hence, with a little abuse of notation, we may assume that $\bar{\nu} = \mu$. Then one of the following holds:

(i) The intersection of the disks $\bar{B}_u$ is a single point.

(ii) For some $\{u,v,w\} = \{i,j,k\}$, $\bar{B}_u \cap \bar{B}_v \subset \bar{B}_w$ and $\bar{B}_u \cap \bar{B}_v \not\subseteq B_w$.

Before investigating (i) and (ii), we remark that during this process, which we refer to as *μ-increasing process*, even though there might be non-maximal values of ν for which the modified configuration satisfies the conditions of the lemma and also (i) or (ii), we always choose the *maximal* value. This value is determined by the centers of the original disks and the ratios of their radii.

First, consider (i). Then, clearly, the unique intersection point q of the disks lies in T, and note that either q lies in the boundary of all three disks, or two disks touch at q. We describe the proof only in the first case, as in the second one we may apply a straightforward modification of our argument. Thus, in this case we may decompose T into three triangles $[x_i, x_j, q]$, $[x_i, x_k, q]$ and $[x_j, x_k, q]$ satisfying the conditions in Lemma 2.4, and obtain

$$\frac{1}{2} \sum_{u \in \{i,j,k\}} \alpha_u \rho_u^2 \leq \frac{4 \arccos \frac{1+\mu}{2}}{(1+\mu)\sqrt{(1-\mu)(3+\mu)}} \Delta \leq \frac{2\pi}{\sqrt{3}(1+\mu)^2} \Delta,$$

where the second inequality follows from the fact that the two expressions are equal if $\mu = \sqrt{3}-1$, and

$$\left(2 \arccos \frac{1+\mu}{2} - \frac{\pi \sqrt{(1-\mu)(3+\mu)}}{\sqrt{3}(1+\mu)} \right)' > 0$$

if $\mu \in [0, \sqrt{3}-1]$. Here, by Lemma 2.4, equality holds only if $\rho_i = \rho_j = \rho_k$, and T is a regular triangle of side length $(1+\mu)\rho_i$. On the other hand, under these conditions in (2.2) we have equality. This implies Lemma 2.6 for (i).

In the remaining part of the proof, we show that if (ii) is satisfied, the density of the configuration is strictly less than $2\pi / \left(\sqrt{3}(1+\mu)^2\right)$. Let q be a common point of $\mathrm{bd}(\bar{B}_w)$ and, say, $\bar{B}_u$. If q is a relative interior point of an arc in $\mathrm{bd}(\bar{B}_u \cap \bar{B}_v)$, then one of the disks is contained in another one, which contradicts the fact that the disks B_u, B_v, B_w form a μ-arrangement. Thus, we have that either $\bar{B}_u \cap \bar{B}_v = \{q\}$, or that q is a vertex of the digon $B_u \cap B_v$. If $\bar{B}_u \cap \bar{B}_v = \{q\}$, then the conditions of (i) are satisfied, and thus, we assume that q is a vertex of the digon $B_u \cap B_v$. By choosing a suitable coordinate system and rescaling and relabeling, if necessary, we may assume that $B_u = \mathrm{int}(\mathbf{B}^2)$, x_v lies on the positive half of the x-axis, and x_w is written in the form $x_w = (\zeta_w, \eta_w)$, where $\eta_w > 0$,

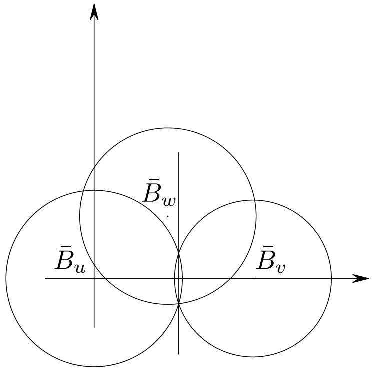

Figure 5: An illustration for the proof of Lemma 2.6.

and the radical line of B_u and B_v separates x_v and x_w (cf. Figure 5). Set $\rho = \rho_w$. We show that $\eta_w > (1+\mu)\rho/2$.

Case 1: if $\rho \geq 1$. Then we have $|x_w| \geq \rho + \mu$.

Let the radical line of B_u and B_v be the line $\{x = t\}$ for some $0 < t \leq 1$. Then, as this line separates x_v and x_w, we have $\zeta_w \leq t$, and by (ii) we have $q = (t, -\sqrt{1-t^2})$. This implies that $|x_w - q| \leq |x_w - x_u|, |x_w - x_v|$, from which we have $0 \leq \zeta_w$. Let S denote the half-infinite strip $S = \{(\zeta, \eta) \in \mathbb{R}^2 : 0 \leq \zeta \leq t, \eta \geq 0\}$, and set $s = (t, -\sqrt{1-t^2} + \rho)$. Note that by our considerations, $x_w \in S$ and $|x_w - q| = \rho$, which yield $\eta_w \leq -\sqrt{1-t^2} + \rho$. From this it follows that $\rho + \mu \leq |x_w| \leq |s|$, or in other words, we have $t^2 + (\rho - \sqrt{1-t^2})^2 \geq (\rho+\mu)^2$. By solving this inequality for t with parameters ρ and μ, we obtain that $t \geq t_0$, $1 \leq \rho \leq \left(1-\mu^2\right)/(2\mu)$ and $0 \leq \mu \leq \sqrt{2} - 1$, where

$$t_0 = \sqrt{1 - \left(\frac{1 - 2\mu\rho - \mu^2}{2\rho}\right)^2}.$$

Let $p = (\zeta_p, \eta_p)$ be the unique point in S with $|p| = \rho + \mu$ and $|p - q| = \rho$, and observe that $\eta_w \geq \eta_p$. Now we find the minimal value of η_p if t is permitted to change and ρ is fixed. Set $p' = (\zeta_p, -\sqrt{1 - \zeta_p^2})$. Since the bisector of $[p', q]$ separates p' and p, it follows that $|p - p'| \geq |p - q| = \rho$ with equality only if $p' = q$ and $p = s$, or in other words, if $t = t_0$. This yields that ζ_p is maximal if $t = t_0$. On the other hand, since $|p| = \rho + \mu$ and p lies in the first quadrant, η_p is minimal if ζ_p is maximal. Thus, for a fixed value of ρ, η_p is minimal if $t = t_0$ and $p = s = (t_0, -\sqrt{1 - t_0^2} + \rho)$, implying that $\eta_w \geq -\sqrt{1 - t_0^2} + \rho = \left(2\rho^2 + \mu^2 + 2\mu\rho - 1\right)/(2\rho)$. Now, $\rho \geq 1$ and $\mu < 1$ yields that

$$\frac{2\rho^2 + \mu^2 + 2\mu\rho - 1}{2\rho} - \frac{(1+\mu)\rho}{2} = \frac{\rho^2 - \mu\rho^2 + 2\mu\rho - 1}{2\rho} \geq \frac{\mu}{2\rho} > 0,$$

implying the statement.

Case 2: if $0 < \rho \leq 1$. In this case the inequality $\eta_w > (1+\mu)\rho/2$ follows by a similar consideration.

In the remaining part of the proof, let

$$\sigma(\mu) = \frac{2\pi}{\sqrt{3}(1+\mu)^2}.$$

Now we prove the lemma for (ii). Suppose for contradiction that for some configuration $\{B_u, B_v, B_w\}$ satisfying (ii) the density is at least $\sigma(\mu)$; here we label the disks as in the previous part of the proof. Let $B'_w = x'_w + \rho_w \operatorname{int}(\mathbf{B}^2)$ denote the reflection of B_w to the line through $[x_u, x_v]$. By the inequality $\eta_w > (1+\mu)\rho/2$ proved in the two previous cases, we have that $\{B_u, B_v, B_w, B'_w\}$ is a μ-arrangement, where we observe that by the strict inequality, B_w and B'_w do not touch each others cores. Furthermore, each triangle $[x_u, x_w, x'_w]$ and $[x_v, x_w, x'_w]$ is covered by the three disks from this family centered at the vertices of the triangle, and the intersection of no two disks from one of these triples is contained in the third one. Thus, the conditions of Lemma 2.6 are satisfied for both $\{B_u, B_w, B'_w\}$ and $\{B_v, B_w, B'_w\}$. Observe that as by our assumption the density in T is $\sigma(\mu)$, it follows that the density in at least one of the triangles $[x_u, x_w, x'_w]$ and $[x_v, x_w, x'_w]$, say in $T' = [x_u, x_w, x'_w]$, is at least $\sigma(\mu)$. In other words, under our condition there is an axially symmetric arrangement with density at least $\sigma(\mu)$. Now we apply the μ-increasing process as in the first part of the proof and obtain a μ'-arrangement $\{\hat{B}_u = x_u + (1+\mu)/(1+\mu')\rho_u \operatorname{int}(\mathbf{B}^2), \hat{B}_w = x_w + (1+\mu)/(1+\mu')\rho_w \operatorname{int}(\mathbf{B}^2), \hat{B}'_w = x'_w + (1+\mu)/(1+\mu')\rho_w \operatorname{int}(\mathbf{B}^2)\}$ with density $\sigma(\mu')$ and $\mu' \geq \mu$ that satisfies either (i) or (ii). If it satisfies (i), we have that the density of this configuration is at most $\sigma(\mu')$ with equality if only if T' is a regular triangle of side length $(1+\mu')\rho$, where ρ is the common radius of the three disks. On the other hand, this implies that in case of equality, the disks centered at x_w and x'_w touch each others' cores which, by the properties of the μ-increasing process, contradicts the fact that B_w and B'_w do not touch each others' μ-cores. Thus, we have that the configuration satisfies (ii).

From Lemma 2.1 it follows that $\hat{B}_w \cap \hat{B}'_w \subset \hat{B}_u$. Thus, applying the previous consideration with $\hat{B}_u$ playing the role of B_w, we obtain that the distance of x_u from the line through $[x_w, x'_w]$ is greater than $(1+\mu')/2\rho_u$. Thus, defining $\hat{B}'_u = x'_u + (1+\mu)/(1+\mu')\rho_u \operatorname{int}(\mathbf{B}^2)$ as the reflection of B'_u about the line through $[x_w, x'_w]$, we have that $\{\hat{B}_u, \hat{B}_w, \hat{B}'_w, \hat{B}'_u\}$ is a μ'-arrangement such that $\{\hat{B}_u, \hat{B}'_u, \hat{B}_w\}$ and $\{\hat{B}_u, \hat{B}'_u, \hat{B}'_w\}$ satisfy the conditions of Lemma 2.6. Without loss of generality, we may assume that the density of $\{\hat{B}_u, \hat{B}'_u, \hat{B}_w\}$ is at least $\sigma(\mu')$. Again applying the μ-increasing procedure described in the beginning of the proof, we obtain a μ''-arrangement of three disks, with $\mu'' \geq \mu'$, concentric with the original ones that satisfy the conditions of the lemma and also (i) or (ii). Like in the previous paragraph, (i) leads to a contradiction, and we have that it satisfies (ii). Now, again repeating the argument we obtain a μ''' -arrangement

$$\left\{ y + \frac{1+\mu}{1+\mu'''}\rho_u \operatorname{int}(\mathbf{B}^2), x_w + \frac{1+\mu}{1+\mu''''}\rho_w \operatorname{int}(\mathbf{B}^2), x'_w + \frac{1+\mu}{1+\mu'''}\rho_w \operatorname{int}(\mathbf{B}^2) \right\},$$

with density at least $\sigma(\mu''')$ and $\mu''' \geq \mu''$, that satisfies the conditions of the lemma, where either $y = x_u$ or $y = x'_u$. On the other hand, since in the μ-increasing process we choose the *maximal* value of the parameter satisfying the required conditions, this yields that $\mu' = \mu'' = \mu'''$. But in this case the property that $\{\hat{B}_u, \hat{B}'_u, \hat{B}_w\}$ satisfies (ii) yields that $\{\hat{B}_u, \hat{B}'_u, \hat{B}_w\}$ does not; a contradiction. □

3 Proof of Theorem 1.2

The idea of the proof follows that in [7] with suitable modifications. In the proof we decompose $U(\mathcal{F}) = \bigcup_{i=1}^{n} B_i$, by associating a polygon to each vertex of certain free digons formed by two disks. Before doing it, we first prove some properties of μ-arrangements.

Let q be a vertex of a free digon, say, $D = B_1 \cap B_2$. We show that the convex angular region R bounded by the closed half lines starting at q and passing through x_1 and x_2, respectively, does not contain the center of any element of $\mathcal{F}$ different from B_1 and B_2 containing q on its boundary. Indeed, suppose for contradiction that there is a disk $B_3 = x_3 + \rho_3 \operatorname{int}(\mathbf{B}^2) \in \mathcal{F}$ with $q \in \operatorname{bd}(B_3)$ and $x_3 \in R$. Since $[q, x_1, x_2] \setminus \{q\} \subset B_1 \cup B_2$, from this and the fact that $\mathcal{F}$ is a Minkowski-arrangement, it follows that the line through $[x_1, x_2]$ strictly separates x_3 from q. As this line is the bisector of the segment $[q, q']$, where q' is the vertex of D different from q, from this it also follows that $|x_3 - q| > |x_3 - q'|$. Thus, $q' \in B_3$.

Observe that in a Minkowski arrangement any disk intersects the boundary of another one in an arc shorter than a semicircle. This implies, in particular, that $B_3 \cap \operatorname{bd}(B_1)$ and $B_3 \cap \operatorname{bd}(B_2)$ are arcs shorter than a semicircle. On the other hand, from this the fact that $q, q' \in B_3$ yields that $\operatorname{bd}(D) \subset B_3$, implying, by the properties of convexity, that $D \subset B_3$, which contradicts our assumption that D is a free digon.

Note that, in particular, we have shown that if a member of $\mathcal{F}$ contains both vertices of a digon, then it contains the digon.

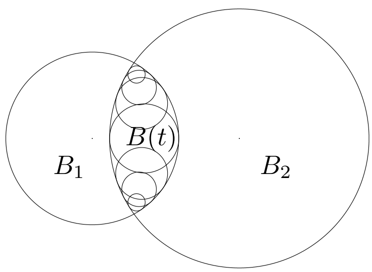

Figure 6: The 1-parameter family of disks inscribed in $B_1 \cap B_2$.

Observe that the disks inscribed in D can be written as a 1-parameter family of disks $B(t)$ continuous with respect to Hausdorff distance, where $t \in (0, 1)$ and $B(t)$ tends to $\{q\}$ as $t \to 0^+$ (cf. Figure 6); here the term 'inscribed' means that the disk is contained in $B_i \cap B_j$ and touches both disks from inside. We show that if some member B_k of $\mathcal{F}$, different from B_1 and B_2, contains $B(t)$ for some value of t, then B_k contains exactly one vertex of D. Indeed, assume that some B_k contains some $B(t)$ but it does not contain any vertex of D. Then for $i \in \{1, 2\}$, $B_k \cap \operatorname{bd}(B_i)$ is a circular arc Γ_i in $\operatorname{bd}(D)$. Let L_i be the half line starting at the midpoint of Γ_i, and pointing in the direction of the outer normal vector of B_i at this point. Note that as D is a plane convex body, $L_1 \cap L_2 = \emptyset$. On the other hand, since B_1, B_2, B_k are a Minkowski arrangement, from this it follows that $x_k \in L_1 \cap L_2$; a contradiction. The property that no B_k contains both vertices of D follows from the fact that D is a free digon. Thus, if $q \in B_k$ for an element $B_k \in \mathcal{F}$, then there is some value $t_0 \in (0,1)$ such that $B(t) \subseteq B_k$ if and only if $t \in (0, t_0]$.

In the proof, we call the disks B_i, B_j *adjacent*, if $B_i \cap B_j$ is a digon, and there is a member of the family $B(t)$ defined in the previous paragraph that is not contained in any element of $\mathcal{F}$ different from B_i and B_j. Here, we remark that any two adjacent disks define a free digon, and if a vertex of a free digon is a boundary point of $U(\mathcal{F})$, then the digon is defined by a pair of adjacent disks.

Consider a pair of adjacent disks, say B_1 and B_2, and let q be a vertex of $D = B_1 \cap B_2$. If q is a boundary point of the union $U(\mathcal{F})$, then we call the triangle $[x_1, x_2, q]$ a *shell triangle*, and observe that by the consideration in the previous paragraph, the union of shell triangles coincides with the inner shell of $\mathcal{F}$.

If q is not a boundary point of $U(\mathcal{F})$, then there is a maximal value $t_0 \in (0,1)$ such that $B(t_0) = x + \rho \mathbf{B}^2$ is contained in an element B_i of $\mathcal{F}$ satisfying $q \in B_i$. Then, clearly, $B(t_0)$ touches any such B_i from inside, and since B_1 and B_2 are adjacent, there is no element of $\mathcal{F}$ containing $B(t_0)$ and the vertex of D different from q. Without loss of generality, assume that the elements of $\mathcal{F}$ touched by $B(t_0)$ from inside are $B_1, B_2, \ldots, B_k$. Since B_1 and B_2 are adjacent and there is no element of $\mathcal{F}$ containing both $B(t_0)$ and the vertex of D different from q, we have that the tangent points of B_1 and B_2 on $\operatorname{bd}(B(t_0))$ are consecutive points among the tangent points of all the disks B_i, where $1 \leq i \leq k$. Thus, we may assume that the tangent points of $B_1, B_2, \ldots, B_k$ on $B(t_0)$ are in this counterclockwise order on $\operatorname{bd}(B(t_0))$. Let x denote the center of $B(t_0)$. Since $\mathcal{F}$ is a Minkowski arrangement, for any $1 \leq i < j \leq k$, the triangle $[x, x_i, x_j]$ contains the center of no element of $\mathcal{F}$ apart from B_i and B_j, which yields that the points $x_1, x_2, \ldots, x_k$ are in convex position, and their convex hull P_q contains x in its interior but it does not contain the center of any element of $\mathcal{F}$ different from $x_1, x_2, \ldots, x_k$ (cf. also [7]). We call P_q a *core polygon*.

We remark that since $\mathcal{F}$ is a μ-arrangement, the longest side of the triangle $[x, x_i, x_{i+1}]$, for $i = 1, 2 \ldots, k$, is $[x_i, x_{i+1}]$. This implies that $\angle x_i x x_{i+1} > \pi/3$, and also that $k < 6$. Furthermore, it is easy to see that for any $i = 1, 2, \ldots, k$, the disks B_i and B_{i+1} are adjacent. Thus, any edge of a core polygon is an edge of another core polygon or a shell triangle. This property, combined with the observation that no core polygon or shell triangle contains any center of an element of $\mathcal{F}$ other than their vertices, implies that core polygons cover the core of $\mathcal{F}$ without interstices and overlap (see also [7]).

Let us decompose all core polygons of $\mathcal{F}$ into triangles, which we call *core triangles*, by drawing all diagonals in the polygon starting at a fixed vertex, and note that the conditions in Lemma 2.6 are satisfied for all core triangles. Now, the inequality part of Theorem 1.2 follows from Lemmas 2.4 and 2.6, with equality if and only if each core triangle is a regular triangle $[x_i, x_j, x_k]$ of side length $(1+\mu)\rho$, where $\rho = \rho_i = \rho_j = \rho_k$, and each shell triangle $[x_i, x_j, q]$, where q is a vertex of the digon $B_i \cap B_j$ is an isosceles triangle whose base is of length $(1+\mu)\rho$, and $\rho = \rho_i = \rho_j$. Furthermore, since to decompose a core polygon into core triangles we can draw diagonals starting at any vertex of the polygon, we have that in case of equality in the inequality in Theorem 1.2, all sides and all diagonals of any core polygon are of equal length. From this we have that all core polygons are regular triangles, implying that all free digons in $\mathcal{F}$ are thick.

On the other hand, assume that all free digons in $\mathcal{F}$ are thick. Then, from Lemma 2.2 it follows that any connected component of $\mathcal{F}$ contains congruent disks. Since an adjacent pair of disks defines a free digon, from this we have that, in a component consisting of disks of radius $\rho > 0$, the distance between the centers of two disks defining a shell triangle, and the edge-lengths of any core polygon, are equal to $(1+\mu)\rho$. Furthermore, since all disks centered at the vertices of a core polygon are touched by the same disk from inside, we also have that all core polygons in the component are regular k-gons of edge-length $(1+\mu)\rho$, where $3 \leq k \leq 5$. This and the fact that any edge of a core polygon connects the vertices of an adjacent pair of disks yield that if the intersection of any two disks centered at two different vertices of a core polygon is more than one point, then it is a free digon. Thus, any diagonal of a core polygon in this component is of length $(1+\mu)\rho$, implying that any core polygon is a regular triangle, from which the equality in Theorem 1.2 readily follows.

4 Remarks and open questions

Remark 4.1. If $\sqrt{3}-1 < \mu < 1$, then by Lemma 2.5, $C(\mathcal{F}) = \emptyset$ for any μ-arrangement $\mathcal{F}$ of order μ.

Remark 4.2. Observe that the proof of Theorem 1.2 can be extended to some value $\mu > \sqrt{3}-1$ if and only if Lemma 2.4 can be extended to this value μ. Nevertheless, from the continuity of the functions in the proof of Lemma 2.4, it follows that there is some $\mu_0 > \sqrt{3}-1$ such that the lemma holds for any $\mu \in (\sqrt{3}-1, \mu_0]$. Nevertheless, we cannot extend the proof for all $\mu < 1$ due to numeric problems.

Remark 4.2 readily implies Remark 4.3.

Remark 4.3. There is some $\mu_0 > \sqrt{3}-1$ such that if $\mu \in (\sqrt{3}-1, \mu_0]$, and $\mathcal{F}$ is a μ-arrangment of finitely many disks, then the total area of the disks is

$$T \leq \frac{4 \cdot \arccos(\frac{1+\mu}{2})}{(1+\mu) \cdot \sqrt{(3+\mu)(1-\mu)}} \operatorname{area}(I(\mathcal{F})) + \operatorname{area}(O(\mathcal{F})),$$

with equality if and only if every free digon in $\mathcal{F}$ is thick.

Conjecture 4.4. *The statement in* Remark 4.3 *holds for any μ-arrangement of finitely many disks with $\sqrt{3}-1 < \mu < 1$.*

Let $0 < \mu < 1$ and let $\mathcal{F} = \{K_i : i = 1, 2, \ldots\}$ be a generalized Minkowski arrangement of order μ of homothets of an origin-symmetric convex body in $\mathbb{R}^d$ with positive homogeneity. Then we define the (upper) density of $\mathcal{F}$ with respect to $U(\mathcal{F})$ as

$$\delta_U(\mathcal{F}) = \limsup_{R \to \infty} \frac{\sum_{B_i \subset R\mathbf{B}^2} \operatorname{area}(B_i)}{\operatorname{area}\left(\bigcup_{B_i \subset R\mathbf{B}^2} B_i\right)}.$$

Clearly, we have $\delta(\mathcal{F}) \leq \delta_U(\mathcal{F})$ for any arrangement $\mathcal{F}$.

Our next statement is an immediate consequence of Theorem 1.2 and Remark 4.3.

Corollary 4.5. *There is some value $\sqrt{3}-1 < \mu_0 < 1$ such that for any μ-arrangement $\mathcal{F}$ of Euclidean disks in $\mathbb{R}^2$, we have*

$$\delta_U(\mathcal{F}) \leq \begin{cases} \frac{2\pi}{\sqrt{3}(1+\mu)^2}, & \text{if } 0 \leq \mu \leq \sqrt{3}-1, \text{and} \\ \frac{4 \cdot \arccos(\frac{1+\mu}{2})}{(1+\mu) \cdot \sqrt{(3+\mu)(1-\mu)}}, & \text{if } \sqrt{3}-1 < \mu \leq \mu_0. \end{cases}$$

For any $0 \leq \mu < 1$, let $u, v \in \mathbb{R}^2$ be two unit vectors whose angle is $\frac{\pi}{3}$, and let $\mathcal{F}_{\text{hex}}(\mu)$ denote the family of disks of radius $(1+\mu)$ whose set of centers is the lattice

$\{ku + mv : k, m \in \mathbb{Z}\}$. Then $\mathcal{F}_{\text{hex}}(\mu)$ is a μ-arrangement, and by Corollary 4.5, for any $\mu \in [0, \sqrt{3} - 1]$, it has maximal density on the family of μ-arrangements of positive homogeneity. Nevertheless, as Fejes Tóth observed in [8] (see also [4] or Section 1), the same does not hold if $\mu > \sqrt{3} - 1$. Indeed, an elementary computation shows that in this case $\mathcal{F}_{\text{hex}}(\mu)$ does not cover the plane, and thus, by adding disks to it that lie in the uncovered part of the plane we can obtain a μ-arrangement with greater density.

Fejes Tóth suggested the following construction to obtain μ-arrangements with large densities. Let $\tau > 0$ be sufficiently small, and, with a little abuse of notation, let $\tau\mathcal{F}_{\text{hex}}(\mu)$ denote the family of the homothetic copies of the disks in $\mathcal{F}_{\text{hex}}(\mu)$ of homothety ratio τ and the origin as the center of homothety. Let $\mathcal{F}^1_{\text{hex}}(\mu)$ denote the μ-arrangement obtained by adding those elements of $\tau\mathcal{F}_{\text{hex}}(\mu)$ to $\mathcal{F}_{\text{hex}}(\mu)$ that do not overlap any element of it. Iteratively, if for some positive integer k, $\mathcal{F}^k_{\text{hex}}(\mu)$ is defined, then let $\mathcal{F}^{k+1}_{\text{hex}}(\mu)$ denote the union of $\mathcal{F}^k_{\text{hex}}(\mu)$ and the subfamily of those elements of $\tau^{k+1}\mathcal{F}_{\text{hex}}(\mu)$ that do not overlap any element of it. Then, as was observed also in [8], choosing suitable values for τ and k, the value of $\delta_U(\mathcal{F}_{\text{hex}}(\mu))$ can be approximated arbitrarily well by $\delta(\mathcal{F}^k_{\text{hex}}(\mu))$. We note that the same idea immediately leads to the following observation.

Remark 4.6. The supremums of $\delta(\mathcal{F})$ and $\delta_U(\mathcal{F})$ coincide on the family of the μ-arrangements $\mathcal{F}$ in $\mathbb{R}^2$ of positive homogeneity.

We finish the paper with the following conjecture.

Conjecture 4.7. *For any* $\mu \in (\sqrt{3} - 1, 1)$ *and any* μ*-arrangement* $\mathcal{F}$ *in* $\mathbb{R}^2$*, we have* $\delta(\mathcal{F}) \leq \delta_U(\mathcal{F}_{\text{hex}}(\mu))$.

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Braid representatives minimizing the number of simple walks*

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Abstract

Given a knot, we develop methods for finding a braid representative that minimizes the number of simple walks. Such braids lead to an efficient method for computing the colored Jones polynomial of the knot, following an approach developed by Armond and implemented by Hajij and Levitt. We use this method to compute the colored Jones polynomial in closed form for the knots $5_2, 6_1$, and 7_2. The set of simple walks can change under reflection, rotation, and cyclic permutation of the braid, and we prove an invariance property which relates the simple walks of a braid to those of its reflection under cyclic permutation. We study the growth rate of the number of simple walks for families of torus knots. Finally, we present a table of braid words that minimize the number of simple walks for knots up to 13 crossings.

Keywords: Knots, braids, simple walk, colored Jones polynomial.

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1 Introduction

The Jones polynomial $V_L(t)$ is an invariant of knots and links defined using quantum representations of braids. It can be uniquely characterized as the polynomial-valued invariant of oriented links with $V_{\bigcirc}(t) = 1$ for $\bigcirc$ the unknot and satisfying the skein relation

$$t^{-1}V_{L_+}(t) - tV_{L_-}(t) = (t^{1/2} - t^{-1/2})V_{L_0}(t),$$

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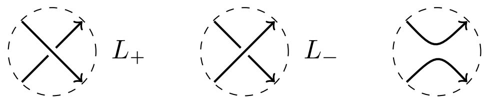
where L_+, L_-, L_0 are identical outside a neighborhood, where they are as pictured



The Jones polynomial admits a combinatorial state sum formula that can be used to compute it, but the complexity of the computation grows exponentially with the crossing number. So this method is impractical for computations that involve links with a large number of crossings.

The *colored Jones polynomial* is a powerful knot invariant packaged as a sequence of Laurent polynomials $J_{N,K}(q)$ for $N \geqslant 2$, with $N = 2$ giving the usual Jones polynomial. It encodes subtle geometric information about the knot complement and appears in several famous open problems in quantum topology, including (i) the Volume Conjecture [18, 23]; (ii) the Slope Conjecture [12, 17]; and (iii) the AJ Conjecture [11]. The first relates the limit of $J_{N,K}(q)$ for $q = e^{2\pi i/N}$ as $N \to \infty$ to the hyperbolic volume of the knot complement; the second posits that every Jones slope of a knot is the slope of an incompressible surface in the knot complement; and the third asserts that the recurrence relation for the N-th colored Jones polynomials is given by the A-polynomial of [9], a plane curve associated to the character variety of $SL(2, \mathbb{C})$ representations of the knot group.

For further background information on the colored Jones polynomial and its relation to the geometry of 3-manifolds, we refer the reader to the books [24] and [10] and their extensive bibliographies. The colored Jones polynomial also has intriguing number theoretic interpretations that will not be discussed in this paper; for more details about these aspects, we refer the reader to the recent papers [3, 4, 20, 21] and their bibliographies.

Our goal in this paper is to study a probabilistic method for computing the colored Jones polynomial. This approach was first developed by Huynh and Lê in [15], and it was later described in terms of walks along braids by Armond [2]. Armond identified the special role played by *simple walks*, resulting in an extremely efficient algorithm for computing $J_{N,K}(q)$, which has been implemented by Hajij and Levitt [14]. The algorithm is exponential in the number of simple walks on the braid, so it is natural to try minimize the number of simple walks before executing the program of [14]. However, as we shall see, this number is highly dependent on the braid representative chosen.

We study how the number of simple walks changes under taking reflection, rotation, and cyclic permutation of a given braid. We also examine the growth rate of the number of simple walks for two families of torus knots. For instance, for the family of $(2, n)$ torus knots, the simple walks satisfy a Fibonacci recurrence and grow exponentially in n. For the family of $(3, n)$ torus knots, the simple walks satisfy a tribonacci recurrence and also grow exponentially in n. We further prove that the total number of simple walks on a braid and its reflection is invariant under cyclic permutation. This fact is used to facilitate finding braid representatives with the least number of simple walks. For knots up to 13 crossings, we developed a program that finds minimal braid representatives. When these braids are used in conjunction with the program of Hajij and Levitt [14], this provides an efficient method for computing the colored Jones polynomial for these knots.

We close this section with a brief synopsis of the rest of this paper. In Section 2, we review the method from [2, 15] for computing the colored Jones polynomial. In Section 3, we use it to compute $J_{N,K}(q)$ in closed form for the knots $5_2, 6_1$, and 7_2. These computations were originally performed by Masbaum using skein theory, see [22]. In Section 4, we recall the basic results about braid representatives for knots and study the effect of the Markov moves on the set of simple walks. In Section 5, we introduce the set of semi-simple walks, and we show that it is invariant under cyclic permutation of the braid word. In Sections 6 and 7, we study the growth rate of the number of simple walks for two families of torus knots. In Section 8, we present the output of a program for finding braid representatives that minimize the number of simple walks.

2 The colored Jones polynomial and walks along braids

Given a knot K and integer $N \geqslant 2$, the colored Jones polynomial $J_{N,K}(q)$ is a Laurent polynomial in the variable $q^{1/2}$. It is normalized so that $J_{N,\bigcirc}(q) = 1$, where $\bigcirc$ is the unknot. When $N = 2$, the colored Jones polynomial agrees with the usual Jones polynomial. In general, the N-th colored Jones polynomial of a knot K can be expressed in terms of the usual Jones polynomial of the $(N-1)$ strand cable of K. However, since the crossing number of the $(N-1)$ strand cable of a knot is $(N-1)^2$ times the crossing number of the knot, this does not lead to a practical method for computing the colored Jones polynomial.

One approach for computing the colored Jones polynomial is presented by Huynh and Lê [15]. Starting with a braid β whose closure is the given knot, Huynh and Lê use methods from quantum algebra to express the colored Jones polynomial as the inverse of the quantum determinant of an almost quantum matrix. The matrix is constructed through the product of Burau matrices, which we obtain from the crossing and orientation properties of β.

A second approach is presented by Armond [2]. It is based on a probabilistic interpretation of the colored Jones polynomial and involves counting *walks along braids*. This method is closely related to the previous one, and in fact it provides a visual representation of the quantum algebra approach. The idea is to view walks along the braid as traversing the strands of the braid from the bottom to the top and to record information about the crossings and their orientations as a product of operators. The end result is the same as that obtained by taking the quantum determinant of the deformation of Burau matrices, but Armond's approach is more accessible and requires less background material on operator theory. One interesting aspect is that the complexity of the computation is sensitive to the choice of braid word, and this will be explored further in Section 4. For now, we focus on describing Armond's approach and the special role played by the *simple walks*.

We begin by introducing a little terminology from braid theory.

Definition 2.1. A *braid* is a set of m strands running from top to bottom with no reversals in vertical direction. The strands may cross each other, but only two strands can participate at each crossing.

Given a braid β, a *braid word* is an expression of the form

$$\beta = \sigma_{i_1}^{\varepsilon_1} \sigma_{i_2}^{\varepsilon_2} \dots \sigma_{i_\ell}^{\varepsilon_\ell},$$

where $\varepsilon_i = \pm 1$ and σ_i is a symbol. Braid words are read from left to right, and braids are drawn from top to bottom. For $1 \leqslant i \leqslant m-1$, σ_i represents the braid with one crossing where the $(i+1)$-st strand crosses over the i-th strand. The inverse σ_i^{-1} represents the braid where the i-th strand crosses over the $(i+1)$-st strand.

The braid word $\beta = \sigma_{i_1}^{\varepsilon_1}\sigma_{i_2}^{\varepsilon_2}\ldots\sigma_{i_\ell}^{\varepsilon_\ell}$ has ℓ crossings, and we say it has *braid length* ℓ. If β is a braid on m strands, we say it has *braid width* m. Note that braid words are not uniquely determined by the braid. Applying a braid relation (see below) will alter the word without changing the braid. The writhe of a braid is defined to be the sum of the signs on all its crossings. For example, the braid word above has writhe $w(\beta) = \sum_{i=1}^{\ell}\varepsilon_i$.

The braid group on m strands is denoted B_m. Abstractly, it is the group with generators $\sigma_1, \ldots, \sigma_{m-1}$ and relations

(i) $\sigma_i\sigma_j = \sigma_j\sigma_i$ for $1 \leqslant i, j \leqslant m-1$ with $|i-j| > 1$ and

(ii) $\sigma_i\sigma_{i+1}\sigma_i = \sigma_{i+1}\sigma_i\sigma_{i+1}$ for $1 \leqslant i \leqslant m-2$.

Relation (i) is called *far commutativity* and (ii) is called the *Yang-Baxter relation* (or *braid relation*). The group operation is given by concatenation of words or, equivalently, by stacking geometric braids, one on top of the other.

Next, we introduce the notions of paths and walks along braids. A *path* starts at the bottom of the braid and traverses arcs of the braid, sometimes jumping down, until it reaches the top of the braid. If the path starts at strand i on the bottom and ends at strand j at the top, we say it is a path from i to j. Whenever the path encounters a crossing, if it is on the overstrand, it is allowed to jump down to the undercrossing arc. If it is on the understrand, then it must stay on that strand. At each crossing the path encounters, a *weight* from the set $\{a_{i,\varepsilon_i}, b_{i,\varepsilon_i}, c_{i,\varepsilon_i} \mid i = 1, \ldots, \ell\}$ is assigned. The weight will depend on the crossing, its sign, and the arcs traversed by the path at that crossing. For example, if the path jumps down at the i-th crossing, it is assigned the weight a_{i,ε_i}. Otherwise, it is assigned the weight b_{i,ε_i} if the path traverses the understrand and c_{i,ε_i} if it traverses the overstrand. Note that, at a given crossing, the path will follow the braid unless it jumps down there. The total weight of the path is the product of the weights of the crossings.

A walk W along β consists of a set $J \subseteq \{1, \ldots, m\}$, a permutation π of J, and a collection of paths with exactly one path in the collection from j to $\pi(j)$ for each $j \in J$. The weight of a walk is $(-1)(-q)^{|J|+\mathrm{inv}(\pi)}$ times the product of the weights of the paths, where $|J|$ is the cardinality of J and $\mathrm{inv}(\pi)$ is the number of inversions in π, i.e., the number of pairs of elements in J with $i < j$ and $\pi(i) > \pi(j)$.

The paths in a walk are ordered from left to right, using their starting strand at the bottom of the braid. This induces an ordering on the weights. The order of the weights is important, and that is because the operators associated to the weights are non-commuting. Operators based at different crossings do commute, but operators at the same crossing do not. Thus, the effect of non-commutativity can be computed locally at each crossing of the braid. Given a walk W and a crossing i of the braid, we use $W_{(i)}$ to denote the local weight of paths of W through crossing i in the given order. If no path of W passes through crossing i, then we set the local weight $W_{(i)} = 1$.

A stack of walks is any ordered collection $W_1 \cdots W_k$ of walks. Visually, this can be viewed as stacking the walks on top of one another with W_1 at the top and W_k on the bottom. The weight of the stack is the product of the weights of the paths in the appropriate order. If two paths belong to different walks, then the path in the higher walk is multiplied to the left of the path in the lower walk. If two paths belong to the same walk, then the path which begins to the left of the other path is said to be above and is multiplied to the left of the other path. Given a stack $\mathcal{S} = W_1 \cdots W_k$ and a crossing i of the braid, we let $\mathcal{S}_{(i)}$ be the local weight of the stack at i; it is equal to the product $(W_1)_{(i)} \cdots (W_k)_{(i)}$ of local weights of the walks of the stack at i in the given order.

With walks along braids established, we now show how they can be used to compute the colored Jones polynomial. Let $R = \mathbb{Z}[q, q^{-1}]$. Let $\hat{x}$ and τ_x be operators on the ring $R[x^{\pm 1}, y^{\pm 1}, u^{\pm 1}]$ given by $\hat{x} f(x, y, \dots) = x f(x, y, \dots)$ and $\tau_x f(x, y, \dots) = f(qx, y, \dots)$. The operators $\hat{y}$, $\hat{u}$, τ_y, τ_u are defined similarly. We associate operators to each of the crossing weights using the formulas:

$$a_+ = (\hat{u} - \hat{y}\tau x^{-1})\tau_y{}^{-1}, \qquad b_+ = \hat{u}^2, \qquad c_+ = \hat{x}\tau_y{}^{-2}\tau_u{}^{-1},$$

$$a_- = (\tau_y - \hat{x}^{-1})\tau_x{}^{-1}\tau_u, \qquad b_- = \hat{u}^2, \qquad c_- = \hat{y}^{-1}\tau_y{}^{-1}\tau_u.$$

By taking the summation of all walks on the braid and writing their weights in terms of the above operators, we obtain the operator P. Letting P act on the constant 1 and making the substitutions $x = z$, $y = z$ and $u = 1$, we obtain a polynomial $\mathcal{E}(P)$. Let $\mathcal{E}_N(P)$ denote the polynomial obtained by making the substitution $z = q^{N-1}$ to $\mathcal{E}(P)$.

The next result shows how to compute the colored Jones polynomial of a knot from its braid representative. It was proved by Huynh and Lê in [15] and appears as Theorem 2.3 in [2].

Theorem 2.2. *Let K be a knot obtained as the closure of a braid $\beta \in B_m$. Its colored Jones polynomial is given by*

$$J_{N,K}(q) = q^{(N-1)(w(\beta)-m+1)/2} \sum_{n=0}^{\infty} \mathcal{E}_N(P^n), \tag{1}$$

where the operator P is the sum of the weights of the walks on β with $J \subseteq \{2, \dots, m\}$.

Stacks of walks are produced when we take the product of the weights of walks. This occurs in the step when we expand the operator P to the power of n.

Huynh and Lê also gave a useful method for evaluating the terms $\mathcal{E}_N(P^n)$ which avoids operator theory. The key result is the following lemma from [15] which computes $\mathcal{E}_N(P^n)$ directly from the weights once they have been put in a preferred order. In the following, we suppress the dependence of the weights on the crossing and write $a_\pm, b_\pm, c_\pm$ instead of $a_{i,\pm}, b_{i,\pm}, c_{i,\pm}$.

Lemma 2.3.

$$\mathcal{E}_N(b_+^s c_+^r a_+^d) = q^{r(N-1-d)} \prod_{i=0}^{d-1} (1 - q^{N-1-r-i})$$

$$\mathcal{E}_N(b_-^s c_-^r a_-^d) = q^{-r(N-1)} \prod_{i=0}^{d-1} (1 - q^{r+i+1-N})$$

We will apply this lemma to the local weights $\mathcal{S}_{(i)}$ of each stack at each crossing. However, before we can apply Lemma 2.3, we must first put the local weights at a crossing into the preferred order. This can always be achieved using the following relations:

$$a_+ b_+ = b_+ a_+, \qquad a_+ c_+ = q c_+ a_+, \qquad b_+ c_+ = q^2 c_+ b_+$$

$$a_- b_- = q^2 b_- a_-, \qquad a_- c_- = q^{-1} c_- a_-, \qquad b_- c_- = q^{-2} c_- b_-$$

Once the local weights have been put into the preferred order at each crossing, Theorem 2.2 and Lemma 2.3 can be applied locally at each crossing to compute the colored Jones polynomial.

The computation is simplified by the observation that only *simple walks* contribute to the colored Jones polynomial [2, Lemma 2.5(a)]. Here, a walk is said to be *simple* if no two paths intersect in the walk, otherwise it is *non-simple*. It turns out that non-simple walks occur in cancelling pairs, so for the purpose of computing $J_{N,K}(q)$, it is enough to consider only simple walks.

The computation is further simplified by the fact that, for any stack of walks, the evaluation of its weights will vanish if the walks in the stack traverse the same arc on N or more different levels [2, Lemma 2.5(b)]. This is extremely useful because it reduces the complexity of the computation and guarantees that only finitely many terms of $\sum_{n=0}^{\infty} \mathcal{E}_N(P^n)$ contribute to the N-th colored Jones polynomial. In particular, for a fixed N, there will always be an upper bound to the integers n which need to be considered in the infinite sum of Equation (1). In practice, this bound can be determined by comparing the arcs traversed by the set of all simple walks for a given braid word.

3 The colored Jones polynomial in closed form

In this section, we apply Theorem 2.2 and Lemma 2.3 to compute $J_{N,K}(q)$, the colored Jones polynomial, for the knots 5_2, 6_1 and 7_2. This is achieved by choosing favorable braid representatives, namely those with only a few simple walks.

In [22], Masbaum uses skein theory to compute the colored Jones polynomial for all twist knots, a class which includes $5_2, 6_1$, and 7_2. More general calculations of the colored Jones polynomial for the double twist knots can be found in [20, 21].

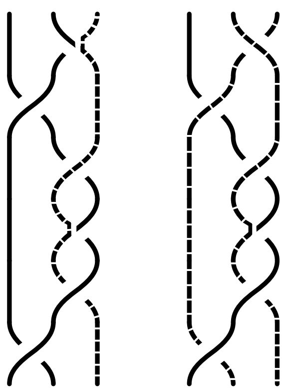


Figure 1: The simple walks A and B shown as arcs with zebra stripes for the braid $\sigma_2^{-1}\sigma_1\sigma_2^3\sigma_1$ with closure the knot 5_2.

Example 3.1. The braid word $\sigma_2^{-1}\sigma_1\sigma_2^3\sigma_1$ represents the knot 5_2 and has two simple walks with $J \subseteq \{2,3\}$. They are $A = qa_{1,-}c_{3,+}a_{4,+}b_{5,+}$ and $B = q^3 b_{1,-}c_{1,-}c_{2,+}c_{3,+}a_{4,+}$ $b_{5,+}b_{6,+}$ (see Figure 1). Notice that A has $J = \{3\}$ and B has $J = \{2,3\}$. Since the walks A and B both traverse the third strand at top and bottom, stacks only need to be considered up to level $N-1$.

Using Theorem 2.2, we can write the colored Jones polynomial as the following:

$$\begin{aligned} J_{N,K}(q) &= q^{(1-N)} \sum_{n=0}^{N-1} \mathcal{E}_N((A+B)^n), \\ &= q^{(1-N)} \sum_{n=0}^{N-1} \mathcal{E}_N((qa_{1,-}c_{3,+}a_{4,+}b_{5,+} + q^3 b_{1,-}c_{1,-}c_{2,+}c_{3,+}a_{4,+}b_{5,+}b_{6,+})^n). \end{aligned}$$

We will expand the above expression using the q-binomial theorem. For that purpose, we introduce the Gaussian binomial coefficients (or q-binomial coefficients), which are defined by

$$\binom{n}{k}_q = \prod_{i=0}^{k-1} \left(\frac{1-q^{n-i}}{1-q^{i+1}} \right).$$

The expansion of the above expression includes a sum of products of A's and B's, which can be interpreted as stacks.

To apply Lemma 2.3, the weights at each crossing must be placed into the order $b^s c^r a^d$, and it is preferable to expand $(A+B)^n$ as a sum of terms of the form $B^k A^{n-k}$. Since the local weights at different crossings commute, the only potential issue with non-commutativity of A and B is at the first crossing. Since $a_{1,-}b_{1,-}c_{1,-} = qb_{1,-}c_{1,-}a_{1,-}$, we have $AB = qBA$, so we can adjust for inversions using the q-binomial coefficient:

$$(A+B)^n = \sum_{k=0}^{n} \binom{n}{k}_q B^k A^{n-k}.$$

Next we use Lemma 2.3 to apply $\mathcal{E}_N(\cdot)$ to evaluate each stack. First, these walks have weights $b_{i,+}$ indexed alone at the fifth and sixth crossings, which evaluates to 1. Additionally, the $c_{i,\pm}$ weights at the first and second crossings in walk B always cancel out since $\mathcal{E}_N(c_{1,-}) = q^{-(N-1)}$ and $\mathcal{E}_N(c_{2,+}) = q^{N-1}$. We still have $c_{3,+}$ in each walk A and walk B. Therefore, for each walk in a stack, the term A or B, q^{N-1} is contributed. Similarly, the weight $a_{4,+}$ appears in both walks, so a stack consisting of n walks will contribute $\prod_{i=1}^{n}(1-q^{N-i})$. Meanwhile, the weight $a_{1,-}$ is only in walk A, so the stack $B^k A^{n-k}$ will contribute $\prod_{i=1}^{n-k}(1-q^{n+i-N})$. Additionally, we need to adjust for the correct order of $b_{1,-}$ and $c_{1,-}$ in the weights in products containing B^k. The number of times the relation is applied increases quadratically with the exponent of B. That is, for a weight containing B^k, its contribution is q^{k^2-k}. Finally, the remaining powers of q arise from the existing variables in the simple walks.

Applying Theorem 2.2, the colored Jones polynomial of 5_2 can be written in closed form as

$$J_{N,K}(q) = q^{N-1} \sum_{n=0}^{N-1} \sum_{k=0}^{n} \binom{n}{k}_q q^{nN+k(k+1)} \prod_{i=1}^{n} \left(1-q^{N-i}\right) \prod_{i=1}^{n-k} \left(1-q^{n+i-N}\right).$$

Example 3.2. The braid word $\sigma_1\sigma_2{\sigma_1}^{-1}{\sigma_3}^{-1}\sigma_2{\sigma_3}^{-1}\sigma_1$ represents the knot 6_1 and has three simple walks with $J \subseteq \{2,3,4\}$. They are $A = qa_{4,-}a_{6,-}$, $B = q^3 c_{2,+}a_{3,-}a_{4,-}b_{5,+}b_{6,-}c_{6,-}$ and $C = q^5 c_{1,+}c_{2,+}b_{3,-}c_{3,-}a_{4,-}b_{5,+}b_{6,-}c_{6,-}b_{7,+}$ (see Figure 2). Notice that A has $J = \{4\}$, B has $J = \{3,4\}$, and C has $J = \{2,3,4\}$. Since the walks A, B and C all traverse the fourth strand at top and bottom, stacks only need to be considered up to level $N-1$.

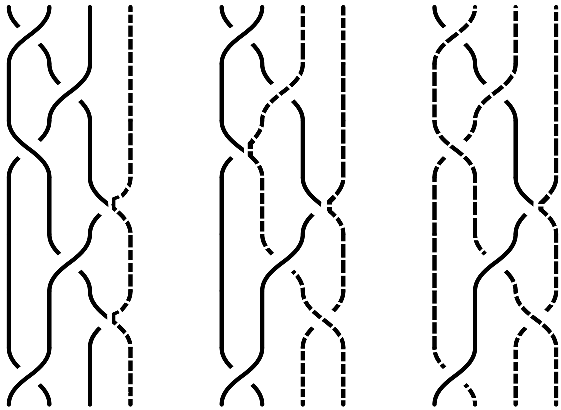


Figure 2: The simple walks A, B and C shown as arcs with zebra stripes for the braid $\sigma_1\sigma_2{\sigma_1}^{-1}{\sigma_3}^{-1}\sigma_2{\sigma_3}^{-1}\sigma_1$ with closure the knot 6_1.

Using Theorem 2.2, the colored Jones polynomial for 6_1 can be written as

$$\begin{aligned}J_{N,K}(q) &= q^{(1-N)}\sum_{n=0}^{N-1}\mathcal{E}_N\left((A+B+C)^n\right),\\ &= q^{(1-N)}\sum_{n=0}^{N-1}\mathcal{E}_N\Big((qa_{4,-}a_{6,-}+q^3c_{2,+}a_{3,-}a_{4,-}b_{5,+}b_{6,-}c_{6,-}\\ &\qquad\qquad + q^5c_{1,+}c_{2,+}b_{3,-}c_{3,-}a_{4,-}b_{5,+}b_{6,-}c_{6,-}b_{7,+})^n\Big).\end{aligned}$$

We use the q-multinomial theorem to expand the terms $(A+B+C)^n$, and to that end we recall the definition of the q-multinomial coefficients.

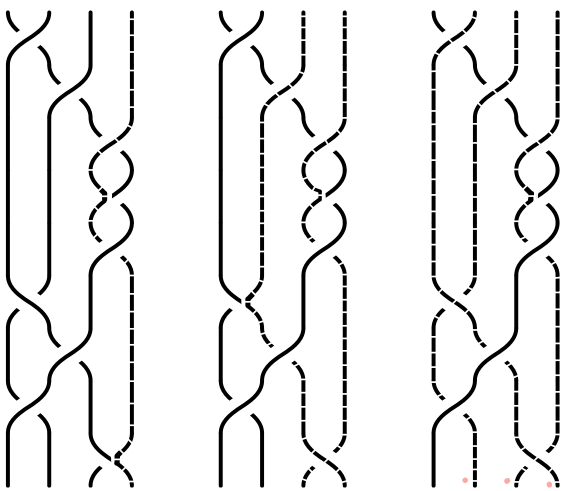


Figure 3: The simple walks A, B and C as arcs with zebra stripes on the braid $\sigma_1\sigma_2\sigma_3^3\sigma_1^{-1}\sigma_2\sigma_1\sigma_3^{-1}$ with closure the knot 7_2.

Given an integer $r \geqslant 1$ and sequence of nonnegative integers $m_1, m_2, \dots, m_r$ such that $n = m_1 + \cdots + m_r$, let

$$\binom{n}{m_1, m_2, \dots, m_r}_q = \frac{[n]_q!}{[m_1]_q![m_2]_q! \dots [m_r]_q!}, \tag{2}$$

where $[n]_q = q^{n-1} + \cdots + q + 1$ and $[n]_q! = [1]_q \cdots [n]_q$. The term $\binom{n}{m_1, m_2, \dots, m_r}_q$ is called the Gaussian multinomial coefficient or q-multinomial coefficient.

With the weights indexed at the third and sixth crossings, the natural order of the walks is C, B, A, as this will allow use of Lemma 2.3 with only a few other adjustments. The use of the q-multinomial coefficient is suitable for this order because inversions with respect to the alphabet C, B, A are reversed with multiplication by q. That is, $AB = qBA$, $AC = qCA$ and $BC = qCB$. The expansion of the trinomial takes the form

$$(A + B + C)^n = \sum_{m=0}^{n} \sum_{k=0}^{m} \binom{n}{n-m, m-k, k}_q C^{n-m} B^{m-k} A^k, \tag{3}$$

where $\binom{n}{n-m, m-k, k}_q$ denotes the q-trinomial coefficient of Equation (2).

We can now expand the trinomial for any power n and use Lemma 2.3 to apply $\mathcal{E}_N(\cdot)$ and evaluate each stack. The $b_\pm$ and $c_\pm$ weights are evaluated the same as in Example 3.1. The weight $a_{4,-}$ appears in each of A, B, C, so for every term $C^{n-m} B^{m-k} A^k$, it will contribute $\prod_{i=1}^{n} (1 - q^{i-N})$. Meanwhile, the weight $a_{3,-}$ only appears in the walk B, so for the term $C^{n-m} B^{m-k} A^k$, it contributes $\prod_{i=1}^{m-k} (1 - q^{n-m+i-N})$. Similarly, the weight $a_{6,-}$ only appears in the walk A, so for the term $C^{n-m} B^{m-k} A^k$, it contributes $\prod_{i=1}^{m-k} (1 - q^{n-k+i-N})$.

Finally, we need to adjust for the correct order of the terms $b_{6,-}$ and $c_{6,-}$ in the products containing $C^{n-m} B^{m-k}$. The number of times the relation is applied increases quadratically with the sum of the exponents of B and C, which is $(n-m) + (m-k) = n-k$. That is, for the term $C^{n-m} B^{m-k} A^k$, applying the relation introduces a factor of $q^{(n-k)^2 - (n-k)}$. We follow the same logic for products C^{n-m} to adjust for the order of the weights $b_{3,-}$ and $c_{3,-}$ at the third crossing.

Applying Theorem 2.2, the colored Jones polynomial of 6_1 can be written in closed form as

$$J_{K,N}(q) = q^{1-N} \sum_{n=0}^{N-1} \sum_{m=0}^{n} \sum_{k=0}^{m} \binom{n}{n-m, m-k, k}_q q^{3n-k-m+(n-k)^2+(n-m)^2} \times \prod_{i=1}^{n} (1 - q^{i-N}) \prod_{i=1}^{m-k} (1 - q^{n-m+i-N}) \prod_{i=1}^{k} (1 - q^{n-k+i-N}).$$

Example 3.3. The braid word $\sigma_1 \sigma_2 \sigma_3^3 \sigma_1^{-1} \sigma_2 \sigma_1 \sigma_3^{-1}$ represents the knot 7_2 and has three simple walks with $J \subseteq \{2, 3, 4\}$. They are $A = qc_{3,+} a_{4,+} b_{5,+} a_{9,-}$, which has has $J = \{4\}$; $B = q^3 c_{2,+} c_{3,-} a_{4,+} b_{5,+} a_{6,-} b_{7,+} b_{9,-} c_{9,-}$, which has has $J = \{3, 4\}$; and $C = q^5 c_{2,+} c_{3,+} a_{4,+} b_{5,+} b_{6,-} c_{6,-} b_{7,+} b_{8,-} b_{9,-} c_{9,-}$, which has $J = \{2, 3, 4\}$ (see Figure 3). Since the walks A, B and C all traverse the fourth strand at top and bottom, stacks only need to be considered up to $N - 1$.

We use Theorem 2.2 to write the colored Jones polynomial for 7_2 as:

$$\begin{aligned} J_{N,K}(q) &= q^{(1-N)}\sum_{n=0}^{N-1}\mathcal{E}_N\left((A+B+C)^n\right), \\ &= q^{(1-N)}\sum_{n=0}^{N-1}\mathcal{E}_N\big((qc_{3,+}a_{4,+}b_{5,+}a_{9,-}+q^3c_{2,+}c_{3,-}a_{4,+}b_{5,+}a_{6,-}b_{7,+}b_{9,-}c_{9,-} \\ &\qquad + q^5c_{2,+}c_{3,+}a_{4,+}b_{5,+}b_{6,-}c_{6,-}b_{7,+}b_{8,-}b_{9,-}c_{9,-})^n\big). \end{aligned}$$

With the weights indexed at the sixth and ninth crossings, the most natural order of the walks is C, B, A. Note that $AB = qBA$, $AC = qCA$ and $BC = qCB$. Therefore, the expansion of the trinomial is as given in equation (3) above.

We expand the trinomial for all powers of n and use Lemma 2.3 to apply $\mathcal{E}_N(\cdot)$ and evaluate each stack. The $b_\pm$ and $c_\pm$ weights are evaluated the same as in Examples 3.1 and 3.2. The weight $a_{4,+}$ appears in each of A, B, C, so for every term $C^{n-m}B^{m-k}A^k$, it will contribute $\prod_{i=1}^{n}(1-q^{N-i})$. Meanwhile, the weight $a_{6,-}$ only appears in the walk B, so for the term $C^{n-m}B^{m-k}A^k$, it contributes $\prod_{i=1}^{m-k}(1-q^{n-m+i-N})$. Similarly, the weight $a_{9,-}$ only appears in the walk A, so for the term $C^{n-m}B^{m-k}A^k$, it contributes $\prod_{i=1}^{k}(1-q^{n-k+i-N})$.

Finally, we need to adjust for the correct order of the terms $b_{9,-}$ and $c_{9,-}$ in the products containing $C^{n-m}B^{m-k}$. The number of times the relation is applied increases quadratically with $(n-m)+(m-k) = n-k$. That is, for the term $C^{n-m}B^{m-k}A^k$, applying the relation introduces a factor of $q^{(n-k)^2-(n-k)}$. We follow the same logic for products C^{n-m} to adjust for the weights at the sixth crossing.

Applying Theorem 2.2, the colored Jones polynomial of 7_2 can be written in closed form as

$$\begin{aligned} J_{K,N}(q) = q^{N-1}\sum_{n=0}^{N-1}\sum_{m=0}^{n}\sum_{k=0}^{m}\binom{n}{n-m,m-k,k}_q q^{nN+2n-m-k+(n-k)^2+(n-m)^2} \\ \times\prod_{i=1}^{n}(1-q^{N-i})\prod_{i=1}^{m-k}(1-q^{n-m+i-N})\prod_{i=1}^{k}(1-q^{n-k+i-N}). \end{aligned}$$

For hyperbolic knots, the Volume Conjecture asserts that

$$\lim_{N\to\infty}\frac{\log|J_{N,K}(e^{2\pi i/N})|}{N} = \frac{\mathrm{Vol}(S^3\smallsetminus K)}{2\pi}.$$

For more information about this important open problem, see the book [24]. The knots in Examples 3.1, 3.2, and 3.3 are all hyperbolic, and the Volume Conjecture has been verified for each of them. For 5_2, this was proved by Ohtsuki [25]; for 6_1, it was proved by Ohtsuki and Yokota [27]; and for 7_2, it follows from Ohtsuki's work on 7-crossing hyperbolic knots [26]. It would be interesting to use the formulas given here to independently verify the Volume Conjecture for these knots.

4 Representing knots as braids

One of the objectives in this paper is to find braid representations of knots that minimize the number of simple walks. To do that, we will apply several different operations that alter the braid word without changing its representative knot. These operations include reflection, rotation, and cyclic permutation of the braid word, and each of them can be used to reduce the number of simple walks. We begin with a review of some standard material on representing knots as braids (see also [5]).

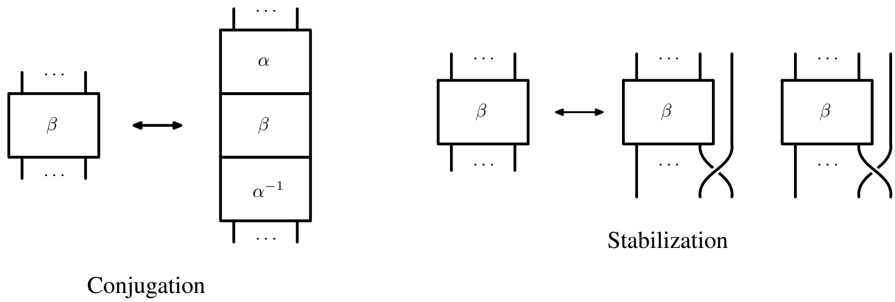


Figure 4: The Markov moves.

Given a braid β, its closure is denoted $\widehat{\beta}$ and is the knot or link obtained by connecting the strands on top with the corresponding strands on bottom without introducing any additional crossings.

The next result is called Alexander's theorem and was first proved in 1923, see [1].

Theorem 4.1. *Every oriented knot or link is equivalent to the closure $\widehat{\beta}$ for some braid $\beta \in B_m$.*

Definition 4.2. The *Markov moves* include *conjugation* and *stabilization* (see Figure 4). Given a braid $\beta \in B_m$, *conjugation* involves replacing it with $\alpha\beta\alpha^{-1}$ for some $\alpha \in B_m$. *Stabilization* involves replacing β with either $\beta\sigma_m$ or $\beta\sigma_m^{-1}$. Note that conjugation preserves the braid width and stabilization increases it by one.

The next result is attributed to Markov. For a proof, see [5, Theorem 2.3].

Theorem 4.3. *Two braids have equivalent link closures if and only if they are related by a sequence of Markov moves.*

Let $\beta \in B_m$, and let

$$SW_\beta = \{W \mid W \text{ is a simple walk on } \beta \text{ with } J \subseteq \{2, \ldots, m\}\} \tag{4}$$

be the set of simple walks on the braid β.

Given a knot, we are interested in finding the braid representative that minimizes the number of simple walks. Of course, the set of simple walks depends on the braid representative chosen. In fact, it depends on the braid word since it is not preserved under insertion (or deletion) of $\sigma_i\sigma_i^{-1}$ or $\sigma_i^{-1}\sigma_i$ into the braid word. This is the analogue, for braids, of the Reidemeister II move. We explain this important point next.

Given a walk on a braid, we say that an arc of the braid is *active* if it is traversed by a path of the walk. Similarly, we say that a crossing is *active* if the walk jumps down from overcrossing arc to undercrossing arc at that crossing. Thus, the active crossings are the ones with the local weight $a_{i,\pm}$. In Figures 1, 2, and 3, the active arcs are depicted with zebra stripes.

Now consider two braid words: $\gamma = \alpha\beta$ and $\gamma' = \alpha\sigma_i\sigma_i^{-1}\beta$. (A similar argument applies to $\gamma' = \alpha\sigma_i^{-1}\sigma_i\beta$.) We will show that $SW_\gamma \subseteq SW_{\gamma'}$.

Suppose W is a simple walk on γ. If both strands $i, i+1$ are active or if they are both not active, then W extends in a unique way to a simple walk on γ'. If one of the strands $i, i+1$ is active and the other is not, then W extends to a simple walk on γ', but possibly in more than one way. This proves the claim, and in particular, we see that the number of simple walks is non-decreasing under an elementary insertion.

Recall that a braid word is said to be *reduced* if it does not contain an occurrence of $\sigma_i\sigma_i^{-1}$ or $\sigma_i^{-1}\sigma_i$. By the above considerations, for any given knot, we can always assume that its braid representative is given by a reduced word.

In a similar way, one can show that the set of simple walks is invariant under far commutativity and the Yang-Baxter relation. For far commutativity, this is straightforward, and we leave the details to the reader. For the Yang-Baxter relation, consider the braid words $\gamma = \alpha\sigma_i\sigma_{i+1}\sigma_i\beta$ and $\gamma' = \alpha\sigma_{i+1}\sigma_i\sigma_{i+1}\beta$ and assume the relevant crossings are $j, j+1$, and $j+2$.

We claim that any simple walk on γ extends in a unique way to a simple walk on γ'. There are several cases, depending on which of the three crossings $j, j+1, j+2$ are active. If none of the crossings are active, then it extends to a simple walk on γ'. If one of the crossings is active, and if we make the corresponding crossing on γ' active, and then it extends to a simple walk on γ'. If two of the crossings of γ are active, then they must be j and $j+2$, and it extends to a simple walk on γ' again with j and $j+2$ active crossings. Note that it is not possible for all three crossings to be active. This shows that $|SW_\gamma| = |SW_{\gamma'}|$ under the Yang-Baxter relation.

One can also apply the Markov moves to a braid and consider their effect on the set of simple walks. For instance, under conjugation, one would expect that the resulting braid word will have a larger set of simple walks. A special case is *cyclic permutation*, which involves replacing $\beta = \sigma_{i_1}^{\varepsilon_1}\sigma_{i_2}^{\varepsilon_2}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}$ with $\beta' = \sigma_{i_2}^{\varepsilon_2}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}\sigma_{i_1}^{\varepsilon_1}$. We will study the effect of cyclic permutation on the set of simple walks in the next section.

Under stabilization, we will show that the set of simple walks is non-decreasing. Let $\beta \in B_m$, $\beta' = \beta\sigma_m^{\pm 1} \in B_{m+1}$, and suppose W is a simple walk on β. If $m \notin J$, then W extends uniquely to a simple walk on β'. If $m \in J$ and $\beta' = \beta\sigma_m$, then we can extend W to a simple walk on β' by either making the extra crossing active or by setting $J' = J \cup \{m+1\}$. If $m \in J$ and $\beta' = \beta\sigma_m^{-1}$, then we can extend W to a simple walk on β' with $J' = J \cup \{m+1\}$. Notice that for $\beta' = \beta\sigma_m^{-1}$, we have one additional simple walk that does not come from β, namely the one with $J = \{m+1\}$ and the extra crossing made active. In particular, it follows that $|SW_\beta| \leqslant |SW_{\beta'}|$.

Let K be a knot and suppose $\beta \in B_{m+1}$ is a braid representative for K with $m \geqslant 1$. If β is conjugate to a braid of the form $\gamma\sigma_m^{\pm}$ for some braid $\gamma \in B_m$, then β is said to be *reducible*. The braid β is said to be *irreducible* if it is not reducible.

The next result summarizes our discussion.

Proposition 4.4. *If K is a knot, then any braid representative for K that minimizes the number of simple walks can be assumed to be given by a reduced and irreducible braid word.*

In addition, one can apply symmetry operations to alter the braid word without changing its knot or link closure. We will use these operations to find braid representatives that minimize the number of simple walks. The three operations we will consider are called reflection, rotation, and reversal, and we introduce them next.

For a given braid β, its reflection is denoted β^* and is obtained by switching all the crossings of β. If β represents the knot K, then β^* represents its mirror image K^*. If $\beta = \sigma_{i_1}^{\varepsilon_1} \cdots \sigma_{i_\ell}^{\varepsilon_\ell}$, then its reflection is the braid word given by $\beta^* = \sigma_{i_1}^{-\varepsilon_1} \cdots \sigma_{i_\ell}^{-\varepsilon_\ell}$ (see Figure 5).

For the purposes of computing the colored Jones polynomial, one can use either β or β^*, since the invariants are related by the simple formula $J_{N,K}(q) = J_{N,K^*}(q^{-1})$. The two braids will have completely different sets of simple walks. In fact, as we shall see in the next section, the simple walks on β and β^* are disjoint and complementary to one another. There is an obvious computational advantage to working with the braid having fewer simple walks.

In fact, there are other symmetries that can be applied to get a new braid representative for a knot (or its mirror image). For example, given a braid word β representing a knot, if one rotates it 180° in the plane, one obtains a new braid word representing the same knot. Specifically, if $\beta = \sigma_{i_1}^{\varepsilon_1} \cdots \sigma_{i_\ell}^{\varepsilon_\ell}$, then the rotated braid word is denoted $\beta^\dagger$ and is given by $\beta^\dagger = \sigma_{m-i_\ell}^{\varepsilon_\ell} \cdots \sigma_{m-i_1}^{\varepsilon_1}$ (see Figure 5).

Another example is braid reversal, which is given by reversing the order of the braid word. Again, the new braid represents the same knot. If $\beta = \sigma_{i_1}^{\varepsilon_1} \cdots \sigma_{i_\ell}^{\varepsilon_\ell}$, then its reversal is denoted β^r and is given by $\beta^r = \sigma_{i_\ell}^{\varepsilon_\ell} \cdots \sigma_{i_1}^{\varepsilon_1}$ (see Figure 5). Notice that β^r is the braid obtained from β by rotating it 180° around a horizontal line in the plane.

There is a one-to-one correspondence between the sets of simple walks on β and β^r. Under the correspondence, the walks have the same set of active crossings, and the weights for the over- and undercrossings $(b_{i,\pm}, c_{i,\pm})$ are switched. In fact, as we shall see, a simple walk is completely determined by its set of active crossings, and it follows that $|SW_\beta| = |SW_{\beta^r}|$.

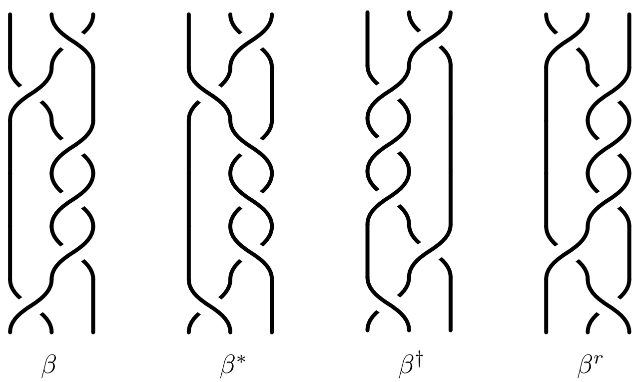


Figure 5: A braid β representing the knot 5_2 and its reflection β^*, rotation $\beta^\dagger$, and reversal β^r.

Given a braid word for a knot, applying reflection, rotation, or cyclic permutation will alter its set of simple walks. Since the computation of the colored Jones polynomial is exponential in the number of simple walks, it is advantageous to choose the braid representative that minimizes the number of simple walks.

5 Semi-simple walks and cyclic permutation

The main result in this section is an invariance property which asserts that under the cyclic permutation, the total number of simple walks on a braid β and its reflection β^* does not change. To see this, we introduce the notion of semi-simple walks and study their behavior under reflection.

Recall the definition of SW_β in Equation (4). Previously, we identified walks W with their weights, given by the ordered product of operators $\{a_{i,\pm}, b_{i,\pm}, c_{i,\pm}\}$ for each crossing traversed. However, it will be more convenient to record W using only the operators $a_{i,\pm}$, and we can do so with no loss of information. In the following, we write a_i instead of $a_{i,\pm}$; it is notationally more compact and the sign $\pm$ can be recovered from the braid word. Thus, there is a one-to-one correspondence between simple walks on β and (certain) monomials in $\{a_1, \dots, a_\ell\}$, as we shall now explain.

Given a simple walk W, recall that the active crossings are where the walk jumps down from the overcrossing arc to the undercrossing arc. If the i-th crossing is active, we record this with a_i. As usual, the crossings are labeled $1, 2, \dots, \ell$ from top to bottom of the braid. The collection of active crossings of W determines a monomial in $\{a_1, \dots, a_\ell\}$, and thus we see that a simple walk determines a monomial. Conversely, the monomial in $\{a_1, \dots, a_\ell\}$ uniquely determines the simple walk W. We will explain this below, but before we do, notice that not every monomial corresponds to a simple walk. For example, the trefoil braid σ_1^3 has three crossings and so there are $2^3 = 8$ possible monomials. However, it has only one simple walk corresponding to the monomial a_2.

Suppose then that $a_{i_1} \cdots a_{i_k}$ is a monomial, indicating that crossings $i_1, \dots, i_k$ are active. We perform an oriented smoothing at each active crossing. Since the walk jumps down there, the crossing type determines which of the arcs are active and which are not. Specifically, if the crossing is positive, the active arc is the one on the left, and if the crossing is negative, the active arc is the one on the right (see Figure 6). At each active crossing, we mark the active arc using some marking scheme. (In all figures, the active arcs have zebra stripes.) We then extend the marking along the arc through any inactive crossings and around the back of the braid closure, continuing again through the braid and around the back as many times as necessary, until reaching another active crossing.

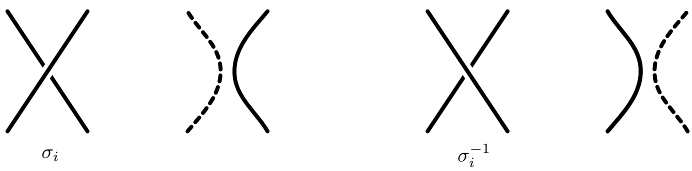


Figure 6: An active crossing and its oriented smoothing for σ_i and σ_i^{-1}. The active arc has zebra stripes and the inactive arc is solid.

One of two things will happen at this active crossing. Either the extended marking is on an inactive arc, in which case the monomial does not correspond to a valid simple walk, or it is on the active arc. If the second case holds for all extended arcs, then this is a valid simple walk. Notice that, in that case, every arc of the partial smoothing of the braid closure is connected to either an active or an inactive arc. To see that we argue by contradiction. If the partial smoothing of $\widehat{\beta}$ contains an arc that is not connected to an active or an inactive arc, then we can follow it along $\widehat{\beta}$ and it will only pass through inactive crossings before returning to itself. Therefore, it determines a sublink of the closure of β, which contradicts the assumption that the closure of β is a knot.

Note that, in the second case, the simple walk is determined by the active or marked arcs, and once those are specified we can read the full operator by recording all the crossings it passes through. This explains why the simple walk is determined by its active crossings. Note that, in order for the marked arcs to be a simple walk, the first strand of the braid at the top and bottom must be inactive.

This process can alternatively be understood in terms of taking the partial smoothing of a knot K at a subset of crossings. Given a subset of crossings, we can perform the partial oriented smoothing of K at the selected crossings. In general, this will produce a link. Our assumption is that the resulting link can be partitioned into two sublinks, one containing the active (or marked) arcs the other containing the inactive (or unmarked) arcs.

So, for a given monomial to correspond to a simple walk, it must be the case that the active and inactive arcs of the braid are contained in different components of the partial smoothing. Further, it must be the case that the first strand of the braid (at bottom) is inactive.

We can apply this to understand the behavior of simple walks under taking reflection. In the mirror image, all the crossings are switched. So, using same monomials to record simple walk on β and β^*, it follows that taking reflection is equivalent to switching the active and inactive arcs. That is because each positive crossing of β is negative in β^* and vice versa. This is illustrated by switching from left to right or vice versa in Figure 6.

The walks on β and β^* with the same monomial are *dual*. We explain this from the point of view of the full set of weights. Let W be a walk on β with monomial $a_{i_1} \cdots a_{i_k}$, and let W^* be the corresponding walk on β^* with monomial $a_{i_1} \cdots a_{i_\ell}$. Then W and W^* trace out disjoint arcs of the braid obtained from β by smoothing the crossings $i_1, \ldots, i_k$. In terms of the weights, the walks W and W^* have the same set of active crossings, but at the inactive crossings, their local weights are opposite. Specifically, if i is an inactive crossing and the local weight $W_{(i)} = b_i$, then $W^*_{(i)} = c_i$. If instead $W_{(i)} = c_i$, then $W^*_{(i)} = b_i$. Likewise, if $W_{(i)} = 1$, then $W^*_{(i)} = b_i c_i$, and if $W_{(i)} = b_i c_i$ then $W^*_{(i)} = 1$.

Lemma 5.1. *The simple walks with $J \subseteq \{2, \ldots, m\}$ on a braid β and its reflection β^* are disjoint. In other words, $SW_\beta \cap SW_{\beta^*} = \varnothing$.*

Proof. Suppose W is a simple walk on β with monomial $a_{i_1} \cdots a_{i_k}$. Then the partial smoothing of β at the crossings $i_1, \ldots, i_k$ can be partitioned into active and inactive arcs. Here, we mark the active arcs, with the first strand of the braid at the top inactive. For the same monomial on the mirror image β^*, the active and inactive arcs will be switched. In particular, the first strand on β^* will be active at the top and marked as such. Therefore, the monomial $a_{i_1} \cdots a_{i_k}$ will not correspond to a valid simple walk on β^*. It follows that $SW_\beta \cap SW_{\beta^*} = \varnothing$, and this completes the proof. □

Definition 5.2. Given a braid word β, we say that a walk W on β is *semi-simple* if it is a simple walk on β or on β^* with $J \subseteq \{2, \ldots, m\}$. We use $\mathfrak{S}_\beta$ to denote the set of semi-simple walks on β. Therefore, $\mathfrak{S}_\beta = SW_\beta \cup SW_{\beta^*}$.

Since SW_β and SW_{β^*} are disjoint, it follows that $|\mathfrak{S}_\beta| = |SW_\beta| + |SW_{\beta^*}|$, where $|S|$ denotes the cardinality of the finite set S.

We leave it as an exercise to show that every monomial a_i for $1 \leqslant i \leqslant \ell$ corresponds to a simple walk on either β or β^*. Thus $|\mathfrak{S}_\beta| \geqslant n$.

Theorem 5.3. *The set of semi-simple walks $\mathfrak{S}_\beta$ is invariant under cyclic permutation of the braid word.*

The theorem is a direct consequence of the next two lemmas. The first lemma implies that cyclic permutation of β does not alter the set of simple walks unless β starts with σ_1 or σ_1^{-1}.

Lemma 5.4. *Suppose $\beta = \sigma_{i_1}^{\varepsilon_1}\sigma_{i_2}^{\varepsilon_2}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}$ is a braid word with $i_1 \neq 1$. Let $\beta' = \sigma_{i_2}^{\varepsilon_2}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}\sigma_{i_1}^{\varepsilon_1}$ be the braid obtained by cyclic permutation. Then $SW_\beta = SW_{\beta'}$.*

Proof. Suppose $W \in SW_\beta$ is a simple walk on β with $J \subseteq \{2,\ldots,m\}$. Let W' be the corresponding simple walk on β', with underlying set J'. There are three possible cases, depending on whether i_1 and i_1+1 lie in J. First, if neither i_1 nor i_1+1 lie in J, then cyclic permutation has no effect and W' is a simple walk on β' with $J' = J$. Second, if exactly one of i_1, i_1+1 lies in J, then $J' \neq J$, but W' is nevertheless a simple walk on β' with $J' \subseteq \{2,\ldots,m\}$. Third, if both i_1 and i_1+1 are in J, then $J' = J$ and W is a valid simple walk on β'. This completes the proof of the lemma. □

The second lemma studies the effect of cyclic permutation for braids that start with σ_1 or σ_1^{-1}. We will show that cyclic permutation of a braid β has the potential to exchange simple walks between SW_β and $SW_{\beta *}$, but it does not alter the set of semi-simple walks.

Lemma 5.5. *Suppose $\beta = \sigma_{i_1}^{\varepsilon_1}\sigma_{i_2}^{\varepsilon_2}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}$ is a braid word with $i_1 = 1$. Let $\beta' = \sigma_{i_2}^{\varepsilon_2}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}\sigma_{i_1}^{\varepsilon_1}$ be the braid obtained by cyclic permutation. Then $\mathfrak{S}_\beta = \mathfrak{S}_{\beta'}$.*

Proof. Suppose $W \in SW_\beta$ is a simple walk on β with $J \subseteq \{2,\ldots,m\}$. Let W' be the corresponding simple walk on β', with underlying set J'. There are two possible cases, depending on whether or not J contains 2. If $2 \notin J$, then $J' = J$ and so $W' \in SW_{\beta'}$. Similarly, if $2 \in J$ and the monomial for W contains a_1 (in which case β necessarily begins with σ_1^{-1}), then again $J' = J$ and $W' \in SW_{\beta'}$. However, if $2 \in J$ and the monomial for W does not contain a_1, then $1 \in J'$ and so $W' \notin SW_{\beta'}$. However, the dual walk $(W')^*$ is simple walk on $(\beta')^*$ with $(J')^* \subseteq \{2,\ldots,m\}$, and hence $(W')^* \in SW_{(be')^*}$. In particular, it follows that the set $\mathfrak{S}_\beta = SW_\beta \cup SW_{\beta *}$ of semi-simple walks is unchanged by cyclic permutation. This completes the proof of the lemma. □

The next result states that, up to reordering the crossings, the set of semi-simple walks on a braid word and its rotation are equal.

Proposition 5.6. *Let $\beta = \sigma_{i_1}^{\varepsilon_1}\cdots\sigma_{i_\ell}^{\varepsilon_\ell}$ be a braid word on m strands, and let $\beta^\dagger = \sigma_{m-i_1}^{\varepsilon_1}\cdots\sigma_{m-i_\ell}^{\varepsilon_\ell}$ be its rotation. Then the sets of semi-simple walks of β and $\beta^\dagger$ are equal, namely $\mathfrak{S}_\beta = \mathfrak{S}_{\beta^\dagger}$.*

Proof. The braid rotation $\beta^\dagger$ is obtained from β by rotating it 180° in the plane. In order to relate the semi-simple walks on β and $\beta^\dagger$, we index the crossings of $\beta^\dagger$ from top to bottom using $n,\ldots,1$, and we identify semi-simple walks on β and $\beta^\dagger$ with the subsets of active crossings. In this way, every semi-simple walk on β and $\beta^\dagger$ corresponds to a monomial $a_{i_1}\ldots a_{i_k}$ indicating that $i_1,\ldots,i_k$ are the active crossings.

Given a monomial $a_{i_1}\ldots a_{i_k}$, the semi-simple walk on β is obtained by taking the smoothing of β at each crossing $i_1,\ldots,i_k$ and locally marking the active and inactive arcs using a marking scheme that differentiates them. (We mark the active arcs using zebra stripes.) Then extend the markings around the braid closure. Since $a_{i_1} \dots a_{i_k}$ corresponds to a semi-simple walk, the markings on the active and inactive arcs will not coincide.

The same will be true for $\beta^\dagger$, provided one follows the same procedures at the corresponding crossings. Since $\beta^\dagger$ is obtained by a 180° rotation which interchanges the first and last strands of the braid, this will not preserve SW_β since the new walk may not satisfy $J \subseteq \{2, \dots, m\}$. Nevertheless, the semi-simple walks of β and $\beta^\dagger$ are preserved. This completes the proof. □

6 Simple walks on $(2, n)$ torus braids

In this section, we show that the number of simple walks on the braid β_n with closure the $(2, n)$ torus link is given by the n-th term in the Fibonacci sequence $1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, \dots$ We will find a closed form solution for the number of simple walks and use it to show they grow exponentially in n.

For $n \geqslant 1$ let $\beta_n = \sigma_1^{-n}$. The closure of β_n is the $(2, n)$ torus knot if n is odd and the $(2, n)$ torus link if n is even. For that reason, we refer to β_n as the (negative) $(2, n)$ torus braid.

Proposition 6.1. *Let $f(n)$ be the number of simple walks on the $(2, n)$ torus braid β_n. Then*

$$f(n) = \left(\frac{5+\sqrt{5}}{10}\right)\left(\frac{1+\sqrt{5}}{2}\right)^n + \left(\frac{5-\sqrt{5}}{10}\right)\left(\frac{1-\sqrt{5}}{2}\right)^n.$$

Proof. The first step is to show that the simple walks on β_n satisfy the Fibonacci recurrence relation

$$f(n) = f(n-1) + f(n-2). \tag{5}$$

To do this, we establish a bijective correspondence between the set of simple walks on β_n and the union of the sets of simple walks on β_{n-1} and β_{n-2}. This is accomplished by extending simple walks on β_{n-1} and β_{n-2} to simple walks on β_n.

In the following, we identify simple walks with their weights, which we write as monomials in $\{a_i, b_i, c_i \mid i = 1, \dots, n\}$. Notice that all simple walks under consideration will have $J = \{2\}$.

Given a simple walk w' on β_{n-1}, set $w = w'a_n$. Then w is a simple walk on β_n. See Figure 7 (left). Since $J = \{2\}$, this is actually the only way to extend w' to a simple walk on β_n .

Similarly, given a simple walk w' on β_{n-2}, set $w = w'b_{n-1}c_n$. Then w is again a simple walk on β_n. See Figure 7 (right). This is the only way to extend w' to a simple walk on β_n which avoids simple walks extended from β_{n-1}.

Figure 7: Extending simple walks from β_{n-1} and β_{n-2} to β_n.

The two sets of simple walks are disjoint. This can be verified by noting that they traverse different strands between the $(n-1)$-st and n-th crossings. Equivalently, one can see this by comparing their weights at the n-th crossing. The simple walks extended from β_{n-1} have weight a_n, whereas those extended from β_{n-2} have weight c_n.

Every simple walk on β_n is an extension of one on β_{n-1} or β_{n-2}. To that end, let w be a simple walk on β_n. Since $J = \{2\}$, at the n-th crossing, either the walk jumps down and has weight a_n, or it stays on the overstrand and has weight c_n. In the first case, $w = w'a_n$ for a simple walk w' on β_{n-1}. In the second, $w = w'b_{n-1}c_n$ for some simple walk w' on β_{n-2}. This establishes the bijective correspondence, and Equation (5) follows directly.

The second step is to solve the recurrence Relation (5). It is a homogeneous linear recurrence relation with constant coefficients and characteristic polynomial

$$p(t) = t^n - t^{n-1} - t^{n-2} = t^{n-2}(t^2 - t - 1).$$

This polynomial has two non-zero roots:

$$t = \frac{1 \pm \sqrt{5}}{2}.$$

Therefore, its general solution is given by $f(n) = c_1(\frac{1+\sqrt{5}}{2})^n + c_2(\frac{1-\sqrt{5}}{2})^n$. Using the values $f(1) = 1$ an $f(2) = 2$, it follows that

$$1 = c_1\left(\frac{1+\sqrt{5}}{2}\right) + c_2\left(\frac{1-\sqrt{5}}{2}\right),$$
$$2 = c_1\left(\frac{1+\sqrt{5}}{2}\right)^2 + c_2\left(\frac{1-\sqrt{5}}{2}\right)^2.$$

Solving for c_1, c_2, we find that

$$c_1 = \frac{5+\sqrt{5}}{10} \quad \text{and} \quad c_2 = \frac{5-\sqrt{5}}{10}.$$

The formula for $f(n)$ follows, and this completes the proof. □

7 Simple walks on $(3, n)$ torus braids

In this section, we show that the number of simple walks on the braid γ_n with closure the $(3, n)$ torus link is given by the n-th term of the sequence $0, 1, 4, 5, 10, 19, 34, 63, 116, 213, 392, 721, 1326, \ldots$ We will find a closed form solution for the number of simple walks and use it to show they grow exponentially in n.

For $n \geqslant 1$, let $\gamma_n = (\sigma_1^{-1}\sigma_2^{-1})^n$. The closure of γ_n is the $(3, n)$ torus knot if $n \not\equiv 0 \pmod 3$ and the $(3, n)$ torus link if $n \equiv 0 \pmod 3$. For that reason, we refer to γ_n as the (negative) $(3, n)$ torus braid.

Proposition 7.1. *Let $g(n)$ be the number of simple walks on the $(3, n)$ torus braid γ_n. Then*

$$g(n) = c_1\alpha^n + c_2\beta^n + c_3\gamma^n,$$

where α, β, γ are the roots of $t^3 - t^2 - t - 1$ (see Equation (7) *for explicit formulas for the roots) and where*

$$c_1 = \frac{1 + 3\alpha^{-1}}{-\alpha^2 + 4\alpha - 1}, \quad c_2 = \frac{1 + 3\beta^{-1}}{-\beta^2 + 4\beta - 1}, \quad c_3 = \frac{1 + 3\gamma^{-1}}{-\gamma^2 + 4\gamma - 1}.$$

Proof. We claim that $g(n)$ satisfies the tribonacci recurrence relation:

$$g(n) = g(n-1) + g(n-2) + g(n-3). \tag{6}$$

The proof of the claim is long, so we first show how to solve the recurrence relation to get the formula for $g(n)$.

The tribonacci numbers $T(n)$ are the sequence $0, 1, 1, 2, 4, 7, 13, \ldots$ for $n \geqslant 0$, and they also satisfy (6). We will use the closed form solution for $T(n)$ to find a closed form solution for $g(n)$. The recurrence Relation (6) has characteristic polynomial $p(t) = t^n - t^{n-1} - t^{n-2} - t^{n-3} = t^{n-3}(t^3 - t^2 - t - 1)$. It has one nonzero real root α and two complex roots β and γ given by

$$\begin{aligned} \alpha &= \tfrac{1}{3}(1 + \sqrt[3]{19 + 3\sqrt{33}} + \sqrt[3]{19 - 3\sqrt{33}}), \\ \beta &= \tfrac{1}{2}(1 - \alpha + \sqrt{-3\alpha^2 + 2\alpha + 5}), \\ \gamma &= \tfrac{1}{2}(1 - \alpha - \sqrt{-3\alpha^2 + 2\alpha + 5}). \end{aligned} \tag{7}$$

The closed form solution for $T(n)$ is a linear combination of powers of the roots of the characteristic polynomial:

$$T(n) = \frac{\alpha^n}{-\alpha^2 + 4\alpha - 1} + \frac{\beta^n}{-\beta^2 + 4\beta - 1} + \frac{\gamma^n}{-\gamma^2 + 4\gamma - 1}.$$

The sequence $g(n)$ is related to the tribonacci sequence by the equation

$$g(n) = T(n) + 3T(n-1).$$

From this we can write $g(n) = c_1\alpha^n + c_2\beta^n + c_3\gamma^n$ and use the values $g(1) = 0, g(2) = 1, g(3) = 4$ to solve for the coefficients c_1, c_2, c_3:

$$c_1 = \frac{1 + 3\alpha^{-1}}{-\alpha^2 + 4\alpha - 1}, \quad c_2 = \frac{1 + 3\beta^{-1}}{-\beta^2 + 4\beta - 1}, \quad c_3 = \frac{1 + 3\gamma^{-1}}{-\gamma^2 + 4\gamma - 1}.$$

It remains to prove the claim, namely to show that the simple walks on γ_n satisfy the recurrence Relation (6) for all $n \geqslant 4$. To do this, we establish a bijective correspondence between the simple walks on γ_n and the union of the sets of simple walks on γ_{n-1}, γ_{n-2} and γ_{n-3}. In general, for braids on three strands, the simple walks will have $J = \{2\}$, $J = \{3\}$ or $J = \{2, 3\}$. For the $(n, 3)$ torus braids, all three occur.

We claim that every simple walk on γ_{n-1}, γ_{n-2} and γ_{n-3} can be extended to a simple walk along γ_n. We prove this by considering the three cases separately. As before, we will identify simple walks with their weights, which we write as monomials in $\{a_i, b_i, c_i \mid i = 1, \ldots, 2n\}$.

Suppose w' is a simple walk on γ_{n-1}. If $J = \{2\}$, then it is on the understrand at the $(2n-2)$-nd crossing, and so $w' = w'' b_{2n-2}$. We set $w = w'' a_{2n-2} b_{2n}$ and note that w is a simple walk on γ_n with $J = \{2\}$. If $J = \{3\}$, then we set $w = w' a_{2n}$. If $J = \{2, 3\}$, then we set $w = w' b_{2n} \cdot a_{2n-1} c_{2n}$. Note that in this last case, the paths become inverted, but this is allowable for the walks with $J = \{2, 3\}$. Figure 8 shows how the simple walks are extended. In all three cases it is clear that w is a simple walk on γ_n.

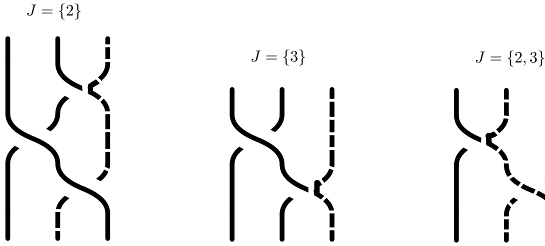


Figure 8: Extending simple walks from γ_{n-1} to γ_n.

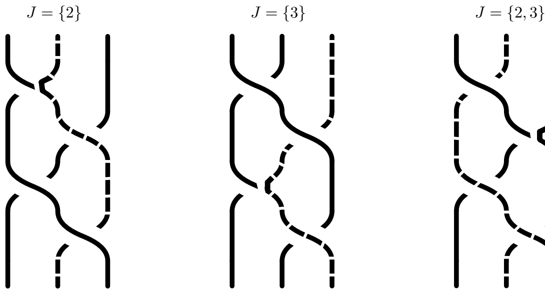


Figure 9: Extending simple walks from γ_{n-2} to γ_n.

In a similar way, we can extend simple walks on γ_{n-2}. Let w' be a simple walk on γ_{n-2}. If $J = \{2\}$, then we set $w = w'a_{2n-3}c_{2n-2}b_{2n}$. If $J = \{3\}$, then we set $w = w'b_{2n-2}a_{2n-1}c_{2n}$. If $J = \{2,3\}$, then we set $w = w'a_{2n-2}b_{2n} \cdot b_{2n-3}c_{2n-1}c_{2n}$. In this last case, notice that the paths become inverted. Figure 9 shows how the simple walks are extended. In all three cases, it is clear that w is a simple walk on γ_n.

Lastly, let w' be a simple walk on γ_{n-3}. Then since $\gamma_n = \gamma_{n-3}(\sigma_1^{-1}\sigma_2^{-1})^3$ with $(\sigma_1^{-1}\sigma_2^{-1})^3$ inducing the identity permutation, we can extend w' to a simple walk on γ_n by remaining on the same strands. If $J = \{2\}$, then we set $w = w'b_{2n-5}c_{2n-3}c_{2n-2}b_{2n}$. If $J = \{3\}$, then we set $w = w'b_{2n-4}b_{2n-3}c_{2n-1}c_{2n}$. If $J = \{2,3\}$, then we set $w = w'b_{2n-5}c_{2n-3}c_{2n-2}b_{2n} \cdot b_{2n-4}b_{2n-3}c_{2n-1}c_{2n}$. Figure 10 shows how the simple walks are extended. In all three cases, it is clear that w is a simple walk on γ_n.

It is not difficult to see that the sets of extended simple walks from $\gamma_{n-1}, \gamma_{n-2}$, and γ_{n-3} are all disjoint. For instance, this follows by comparing their weights, and noting they are pairwise unequal.

The last step is to show that this accounts for all simple walks on γ_n. We will see that every simple walk on γ_n is an extension of a simple walk on γ_{n-1}, γ_{n-2} or γ_{n-3}.

Suppose w is a simple walk on γ_n. If $J = \{2\}$, then it must traverse the understrand at the $2n$-th crossing and is on the overstrand just below the $(2n-2)$-nd crossing. If it jumps down at the $(2n-2)$-nd crossing, then $w = w''a_{2n-2}b_{2n}$, and w is the extension of the simple walk $w' = w''n_{2n-2}$ on γ_{n-1}. Otherwise, if it remains on the overstrand at the $(2n-2)$-nd crossing, then either $w = w'a_{2n-3}c_{2n-2}b_{2n}$ for w' a simple walk on γ_{n-2}, or $w = w'b_{2n-5}c_{2n-3}c_{2n-2}b_{2n}$ for w' a simple walk on γ_{n-3}.

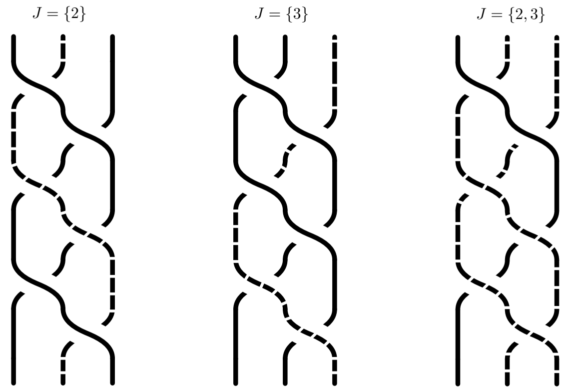


Figure 10: Extending simple walks from γ_{n-3} to γ_n.

If instead $J = \{3\}$, then it is on the overstrand just below the $(2n)$-th crossing. If it jumps down at the $(2n)$-th crossing, then $w = w'a_{2n}$ for w' a simple walk on γ_{n-1}. Otherwise, if it remains on the overstrand at the $(2n)$-th crossing, then either $w = w'b_{2n-2}a_{2n-1}c_{2n}$ for w' a simple walk on γ_{n-2}, or $w = w'b_{2n-4}b_{2n-3}c_{2n-1}c_{2n}$ for w' a simple walk on γ_{n-3}.

Lastly, suppose $J = \{2, 3\}$. Then w consists of two paths, ends with $b_{2n}c_{2n}$, and is on the overstrand below the $(2n-1)$-st crossing. If it jumps down at the $(2n-1)$-st crossing, then $w = w'b_{2n} \cdot a_{2n-1}c_{2n}$ for w' a simple walk on γ_{n-1}. If it remains on the overstrand at the $(2n-1)$-st crossing, then it is also on the overstrand at the $(2n-2)$-nd crossing. If it jumps down at the $(2n-2)$-nd crossing, then $w = w'a_{2n-2}b_{2n} \cdot b_{2n-3}c_{2n-1}c_{2n}$ for w' a simple walk on γ_{n-2}. If it remains on the overstrand at the $(2n-2)$-nd crossing, then it approaches the $(2n-4)$-th and $(2n-5)$-th crossings on understrands, and it follows that $w = w'b_{2n-5}c_{2n-3}c_{2n-2}b_{2n} \cdot b_{2n-4}b_{2n-3}c_{2n-1}c_{2n}$ for w' a simple walk on γ_{n-3}.

This shows that every simple walk on γ_n is obtained by extending a simple walk on $\gamma_{n-1}, \gamma_{n-2}$ or γ_{n-3}. It follows that there is a bijection correspondence between the set of simple walks on γ_n and the union of the simple walks on $\gamma_{n-1}, \gamma_{n-2}$ and γ_{n-3}. The bijective correspondence implies that the sequence $g(n)$ of simple walks on γ_n satisfy the recurrence Relation (6). □

8 Minimal braid representatives

In Table 5, we list knots up to 9 crossings with the braid representatives giving minimal numbers of simple walks. More extensive tables of knots up to 13 crossings and braid representatives for them can be found online at [7]. (In [7] and Table 1 below, we use the notation for braid words from sagemath, meaning that a braid word $\sigma_{a_1}^{\varepsilon_1} \cdots \sigma_{a_\ell}^{\varepsilon_\ell}$ is denoted by $[\varepsilon_1 a_1, \ldots, \varepsilon_\ell a_\ell]$. Tables 4 and 5 use even more compactified notation similar to that at the end of [16].)

These results are empirical. The braid words listed in Table 5 and [7] are the output of a sagemath program developed by the second author. It takes as input braid representatives

Knot	Braid Word	$\lvert SW_\beta \rvert$
$11a_{322}$	$[-1,-1,2,-3,4,-3,2,-3,4,1,2,-3,-2,-2]$	51
$12a_{23}$	$[-1,-3,2,-3,-5,2,4,1,2,-3,-4,5,4,-3,-5,4,2]$	153
$12a_{155}$	$[-1,2,2,-3,4,-3,4,-5,-4,3,2,1,-4,5,2,-3,2]$	127
$12a_{288}$	$[-1,2,2,-3,2,-3,2,1,2,-3,4,2,-3,4]$	71
$12a_{449}$	$[-1,2,4,-3,4,5,4,2,-3,-4,-4,-5,1,2,4,-3,2]$	125
$12a_{494}$	$[-1,2,-3,4,5,2,-3,-4,-4,1,2,-3,4,-5,4,-3,2]$	137
$12a_{750}$	$[-1,2,-3,2,-3,5,4,-3,-4,-4,-5,-4,-4,-3,1,4,-2,3,-2]$	183
$12n_{546}$	$[-1,2,3,1,-2,1,1,1,1,-2,-3,-3,2]$	41
$12n_{601}$	$[-1,-1,2,3,3,3,2,-4,-4,-3,1,2,3,3,-4,2]$	67
$12n_{622}$	$[-1,-1,2,2,3,3,2,-4,1,-2,3,-4,-2,3]$	47

Table 1: Knots up to 12 crossings whose minimizing braid word begins with σ_1^{-1}.

for knots (given by the braids from [19] and [29]) and applies cyclic permutation, reflection, and rotation. It then selects the braid word that minimizes the number of simple walks. The output braid word may represent the knot K or its mirror image K^*, whichever has fewest simple walks.

The braids listed have the fewest simple walks among all *known* braid representatives for the given knots. In general, the question of finding a complete list of braid representatives for a given knot is a delicate and open problem. As we shall see, it is not enough to consider only braid representatives of minimal width. Even if it were, it is an open problem to develop an algorithm for computing the braid width of a knot (see Open Problem 1 in [6]). Nevertheless, these problems have been studied extensively, and much is known about minimal braid representatives of low-crossing knots; see [13, 16] and [29].

Given a knot, one can look for braid representatives that minimize its braid width or the braid length. For many knots, there is a braid representative that simultaneously minimizes both the width and length, but in general, the braid representatives that minimize width need not be the same as the ones that minimize length. The earliest known examples are the knots 16_{472381} and $16_{1223549}$, which were discovered by Stoimenow and have braid width 4 but no minimal length braid representative of width 4, [28, Figure 7].

This interesting aspect has been further studied by Gittings [13] and Van Cott [30], and the "smallest" example is the knot 10_{136}. For all other knots with up to 10 crossings, there is a braid representative that simultaneously minimizes the braid width and length. Further examples of knots whose minimal width braid representatives are not minimal length are listed in Table 4. (These examples come from [19].)

Interestingly, the braid representative that minimizes the number of simple walks is not always a minimal length braid, nor is it always a minimal width braid either. For example, consider the knots 10_{136} and $11n_8$ and their braid representatives in Table 4. For 10_{136}, the number of simple walks is minimized on a braid representative of minimal length but not one of minimal width, whereas for $11n_8$, the number of simple walks is minimized on a braid representative of minimal width but not one of minimal length. Similar examples can be found among the other knots listed in Table 4.

Our computations suggest that, for any knot, one can always minimize the number of simple walks on a braid representative of minimal width or minimal length. This is an interesting problem for future investigation. In order to make progress, we need more information about the minimal width and minimal length braid representatives for knots. At present, we do not have complete information on the 13-crossing knots. In particular, we do not know which 13-crossing knots have minimal length braid representatives that are not minimal width. The braid representatives for the 13-crossing knots from [29] are known to be of minimal width, but they are not known to be of minimal length.

Notice that for every knot in Table 5, the braid representative that minimizes the number of simple walks begins with σ_1. This is actually true for all knots up to 10 crossings, but not immediately true for knots with 11 or more crossings (see [7]).

In general, by Lemma 5.4, the minimizing braid representative can always be chosen to begin with either σ_1 or σ_1^{-1}. For knots with 11 and 12 crossings, there are only a handful of examples whose minimizing braid representative begins with σ_1^{-1} and not σ_1. They are listed in Table 1. (There are in addition 82 examples among the knots with 13 crossings, see [7].) In each case, we can find a minimizing braid representative that begins with σ_1 by reversing the braid word and applying cyclic permutation. We explain these steps in more detail.

Take, for example, the first knot in Table 1, namely $11a_{322}$. Its minimizing braid representative is the braid word $\sigma_1^{-2}\sigma_2\sigma_3^{-1}\sigma_4\sigma_3^{-1}\sigma_2\sigma_3^{-1}\sigma_4\sigma_1\sigma_2\sigma_3^{-1}\sigma_2^{-2}$. The reversed braid word will have the same number of simple walks, so it follows that $\sigma_2^{-2}\sigma_3\sigma_2\sigma_1$ $\sigma_4\sigma_3^{-1}\sigma_2\sigma_3^{-1}\sigma_4\sigma_3^{-1}\sigma_2\sigma_1^{-2}$ is also a minimizing braid word for $11a_{322}$. Now repeated application of Lemma 5.4 shows that the braid word $\sigma_1\sigma_4\sigma_3^{-1}\sigma_2\sigma_3^{-1}\sigma_4\sigma_3^{-1}\sigma_2\sigma_1^{-2}\sigma_2^{-2}\sigma_3\sigma_2$ is also minimizing for $11a_{322}$.

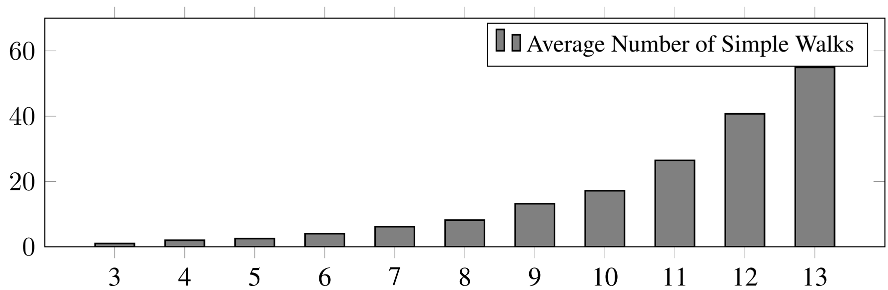


Table 2: Average number of simple walks by crossing number.

The same method applies to the other knots in Table 1. Each one admits a minimizing braid word that starts with σ_1. A similar argument applies to the braid representatives for the 13 crossing knots that begin with σ_1^{-1}. This follows by a routine but somewhat tedious exercise.

Table 2 shows the growth rate of the number of simple walks as a function of the crossing number of the knot. Table 3 shows the growth rate of the number of simple walks as a function of the braid length. Note that Table 3 contains information for knots with up to 12 crossings but not the 13-crossing knots. The reason is that we do not have definitive information about the braid representatives of minimal length for the 13-crossing knots.

We end this paper with a few questions and open problems for future investigation. One is whether braid words that minimize the number of simple walks have a preferred shape or form. By Proposition 4.4, we can assume the braid word is reduced and irreducible, and by Lemma 5.4, we can assume it begins with σ_1 or σ_1^{-1}. We conjecture the braid word can always be chosen to begin with σ_1. Further results as to the shape of minimizing braid words would be helpful for developing efficient search algorithms.

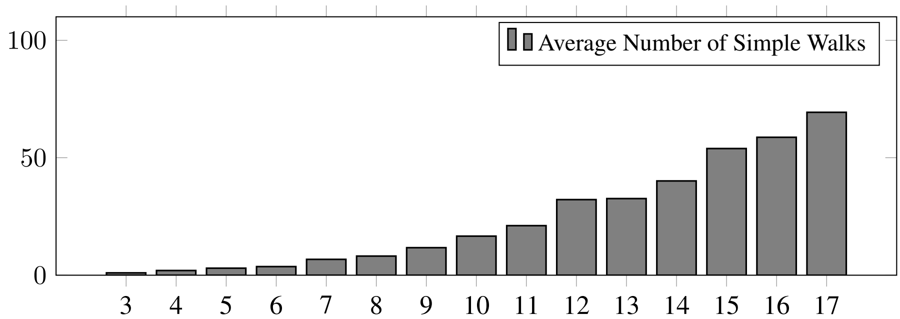


Table 3: Average number of simple walks by braid length.

More generally, it would be extremely useful to automate the generation of minimal width and/or minimal length braid representatives for a given knot. Such tools would allow fast computation of the colored Jones polynomial and other quantum knot invariants, enabling calculations for higher crossing knots, including those in the knot tables of Burton [8], who has recently extended the classification of knots to 19 crossings.

Auxilliary files

Sagemath programs and datasets are available online [7]. This includes a program that generates all the simple walks as operators for a given braid and another that selects braid words that minimize the number of simple walks. It also includes input datasets used to create Tables 4 and 5, as well as output datasets of braid words that minimize the number of simple walks for knots up to 13 crossings.

Knot	Minimal width braid	|SW|	Minimal length braid	|SW|
10_{136}	$123^{-1}21^{-1}2^23^{-1}2^{-2}1$	21	$12^{-1}3^{-1}2^243^{-1}412^{-1}$	17
$11n_8$	$123^{-1}2^{-1}12^{-1}1^{-1}23^22^21$	20	$121^{-1}213^{-1}2^243^{-1}41$	23
$11n_{121}$	$123^22^{-1}12^{-1}1^{-1}2^23^{-1}21$	20	$121^23^{-1}21^{-1}243^{-1}41$	21
$11n_{131}$	$123^22^{-2}1^22^{-1}3^{-1}212^{-1}$	17	$123^{-1}213^22^{-1}3^{-1}43^{-1}4$	21
$12n_{17}$	$2^{-1}12^{-1}34^{-2}32^{-2}3^{-1}43^{-1}41$	63	$(12^{-1})^23^{-1}2^243^25^{-1}45^{-1}$	52
$12n_{20}$	$3^{-1}12^{-1}(32^{-1})^21^{-1}23^{-1}2^21$	26	$(12^{-1})^2(3^{-1}2)^243^{-1}41$	32
$12n_{24}$	$12^{-1}32^{-2}32^{-1}3^{-1}1^{-1}23^{-1}21$	35	$2^{-1}12^{-1}3^{-1}2^243^{-3}41$	32
$12n_{65}$	$2^{-1}123^{-1}4243^{-1}23^{-1}4^{-1}23^{-1}1$	26	$121^{-1}3^{-1}23^{-1}4^{-1}3^254^{-1}51$	25
$12n_{119}$	$2^{-1}1^22^{-1}313(12^{-1})^23^{-1}1$	31	$2^{-1}13^{-1}243^{-1}41^22^{-1}1^2$	23
$12n_{284}$	$(12^{-2})^23132^{-1}12^{-1}3^{-1}$	36	$2^{-1}12^{-1}3^{-1}23^{-1}43^{-1}23^{-1}41$	32
$12n_{311}$	$4121^{-1}23^{-1}42^{-1}3^{-1}432^{-1}3^{-1}1$	37	$2^{-1}1324^{-1}3^{-1}23^{-1}54^{-1}351$	30
$12n_{314}$	$2^{-1}3^{-1}(12^{-1})^33132^{-1}1$	34	$(12^{-1})^23^{-1}2143^{-1}2^{-1}43$	24
$12n_{358}$	$2^{-1}3^{-1}121^{-1}212^{-1}3132^{-1}1$	24	$3^{-1}2^{-1}1432^{-1}34^{-1}3421$	20
$12n_{362}$	$123^{-2}21^{-1}2^23^{-1}2^{-1}32^{-1}1$	42	$3^{-1}2^{-1}12^{-2}43^{-1}41^221$	24
$12n_{403}$	$12^{-1}3^42^{-1}3^{-1}1^{-1}23^{-1}21$	37	$1213^{-1}2^{-1}12^{-1}43^{-1}241$	20
$12n_{482}$	$2^{-1}3^{-1}13^{-1}2^21^{-2}232^{-1}1^2$	29	$2^{-1}12^{-1}3^{-1}243^{-1}23^{-2}41$	32

Table 4: Simple walks for representatives of minimal braid width and length.

Knot	Braid Word	|SW|
$\mathbf{3_1}$	1^3	1
$\mathbf{4_1}$	$(12^{-1})^2$	2
$\mathbf{5_1}$	1^5	3
$\mathbf{5_2}$	12^312^{-1}	2
$\mathbf{6_1}$	$121^{-1}3^{-1}23^{-1}1$	3
$\mathbf{6_2}$	$1^32^{-1}12^{-1}$	4
$\mathbf{6_3}$	$1^22^{-1}12^{-2}$	5
$\mathbf{7_1}$	1^7	8
$\mathbf{7_2}$	$123^31^{-1}213^{-1}$	3
$\mathbf{7_3}$	$1^421^{-1}21$	6
$\mathbf{7_4}$	$12^232^{-1}3212^{-1}$	5
$\mathbf{7_5}$	$1^321^{-1}2^21$	5
$\mathbf{7_6}$	$1^22^{-1}132^{-1}3$	8
$\mathbf{7_7}$	$(12^{-1})^232^{-1}3$	8
$\mathbf{8_1}$	$1234^{-1}2^{-1}3212^{-1}4^{-1}$	4
$\mathbf{8_2}$	$1^52^{-1}12^{-1}$	9
$\mathbf{8_3}$	$121^{-1}3^{-1}23^{-1}4^{-1}34^{-1}1$	9
$\mathbf{8_4}$	$123^{-1}23^{-3}12^{-1}$	7
$\mathbf{8_5}$	$(1^32^{-1})^2$	8
$\mathbf{8_6}$	$1^321^{-1}3^{-1}23^{-1}1$	7
$\mathbf{8_7}$	$1^42^{-1}12^{-2}$	10
$\mathbf{8_8}$	$1^221^{-1}3^{-1}23^{-2}1$	10
$\mathbf{8_9}$	$1^32^{-1}12^{-3}$	9
$\mathbf{8_{10}}$	$1^32^{-1}1^22^{-2}$	9
$\mathbf{8_{11}}$	$121^{-1}2^23^{-1}23^{-1}1$	7
$\mathbf{8_{12}}$	$(12^{-1}34^{-1})^2$	14
$\mathbf{8_{13}}$	$12^23^{-1}23^{-2}12^{-1}$	8
$\mathbf{8_{14}}$	$1^221^{-1}(23^{-1})^21$	8
$\mathbf{8_{15}}$	$12^3132^{-1}3^2$	9
$\mathbf{8_{16}}$	$1^22^{-1}12^{-1}1^22^{-1}$	9
$\mathbf{8_{17}}$	$1(12^{-1})^32^{-1}$	9
$\mathbf{8_{18}}$	$(12^{-1})^4$	10
$\mathbf{8_{19}}$	$(12^3)^2$	5
$\mathbf{8_{20}}$	12^312^{-3}	5
$\mathbf{8_{21}}$	$1^221^{-2}2^21$	6
$\mathbf{9_1}$	1^9	21
$\mathbf{9_2}$	$12343^{-1}42^{-1}3^2212^{-1}$	5
$\mathbf{9_3}$	$1^621^{-1}21$	14
$\mathbf{9_4}$	$123^22^43^{-1}12$	9
$\mathbf{9_5}$	$121^{-1}2342^{-1}3^{-1}4321$	10
$\mathbf{9_6}$	$1^521^{-1}2^21$	12
$\mathbf{9_7}$	$123^42^23^{-1}12^{-1}$	9
$\mathbf{9_8}$	$1412^{-1}3^{-1}423^{-1}12^{-1}$	13
$\mathbf{9_9}$	$12^31^{-1}21^4$	12
$\mathbf{9_{10}}$	$1232^{-1}32^31^{-1}21$	11
$\mathbf{9_{11}}$	$12^{-1}1^3312^{-1}3$	15
$\mathbf{9_{12}}$	$123^{-1}41^{-1}23^{-1}414$	13
$\mathbf{9_{13}}$	$1232^{-1}321^{-1}2^31$	10
$\mathbf{9_{14}}$	$121^{-1}3^{-1}23^{-1}43^{-1}41$	11
$\mathbf{9_{15}}$	$1^223^{-1}41^{-1}23^{-1}41$	16
$\mathbf{9_{16}}$	$12^31^{-1}2^21^3$	10
$\mathbf{9_{17}}$	$(12^{-1})^22^{-1}(32^{-1})^2$	17
$\mathbf{9_{18}}$	$12^23^22^312^{-1}3^{-1}$	10
$\mathbf{9_{19}}$	$12^{-2}3^{-1}243^{-1}412^{-1}$	14
$\mathbf{9_{20}}$	$1^32^{-1}3132^{-1}3$	15
$\mathbf{9_{21}}$	$121^{-1}23^{-1}243^{-1}41$	12
$\mathbf{9_{22}}$	$12^{-1}312^{-3}32^{-1}$	17
$\mathbf{9_{23}}$	$12^21^{-1}23^{-1}2^213^2$	15
$\mathbf{9_{24}}$	$1312^{-1}312^{-3}$	17
$\mathbf{9_{25}}$	$12^334^{-1}12^{-1}34^{-1}$	14
$\mathbf{9_{26}}$	$12^{-1}1^2312^{-1}32^{-1}$	13
$\mathbf{9_{27}}$	$1^22^{-1}12^{-2}32^{-1}3$	15
$\mathbf{9_{28}}$	$12^{-1}1312^{-2}3^2$	17
$\mathbf{9_{29}}$	$(12^{-1}32^{-1})^22^{-1}$	16
$\mathbf{9_{30}}$	$1^22^{-2}12^{-1}32^{-1}3$	16
$\mathbf{9_{31}}$	$12^{-1}1312^{-1}3^22^{-1}$	15
$\mathbf{9_{32}}$	$1(12^{-1})^2312^{-1}3$	14
$\mathbf{9_{33}}$	$(12^{-1})^22^{-1}312^{-1}3$	16
$\mathbf{9_{34}}$	$12^{-1}3(12^{-1})^232^{-1}$	13
$\mathbf{9_{35}}$	$1234^{-1}341^{-1}42^{-1}32123^{-1}$	17
$\mathbf{9_{36}}$	$1^32^{-1}1312^{-1}3$	14
$\mathbf{9_{37}}$	$(12^{-1}3)^243^{-1}23^{-1}2^{-1}4^{-1}$	29
$\mathbf{9_{38}}$	$123^221^{-1}23^{-1}2^21$	13
$\mathbf{9_{39}}$	$123^{-1}2143^{-1}2^{-1}4^{-1}34^2$	18
$\mathbf{9_{40}}$	$12^{-1}312^{-1}132^{-1}3$	14
$\mathbf{9_{41}}$	$13^{-1}423^{-1}23^{-2}12^{-1}34$	20
$\mathbf{9_{42}}$	$123^{-1}212^{-3}3^{-1}$	7
$\mathbf{9_{43}}$	$12^33^{-1}123^{-1}2$	8
$\mathbf{9_{44}}$	$123^{-1}2^212^{-1}3^{-1}2^{-1}$	7
$\mathbf{9_{45}}$	$12^3312^{-1}32^{-1}$	8
$\mathbf{9_{46}}$	$123^{-1}212^{-1}32^{-1}3$	8
$\mathbf{9_{47}}$	$(123^{-1}2)^23^{-1}$	8
$\mathbf{9_{48}}$	$123^22^{-1}12^{-1}3^{-1}1^{-1}21$	9
$\mathbf{9_{49}}$	$12^21312^{-1}3212^{-1}$	9

Table 5: Knots up to 9 crossings and braid words minimizing the number of simple walks.

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Petra Šparl Award 2024: Call for Nominations

The Petra Šparl Award was established in 2017 to recognise in each even-numbered year the best paper published in the previous five years by a young woman mathematician in one of the two journals *Ars Mathematica Contemporanea* (*AMC*) and *The Art of Discrete and Applied Mathematics* (*ADAM*). It was named after Dr Petra Šparl, a talented woman mathematician who died mid-career in 2016.

The award consists of a certificate with the recipient's name, and invitations to give a lecture at the Mathematics Colloquium at the University of Primorska, and lectures at the University of Maribor and University of Ljubljana. The first award was made in 2018 to Dr Monika Pilśniak (AGH University, Poland) for a paper on the distinguishing index of graphs, and then two awards were made for 2020, to Dr Simona Bonvicini (Università di Modena e Reggio Emilia, Italy) for her contributions to a paper giving solutions to some Hamilton-Waterloo problems, and Dr Klavdija Kutnar (University of Primorska, Slovenia), for her contributions to a paper on odd automorphisms in vertex-transitive graphs. The award for 2022 was made to Dr Jelena Sedlar (University of Split, Croatia) for resolving two open conjectures regarding the Wiener index of trees.

The Petra Šparl Award Committee is now calling for nominations for the next award.

Eligibility: Each nominee must be a woman author or co-author of a paper published in either *AMC* or *ADAM* in the calendar years 2019 to 2023, who was at most 40 years old at the time of the paper's first submission.

Nomination Format: Each nomination should specify the following:

(a) the name, birth-date and affiliation of the candidate;
(b) the title and other bibliographic details of the paper for which the award is recommended;
(c) reasons why the candidate's contribution to the paper is worthy of the award, in at most 500 words; and
(d) names and email addresses of one or two referees who could be consulted with regard to the quality of the paper.

Procedure: Nominations should be submitted by email to any one of the three members of the Petra Šparl Award Committee (see below), **by 31 October 2023**.

Award Committee:

- Marston Conder, m.conder@auckland.ac.nz
- Asia Ivić Weiss, weiss@yorku.ca
- Aleksander Malnič, aleksander.malnic@guest.arnes.si

Marston Conder, Asia Ivić Weiss and Aleksander Malnič
Members of the *2024 Petra Šparl Award Committee*

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