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Connected Turán number of trees

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Abstract

The connected Turán number is a variant of the much studied Turán number, $\mathrm{ex}(n, F)$, the largest number of edges that an n-vertex F-free graph may contain. We start a systematic study of the connected Turán number $\mathrm{ex}_c(n, F)$, the largest number of edges that an n-vertex *connected* F-free graph may contain. We focus on the case where the forbidden graph is a tree. Prior to our work, $\mathrm{ex}_c(n, T)$ was determined only for the case T is a star or a path. Our main contribution is the determination of the exact value of $\mathrm{ex}_c(n, T)$ for small trees, in particular for all trees with at most six vertices, as well as some trees on seven vertices and several infinite families of trees. We also collect several lower-bound constructions of connected T-free graphs based on different graph parameters.

The celebrated conjecture of Erdős and Sós states that for any tree T, we have $\mathrm{ex}(n, T) \leq (|T| - 2)\frac{n}{2}$. We address the problem how much smaller $\mathrm{ex}_c(n, T)$ can be, what is the smallest possible ratio of $\mathrm{ex}_c(n, T)$ and $(|T| - 2)\frac{n}{2}$ as $|T|$ grows.

Keywords: Extremal graph theory, connected host graphs, trees.

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1 Introduction

For a graph G, we write $e(G)$ and $|G|$ to denote the number of edges and vertices in G. For a pair U, V of disjoint sets of vertices in G, we use $e_G(U, V)$ to denote the number of edges in G with one endpoint in U and the other in V. G will be omitted from the subscript if it is clear from context.

One of the most studied problems in extremal graph theory is to determine the Turán number $\mathrm{ex}(n, F)$, the largest number of edges that an n-vertex graph can have without containing a subgraph isomorphic to F. In this paper, we start a systematic study of a variant of this parameter: the connected Turán number $\mathrm{ex}_c(n, F)$ is the largest number of edges that a *connected* n-vertex graph can have without containing F as a subgraph. Observe that if F is 2-edge-connected, then any maximal F-free graph G is connected, as if G has at least two connected components, then adding an edge between them would not create any copy of F. Also, if the chromatic number of F is at least 3, then by the famous theorem by Erdős, Stone, and Simonovits [6, 7], we know that $\mathrm{ex}(n, F)$ is attained asymptotically (and for some graphs precisely) at the Turán graph that is connected. These two observations imply the following proposition.

Proposition 1.1.

(1) *If all connected components of F are 2-edge-connected, then* $\mathrm{ex}(n, F) = \mathrm{ex}_c(n, F)$.

(2) *If $\chi(F) \geq 3$, then* $\mathrm{ex}_c(n, F) = (1 + o(1))\,\mathrm{ex}(n, F)$.

The asymptotics of $\mathrm{ex}(n, F)$ is unknown for most bipartite F (for a general overview of the so-called degenerate Turán problems, see the survey by Füredi and Simonovits [8]). However, it is known that for any graph F that contains a cycle, $\mathrm{ex}(n, F)$ grows superlinearly. If $\mathrm{ex}(n, F)$ is attained at a non-connected graph with a connected component of size m, then we have $\mathrm{ex}(n, F) \leq \mathrm{ex}(m, F) + \mathrm{ex}(n - m, F)$, which does not hold for 'nice' superlinear functions. There is a relatively large literature on the Turán number of forests (see e.g. [3, 11, 12, 14, 15]), and in many cases the extremal graphs turned out to be connected, so for those forests F, we have $\mathrm{ex}(n, F) = \mathrm{ex}_c(n, F)$. In this paper, we concentrate on the family of trees. A famous conjecture of Erdős and Sós (that appeared in print first in [4]) states that any n-vertex graph with more than $\frac{(k-2)n}{2}$ edges contains any tree T on k vertices. A proof was announced in the early 1990's by Ajtai, Komlós, Simonovits, and Szemerédi, but only arguments of special cases have appeared. A recent survey of these and other degree conditions that imply embeddings of trees is given in [13]. The universal construction that shows the tightness of the Erdős–Sós conjecture is the union of vertex-disjoint cliques of size $k - 1$. This is not a connected graph and we are only aware of two explicit results concerning $\mathrm{ex}_c(n, T)$ (but there exist results on Turán problems in connected host graphs, see e.g. [2]). The connected Turán number of stars follows from the existence of (nearly) regular connected graphs. Apart from stars, paths on k vertices, denoted by P_k, have been considered. The value of $\mathrm{ex}_c(n, P_k)$ was determined by Kopylov, and independently by Balister, Győri, Lehel, and Schelp with the latter group also showing the uniqueness of extremal constructions.

Theorem 1.2 ([1, Balister, Győri, Lehel, Schelp], [10, Kopylov])**.** *If G is an n-vertex connected graph that does not contain any paths on $k + 1$ vertices, then*

$$e(G) \leq \max\left\{\binom{k-1}{2} + n - k + 1, \binom{\lceil \frac{k+1}{2} \rceil}{2} + \left\lfloor \frac{k-1}{2} \right\rfloor \left(n - \left\lceil \frac{k+1}{2} \right\rceil\right)\right\}$$

holds.

In the remainder of the introduction, we shall present the various results obtained concerning $\mathrm{ex}_c(n,T)$. Lower bound constructions are given in Section 2 and exact determination of $\mathrm{ex}_c(n,T)$ including all trees on up to six vertices and some trees having seven vertices is included in Section 3.

Our first result gathers several constructions, all based on some graph parameters, that provide lower bounds on $\mathrm{ex}_c(n,T)$. For those parameters we use the following notation.

Definition 1.3.

- $p(G)$ denotes the maximum number of vertices in a path P of G such that for all $x \in V(P)$ we have $d_G(x) \le 2$.
- $\Delta(G)$ and $\delta(G)$ denote the maximum and the minimum degree in G.
- $\nu(G)$ denotes the number of edges in a largest matching of G.
- $\delta_2(T)$ denotes the smallest degree in T that is larger than 1.
- For a vertex $v \in V(T)$ let $m_T(v)$ be the size of largest component of $T - v$ and let $m(T) = \min\{m_T(v) : v \in V(T)\}$.
- For a vertex $v \in V(T)$ let $m_{T,2}(v)$ be the sum of the sizes of two largest components of $T - v$ and let $m_2(T) = \min\{m_{T,2}(v) : v \in V(T)\}$.
- For an edge $e = xy \in E(G)$ we write $w(e) = \min\{d_G(x), d_G(y)\}$ and define $w(G) = \max\{w(e) : e \in E(G)\}$.

Notation. For graphs H and G, their disjoint union is denoted by $H \cup G$. The join of H and G, denoted by $H+G$, is $H \cup G$ with all edges hg $h \in H, g \in G$ added. For a graph H and a positive integer k, kH denotes the pairwise vertex-disjoint union of k copies of H. S_k denotes the star with k leaves, P_k, C_k, K_k, E_k denote the path, the cycle, the complete graph and the empty graph on k vertices, respectively. The complete bipartite graph with parts of size a and b is denoted by $K_{a,b}$.

In the following remark, we gather the consequences of known constructions (mostly used for distinct purposes).

Remark 1.4.

(1) The existence of connected (nearly)-regular graphs show $\mathrm{ex}_c(n,T) \ge \lfloor \frac{n(\Delta(T)-1)}{2} \rfloor$.

(2) The construction of Theorem 1.2 shows that if T has diameter d, then $\mathrm{ex}_c(n,T) \ge \binom{\lceil \frac{d+1}{2} \rceil}{2} + \lfloor \frac{d-1}{2} \rfloor (n - \lceil \frac{d+1}{2} \rceil)$.

(3) $K_{a-1,n-a+1}$ shows that if the bipartition of T consists of classes of sizes a and b with $a \le b$, then $\mathrm{ex}_c(n,T) \ge (a-1)(n-a+1)$. In particular, we have $\mathrm{ex}_c(n,T) \ge (w(T)-1)(n-w(T)+1)$ and $\mathrm{ex}_c(n,T) \ge (\nu(T)-1)(n-\nu(T)+1)$. The latter can be improved to $\mathrm{ex}_c(n,T) \ge (\nu(T)-1)(n-\nu(T)+1) + \binom{\nu(T)-1}{2}$ shown by $K_{\nu(T)-1} + E_{n-\nu(T)+1}$, the largest graph with matching number less than $\nu(T)$ if n is large as proved by Erdős and Gallai [5].

Observe that if T is balanced, i.e. $a = b$ in its bipartition, then the number of edges in $K_{a-1,n-a+1}$ is just a constant smaller than the number of edges in $\frac{n}{k-1}K_{k-1}$, the extremal graph of the Erdős-Sós conjecture. The next proposition states lower bounds due to new constructions. The proof of Proposition 1.5 will be given in Scetion 2.

Proposition 1.5. *Suppose T is a tree on $k \geq 4$ vertices.*

(1) *If T is not a path and thus $p(T) \leq k-3$, then $\mathrm{ex}_c(n,T) \geq (\binom{k-2p(T)-3}{2} + p(T)+2)\lfloor \frac{n}{k-p(T)-2} \rfloor$. Furthermore, if T contains at least two vertices of degree at least three, then $\mathrm{ex}_c(n,T) \geq \frac{\binom{k-p(T)-1}{2}+p(T)+2}{k} n - O(k)$.*

(2) *If T is not a star and $\delta_2(T) > 2$, then $\mathrm{ex}_c(n,T) \geq \lfloor \frac{n-1}{k-1} \rfloor (\binom{k-2}{2} + \delta_2(T) - 1)$.*

(3) *If T is not a path, then $\mathrm{ex}_c(n,T) \geq n-1+\lfloor \frac{n-1}{m(T)-1} \rfloor \binom{m(T)-1}{2}$.*

(4) $\mathrm{ex}_c(n,T) \geq \lfloor \frac{n}{k-m_2(T)} \rfloor (1 + \binom{k-m_2(T)}{2})$.

Next, we determine $\mathrm{ex}_c(n,T)$ for all trees on k vertices with $4 \leq k \leq 6$ (note that there do not exist P_3-free connected graphs), some trees on 7 vertices and for some infinite families of trees. We need some notation first.

Let $D_{a,b}$ denote the *double star* on $a+b+2$ vertices such that the two non-leaf vertices have degree $a+1$ and $b+1$. $S_{a_1,a_2,\ldots,a_j}$ with $j \geq 3$ denotes the *spider* obtained from j paths with $a_1, a_2, \ldots, a_j$ edges by identifying one endpoint of all paths. So $S_{a_1,a_2,\ldots,a_j}$ has $1+\sum_{i=1}^{j} a_i$ vertices and maximum degree j. The only vertex of degree at least 3 is the *center* of the spider, the maximal paths starting at the center are the *legs* of the spider. M_n denotes the matching on n vertices (so if n is odd, then an isolated vertex and $\lfloor \frac{n}{2} \rfloor$ isolated edges).

The values of $\mathrm{ex}_c(n, P_{k+1})$ were determined by Theorem 1.2, and for $k \geq 3$, the statement $\mathrm{ex}_c(n, S_k) = \lfloor \frac{n(k-1)}{2} \rfloor$ follows from Remark 1.4(1) and that the degree-sum of an S_k-free graph is at most $n(k-1)$. So in the next theorem, we only list those trees that are neither paths nor stars. In particular, all trees have 5 or 6 vertices. Proofs of the following theorems will be given in Section 3.

Theorem 1.6. *For non-star, non-path trees with 5 or 6 vertices, the following exact results are valid.*

(1) *For any $T = S_{2,1,\ldots,1}$ we have $\mathrm{ex}_c(n,T) = \lfloor \frac{n(\Delta(T)-1)}{2} \rfloor$ if $n \geq |T|$. In particular, $\mathrm{ex}_c(n, S_{2,1,1}) = n$ if $n \geq 5$ and $\mathrm{ex}_c(n, S_{2,1,1,1}) = \lfloor \frac{3n}{2} \rfloor$ if $n \geq 6$.*

(2) *We have $\mathrm{ex}_c(n, D_{2,2}) = 2n-4$ if $n \geq 6$.*

(3) *We have $\mathrm{ex}_c(n, S_{3,1,1}) = \lfloor \frac{3(n-1)}{2} \rfloor$ if $n \geq 7$ and $\mathrm{ex}(6, S_{3,1,1}) = 9$.*

(4) *We have $\mathrm{ex}_c(n, S_{2,2,1}) = 2n-3$ if $n \geq 6$.*

Let $D^*_{2,2}$ be the tree obtained from $D_{2,2}$ by attaching a leaf to one leaf of $D_{2,2}$.

Theorem 1.7. *$ex_c(n, D^*_{2,2}) = 2n-3$ for all $n \geq 7$, and $ex_c(n, D^*_{2,2}) = \binom{n}{2}$ for $1 \leq n \leq 6$.*

Theorem 1.8. *$ex_c(n, S_{2,2,2}) = 2n-2$ for all $n \geq 7$, and $ex_c(n, S_{2,2,2}) = \binom{n}{2}$ for $1 \leq n \leq 6$.*

Theorem 1.9. *$ex_c(n, S_{3,2,1}) = 2n-3$ for all $n \geq 7$, and $ex_c(n, S_{3,2,1}) = \binom{n}{2}$ for $1 \leq n \leq 6$.*

Theorem 1.10. *For any* $T = S_{3,1,\dots,1}$ *with* $\Delta(T) \geq 4$, *if* n *is large enough, then* $\mathrm{ex}_c(n,T) = \lfloor \frac{(\Delta(T)-1)n}{2} \rfloor$.

The broom, which we denote by $B(k,a)$, is the special spider $S_{a-1,1,1,\dots,1}$ on k vertices. So its maximum degree is $k-a+1$ and its diameter is a.

Theorem 1.11.

(1) *For any* $a \leq k-2$, $\mathrm{ex}_c(n, B(k,a)) \geq \max\{\lfloor \frac{(k-a)n}{2} \rfloor, \binom{\lceil \frac{a+1}{2} \rceil}{2} + \lfloor \frac{a-1}{2} \rfloor (n - \lfloor \frac{a+1}{2} \rfloor)\}$ *holds.*

(2) *For any* $a \leq k/3$, $\mathrm{ex}_c(n, B(k,a)) = \lfloor \frac{(k-a)n}{2} \rfloor$ *holds if* n *is large enough.*

For a better overview, we include tables with previous results, our results and open cases for trees on up to 7 vertices. $SD_{2,2}$ denotes the tree on 7 vertices obtained from the double star $D_{2,2}$ by subdividing the edge connecting its two centers.

Number of vertices	Tree	$\mathrm{ex}_c(n,T)$	Construction
4	P_4	$n-1$	S_{n-1}
	S_3	n	C_n
5	P_5	n	$K_1 + (K_2 \cup E_{n-3})$
	S_4	$\lfloor \frac{3n}{2} \rfloor$	(nearly) 3-regular
	$S_{2,1,1}$	n	C_n
6	P_6	$2n-3$	$K_2 + E_{n-2}$
	S_5	$2n$	4-regular
	$S_{2,1,1,1}$	$\lfloor \frac{3n}{2} \rfloor$	(nearly) 3-regular
	$S_{2,2,1}$	$2n-3$	$K_2 + E_{n-2}$
	$S_{3,1,1}$	$\lfloor \frac{3(n-1)}{2} \rfloor$	$K_1 + M_{n-1}$
	$D_{2,2}$	$2n-4$	$K_{2,n-2}$

Table 1: The value of $\mathrm{ex}_c(n,T)$ for all trees up to 6 vertices.

Tree	$\mathrm{ex}_c(n,T)$	Construction	Tree	$\mathrm{ex}_c(n,T)$	Construction
S_6	$\lfloor \frac{5n}{2} \rfloor$	(nearly) 5-regular	P_7	$2n-2$	$K_2 + (E_{n-4} \cup K_2)$
$S_{4,1,1}$	$\geq 2n-3$	$K_2 + E_{n-2}$	$S_{3,2,1}$	$2n-3$	$K_2 + E_{n-2}$
$S_{3,1,1,1}$	$\lfloor \frac{3n}{2} \rfloor$	(nearly) 3-regular	$S_{2,1,1,1,1}$	$2n$	4-regular
$S_{2,2,2}$	$2n-2$	$K_2 + (E_{n-4} \cup K_2)$	$S_{2,2,1,1}$	$\geq 2n-3$	$K_2 + E_{n-2}$
$D^*_{2,2}$	$2n-3$	$K_2 + E_{n-2}$	$D_{2,3}$	$\geq 2n-4$	$K_{2,n-2}$
$SD_{2,2}$	$\geq \frac{13n}{7} - O(1)$	Proposition 1.5(1)	$D_{2,3}$	$\geq 2n-2$ if $6 \mid n-1$	Proposition 1.5(2)

Table 2: Exact values and lower bounds on $\mathrm{ex}_c(n,T)$ for trees with 7 vertices.

The starting point of our final subtopic is the Erdős–Sós conjecture, $\mathrm{ex}(n,T) = \frac{k-2}{2}n + O_k(1)$. We would like to know how much smaller $\mathrm{ex}_c(n,T)$ can be than $\mathrm{ex}(n,T)$. For any tree T we introduce

$$\gamma_T := \limsup_n \frac{2}{|T|-2} \cdot \frac{\mathrm{ex}_c(n,T)}{n}$$

where $|T|$ denotes the number of vertices in T. It is well-known that any graph with average degree at least $2d$ contains a subgraph with minimum degree at least d. Also, any tree on k vertices can be embedded to any graph with minimum degree at least k. This shows that $\gamma_T \leq 2$ for any tree T on k vertices. The Erdős–Sós conjecture would imply $\gamma_T \leq 1$.

Let $\mathcal{T}_k$ denote the set of trees on at least k vertices. We write $\gamma_k := \inf\{\gamma_T : T \in \mathcal{T}_k\}$ and $\gamma := \lim_{k\to\infty} \gamma_k$. Observe that γ_k is monotone increasing as $\mathcal{T}_2 \supset \mathcal{T}_3 \supset \mathcal{T}_4 \supset \dots$, and thus the limit γ exists.

Theorem 1.12. *The following upper and lower bounds hold:* $\frac{1}{3} \leq \gamma \leq \frac{2}{3}$.

2 Constructions

Proof of Proposition 1.5. For all lower bounds we need constructions.

For the general lower bound of (1), we construct a graph $G(V, E)$ as follows: let $s := \lfloor \frac{n}{k-p(T)-2} \rfloor$ and let V be partitioned into $\bigcup_{i=1}^{s}(A_i \cup Q_i)$ with $|A_i| = k - 2p(T) - 3$ for all $1 \leq i \leq s$, $|Q_i| = p(T) + 1$ for all $1 \leq i < s$. $G[A_i]$ is a clique for all i. Every clique A_i contains a special vertex x_i, and $G[\{x_i, x_{i+1}\} \cup Q_i]$ is a path with end vertices x_i and x_{i+1} (with $x_{s+1} = x_1$). Then G cannot contain T, as a copy of T could contain the vertices of an A_i and then at most $p(T)$ vertices from both of Q_{i-1} and Q_i, so at least one vertex of T cannot be embedded.

To see the furthermore part of (1), we have the following construction G: we partition the vertex set of G into $\{v\} \cup \bigcup_{i=1}^{s}(A_i \cup Q_i)$, where $s = \lceil \frac{n-1}{k} \rceil$ with $|A_i| = k - p(T) - 1$, $|Q_i| = p(T) + 1$ for all $1 \leq i < s$, and $|Q_i| \leq p(T) + 1$ and if $|A_i| > 0$, then $|Q_i| = p(T) + 1$. The edges of G are defined such that $G[\{v\} \cup \bigcup_{i=1}^{s} Q_i]$ is a spider with center v and legs Q_i, $G[A_i]$ is a clique and exactly one vertex of A_i is connected to the leaf of the leg in Q_i. The number of edges adjacent to $A_i \cup Q_i$ is $\binom{k-p(T)-1}{2} + p(T) + 2$, therefore $e(G)$ is as claimed. Finally, to see that G is T-free, observe that as T contains at least two vertices of degree at least 3, if G contained a copy of T, then this copy should contain a vertex u from one of the A_is. Also, such a copy cannot contain all vertices of Q_i as $p(T) < |Q_i|$. Therefore, the vertices of the copy of T should be contained in $|A_i| + |Q_i| - 1 < k$ vertices — a contradiction.

The lower bound of (2) is shown by the following construction of a connected n-vertex T-free graph G: we partition the vertex set of G into $\{v\} \cup \bigcup_{i=1}^{\lceil \frac{n-1}{k-1} \rceil} A_i$ with $|A_i| = k - 1$ for all $i = 1, 2, \dots, \lfloor \frac{n-1}{k-1} \rfloor$ and every A_i containing a special vertex x_i. The edges of G are defined as follows: $G[A_i \setminus \{x_i\}]$ is a clique, v is adjacent to all x_i, and x_i is adjacent to $\delta_2(T) - 2$ other vertices of A_i, so $d_G(x_i) = \delta_2(T) - 1$. We claim that G is T-free. Indeed, as $G - v$ has components of size at most $k - 1$, a copy of T must contain v. As T is not a star, at least one of v's neighbors is not a leaf and so its degree should be at least $\delta_2(T)$. But all v's neighbors are x_i vertices that have degree $\delta_2(T) - 1$ in G. The number of edges in $G[\{v\} \cup \bigcup_{i=1}^{\lfloor \frac{n-1}{k-1} \rfloor} A_i]$ is $\lfloor \frac{n-1}{k-1} \rfloor (\binom{k-2}{2} + \delta_2(T) - 1)$.

The construction yielding the lower bound of (3) is $G = K_1 + (rK_{m(T)-1} \cup K_s)$, where $r = \lfloor \frac{n-1}{m(T)-1} \rfloor$ and $s \geq 0$. Indeed, if G contained a copy of T, then this copy should contain the vertex v of K_1 as otherwise T would be contained in $m(T) - 1$ vertices. But then we cannot embed the largest branch pending on v as it has size at least $m(T)$.

To obtain the construction yielding the lower bound of (4), we partition the vertex set to $A_1, A_2, \dots, A_s, A_{s+1}$ with $s = \lfloor \frac{n}{k-m_2(T)} \rfloor$ and $|A_i| = k - m_2(T)$ for all $i = 1, 2, \dots, s$. As T is not a path, we have $k - m_2(T) \geq 2$, so in each A_i we can pick two distinct vertices

x_i, y_i, maybe with the exception of A_{s+1}. Then we define G as a "cycle of cliques", so $G[A_i]$ is a clique for all i, and $x_i y_{i+1}$ is an edge (formally there should be three cases depending whether A_{s+1} has size 0, 1, or at least 2). To see that G is T-free, consider the vertex v with $m_2(T) = m_{T,2}(v)$, i.e. the largest two connected components B_1, B_2 in $T - v$ have a total size of $m_2(T)$. Suppose G contains a copy of T and the vertex playing the role of v belongs to A_i. Then, as there are only two edges leaving A_i, T apart from two components of $T - v$ must be embedded into A_i. Moreover, since the two edges leave from distinct vertices, at least one vertex of the two exceptional components must also be embedded to A_i. So A_i should contain at least $k - m_2(T) + 1$ vertices — a contradiction. (If $i = s + 1$ and $x_i = y_i$, then we have the same contradiction, as then A_{s+1} should contain at least $k - m_2(T)$ vertices, but A_{s+1} is strictly smaller than that.) □

3 Proofs

We start by proving Theorem 1.6. We restate and prove its parts separately.

Theorem 3.1. *For $T = S_{2,1,\dots,1}$, the equality* $\mathrm{ex}_c(n, T) = \lfloor \frac{n(\Delta(T)-1)}{2} \rfloor$ *holds if $n \geq |T|$.*

Proof. The constructions giving the lower bounds are connected (nearly) regular graphs of degree $\Delta(T) - 1$.

If $T = S_{2,1,1,\dots,1}$, then the upper bound proof is a special case of Theorem 1.11, but for completeness, we give a simpler proof of this case. If G is a connected, n-vertex, T-free graph and for some x we have $d_G(x) \geq \Delta(T)$, then G is the star. Indeed, the neighbors of x can be adjacent only to other neighbors of x, otherwise T would be a subgraph of G. So by connectivity $N_G[x] = V(G)$. But then if there is at least one edge between two neighbors of x, then, as $|V(G)| \geq |V(T)|$, again T would be a subgraph of G. The star has fewer edges than the claimed maximum, so to have $\mathrm{ex}_c(n, T)$ edges, G must be (nearly) $(\Delta(T) - 1)$-regular. □

Theorem 3.2. *For any $n \geq 6$,* $\mathrm{ex}_c(n, D_{2,2}) = 2n - 4$ *holds.*

Proof. To see the lower bound, observe that $K_{2,n-2}$ is $D_{2,2}$-free as $w(K_{2,n-2}) = 2$, while $w(D_{2,2}) = 3$.

To see the upper bound, observe first that all connected graphs with 6 vertices and at least 9 edges contain a copy of $D_{2,2}$ as can be checked in the table of graphs of [9] on pages 222–224.

Suppose there exists a minimum counterexample: a connected graph G on $n \geq 7$ vertices and $e(G) \geq 2n - 3$ edges with no copy of $D_{2,2}$. We consider several cases.

CASE I: $\delta(G) \leq 2$ and there is a vertex v of degree at most 2 which is not a cut vertex.

Delete this vertex v of degree 1 or 2 to obtain a connected $H = G \setminus v$ with $|H| \geq 6$. By minimality $e(H) \leq 2(n-1)$–4 and $2n-3 \leq e(G) \leq e(H)+2 \leq 2(n-1)$–$4+2 = 2n-4$ — a contradiction.

CASE II: $\delta(G) = 2$ and every vertex of degree 2 is a cut vertex.

Consider v of degree 2 such that in $H = G - v$ out of the two components A and B, $|A|$ is as small as possible. Let w be the vertex in A adjacent to v and let z be the vertex in B adjacent to v.

If $|A| \geq 6$ then by minimality of G, $2n - 3 \leq e(G) \leq 2|A| - 4 + 2|B| - 4 + 2 = 2(|A| + |B| + 1) - 8 = 2n - 8$ — a contradiction. Otherwise $3 \leq |A| \leq 5$ as $|A| \leq 2$

would imply $\delta(G) = 1$ and we were in Case I. Also, $|A| \geq 4$ as $|A| = 3$ would imply that A must contain a vertex of degree 2 which is not a cut vertex and we were in Case I again.

Suppose $|A| = 5$. If $d_G(w) = 2$ then $|A|$ is not minimum, so in the induced subgraph on A all vertices have degree at least 2 and $d_G(w) \geq 3$. But then the induced graph on A either contains a vertex of degree 2 which is not a cut vertex and we are in Case I or all degrees in $G[A \cup \{v\}]$ (except for v) are at least 3. Then one can find a copy of $D_{2,2}$ with w being one of the centers and v being a leaf pending from w. Indeed, by the degree condition, $G[A \setminus \{w\}]$ contains a C_4, so if $N(w)$ contains two non-neighbor vertices x, y of this C_4, then x can be the other center of the copy of $D_{2,2}$ and y the other leaf pending from w. Otherwise w has exactly two neighbors in A, and then by the degree condition $G[A \setminus \{w\}]$ is K_4 and it is trivial to embed $D_{2,2}$.

Finally suppose $|A| = 4$. As $|B| \geq |A| = 4$, it follows that $B^* = B \cup \{v, w\}$ has at least 6 vertices and $|B^*| = n - 3$, and hence by minimality of G, $e(B^*)$ contains at most $2(n-3)-4$ edges and together with at most 6 edges in A gives $e(G) \leq 2n-10+6 = 2n-4$ — a contradiction.

Case III: $\delta(G) \geq 3$.

If all vertices are of degree 3, we have $3n/2$ edges, which is at most $2n - 4$ for $n \geq 8$. For $n = 7$ this is impossible by parity, hence $\delta(G) \geq 3$ and $\Delta(G) \geq 4$. Consider an edge $e = xy$ with $d_G(y) = \Delta(G) \geq 4$ and $d_G(x) \geq 3$.

If $d_G(y) \geq 5$, then for $u, u' \in N(x)$ we have $|N(y) \setminus \{x, u, u'\}| \geq 2$, so x and y are centers of a copy of $D_{2,2}$. If $d_G(y) = 4$ and $d_G(x) = 4$ then either x and y have distinct neighbors s not in $N[y]$ and t not in $N[x]$ and we find a copy of $D_{2,2}$ with centers x, y, or x and y are twins having the same neighbors a, b, c excluding themselves. But as $|G| \geq 7$, at least one vertex, say a, has a neighbor d not adjacent to the other 4 vertices and then a and x can be centers of $D_{2,2}$ with y and d pending from a.

So we can assume that all vertices have degree 3 or 4 and vertices of degree 4 form an independent set Q. Let $P = V \setminus Q$, and consider the bipartite $G[P, Q]$ where $p + q = n$, $|P| = p$ and $|Q| = q$. Clearly, $4q = e(P, Q) \leq 3p$. Hence $3n = 3q + 3p \geq 7q$ and $q \leq 3n/7, p \geq 4n/7$. But then

$$e(G) = \frac{4q + 3p}{2} \leq \frac{12n/7 + 12n/7}{2} = \frac{12n}{7} < 2n - 3$$

for $n \geq 11$. So we are left with $n = 7, 8, 9, 10$.

For $n = 7$: $q \leq 3n/7 = 3$ and q must be an integer. If $q = 3$, then $G = K_{4,3}$ containing $D_{2,2}$. The case $q = 2$ is impossible as the degree sum would be odd (by the number p of odd-degree vertices). Hence $q = 1$ and $p = 6$. Consider a vertex v of degree 4 and its neighbors a, b, c, d all of degree 3. If say a is adjacent to a vertex outside $\{v, b, c, d\}$, then there is $D_{2,2}$. But as this holds for all of a, b, c, d it means $A = \{v, a, b, c, d\}$ has no neighbor in $V \setminus A$ and G is not connected.

For $n = 8$, we still have $q \leq \lfloor \frac{3n}{7} \rfloor = 3$ and $p \geq 5$. But $p = 5, 7$ are impossible, again due to parity, hence $q = 2$ and $p = 6$. Let $Q = \{a, b\}$ be the set of vertices of degree 4. If some vertex x in P is adjacent to both a and b, then consider the only neighbor z of x in P. Here a is adjacent to x and three more vertices in P, so at least two vertices except x and z are neighbors of a and x can use z and b to obtain a copy of $D_{2,2}$ with centers x and a. Hence every vertex in P is adjacent to at most one vertex in Q, yielding $|P| \geq e(P, Q) = 4|Q|$ — a contradiction.

For $n = 9$, we have $q \le \lfloor \frac{3n}{7} \rfloor = 3$. The case $q = 2$ is impossible by parity and $q = 1$, $p = 8$ implies $e(G) = (4 + 24)/2 = 14 = 2n - 4$ as stated by the theorem. So only $q = 3$, $p = 6$ is to be checked. Let $Q = \{a, b, c\}$ be the set of vertices of degree 4. If some vertex v in P has at least two neighbors in Q, say a, b, then we have a copy of $D_{2,2}$ with centers v and a, as all the four neighbors of a are in P and at most two of them belong to $N[x]$. So every vertex in P can have at most one neighbor in Q and as in the previous case we have $|P| \ge e(P, Q) = 4|Q|$ — a contradiction.

For $n = 10$, $q \le \lfloor \frac{3n}{7} \rfloor = 4$, and so parity of the degree sum implies $q = 4$ or $q = 2$. If $q = 2$ then $e(G) = (8 + 24)/2 = 16 = 2n - 4$ as stated in the theorem, so only $q = 4$, $p = 6$ remains to be checked.

Let $Q = \{a, b, c, d\}$ be the set of vertices of degree 4. If some vertex v in P has all its neighbors in Q, say a, b, c, then we obtain a copy of $D_{2,2}$ with centers v and a. Otherwise, we have $4|Q| = e(P, Q) \le 2|P|$ — a contradiction. □

Theorem 3.3. $\mathrm{ex}_c(n, S_{3,1,1}) = \lfloor \frac{3(n-1)}{2} \rfloor$ *if* $n \ge 7$ *and* $ex_c(6, S_{3,1,1}) = 9$.

Proof. The lower bounds are shown by $K_1 + M_{n-1}$ for $n \ge 7$ and by $K_{3,3}$ for $n = 6$. The former is $S_{3,1,1}$-free as shown in Proposition 1.5(3) with $m(S_{3,1,1}) = 3$. The graph $K_{3,3}$ is $S_{3,1,1}$-free as the bipartition of $S_{3,1,1}$ has a part of size 4.

To obtain the upper bound, we consider an $S_{3,1,1}$-free connected graph G. The general idea is to choose a longest cycle $C = v_1v_2, \dots, v_k$ in G, and argue depending on its length k.

If $k = n$, then C is a Hamiltonian cycle. It cannot have short chords; e.g. if v_2v_4 is an edge, then $S_{3,1,1}$ can have center v_2 and legs v_2v_1, v_2v_3, $v_2v_4v_5v_6$. Moreover if $n > 6$, then longer chords cannot occur either. Indeed, if v_2v_j with $j = 5, \dots, n-2$ is an edge, then v_2 with v_j and its two successors can form the leg of length 3. Likewise for $j = 6, \dots, n-1$ such a leg can be formed using the two predecessors of v_j, still keeping the legs v_2v_1 and v_2v_3. This excludes all chords if $n > 6$, hence $|E(G)| = n$. If $n = 6$, then antipodal vertices can be adjacent without creating any copy of $S_{3,1,1}$, but no other chords may occur. In this way we obtain the extremal graph $K_{3,3}$.

Assume next that $4 < k < n$. We show that this is impossible whenever $n \ge 6$. Since G is connected, there is a vertex x not in C but having at least one neighbor in C. If e.g. xv_2 is an edge, we find $S_{3,1,1}$ with center v_2 and legs xv_2, v_2v_1, $v_2v_3v_4v_5$.

Assume now $k = 4$, $C = v_1v_2v_3v_4$, $n \ge 6$. If P is any path with one end in C and all its other vertices in $V(G) \setminus V(C)$, then P can have no more than two edges, otherwise $S_{3,1,1}$ would be found, with the long leg in P and the two short legs in C. We are going to prove that if P is shorter than 3, the number of edges in G is smaller than what is given in the theorem.

If P has length 2, let xyv_1 be a path attached to C. Then the edges xv_2, xv_3, xv_4, yv_2, yv_4 cannot be present because C is a longest cycle. Also the edges v_1v_3 and v_2v_4 are excluded because G is $S_{3,1,1}$-free. This implies $|E(G)| \le 8$ if $n = 6$. If $n > 6$, there should be a further vertex z adjacent to $C \cup P$, but any edge from z to $C \cup P$ would create an $S_{3,1,1}$. (For zx the center is v_1, and for any other edge the center is the neighbor of z.) Hence $n > 6$ is impossible in this case.

Suppose that $P = yv_1$ is a single edge not extendable to a longer path outside C. Then a sixth vertex x can only be adjacent to v_2 or v_4 (or both), otherwise an $S_{3,1,1}$ would occur. And also here, it is not possible to extend this graph to a connected graph of order 7 without creating an $S_{3,1,1}$ subgraph. Hence $n = 6$. Moreover, the diagonals of C must be missing;

e.g. the edges xv_2 and v_2v_4 would yield $S_{3,1,1}$ with center v_2 and legs xv_2, v_2v_3, $v_2v_4v_1y$. Thus the number of edges is only 4 plus the degree sum of x and y, which is at most 7 because the presence of all four edges xv_2, xv_4, yv_1, yv_3 would make G Hamiltonian, hence C would not be a longest cycle.

Finally we have to consider graphs without any cycles longer than 3. It means that each block of G is K_2 or K_3. Let $f(n)$ denote the maximum number of edges in such a graph. We clearly have $f(1) = 0$, $f(2) = 1$, $f(3) = 3$. Let B be an endblock of G, with cut vertex w. Deleting $B - w$ from G we obtain a $S_{3,1,1}$-free connected graph of order $n - |V(B)| + 1$, where $|V(B)|$ is 2 or 3. Hence

$$f(n) \leq \max\{f(n-1) + 1, f(n-2) + 3\}.$$

This recursion implies $f(n) \leq \lfloor 3(n-1)/2 \rfloor$ for every n, completing the proof of the upper bound for $n \geq 7$. □

Theorem 3.4. $\mathrm{ex}_c(n, S_{2,2,1}) = 2n - 3$ *if* $n \geq 6$.

Proof. The lower bound is shown by $K_2 + E_{n-2}$ as it has matching number 2, while $\nu(S_{2,2,1}) = 3$.

To obtain the upper bound on $\mathrm{ex}_c(n, S_{2,2,1})$, we proceed by induction: for $n = 6$ every connected graph on 6 vertices and 10 edges contains $S_{2,2,1}$ (by inspecting the table of graphs of [9] on pages 222–224).

For the induction step assume that the statement of the theorem holds for graphs of at most $n - 1$ vertices and assume on the contrary that G is a connected graph on n vertices and $2n - 2$ edges without $S_{2,2,1}$. Here $2n - 2$ suffices as otherwise if $e(G) \geq 2n - 1$, we can delete an edge on a cycle.

If $\delta(G) \leq 2$ and there is a vertex v of degree at most 2 which is not a cut vertex, then we can apply induction to $H = F - v$ to obtain $e(G) \leq e(H) + 2 \leq 2(n-1) - 3 + 2 = 2n - 3$ — a contradiction.

Suppose $\delta(G) = 2$ and every vertex of degree 2 is a cut vertex. Then let v be such a cut vertex with neighbors x and y. Consider $H = G - v + (xy)$. Here $|H| = n - 1$ and $e(H) = 2n - 2 - 2 + 1 = 2(n-1) - 2 + 1$, hence by induction H contains a copy S of $S_{2,2,1}$. If S does not use the edge xy, then S is also in G — a contradiction. If S uses xy such that one of x and y, say x, is a leaf in S, then replace x by v and the edge xy by vy to obtain a copy S' of $S_{2,2,1}$ in G — a contradiction. Finally, if xy is the edge of a 2-leg of S containing the center, say x and the leg is xyz, then replace this leg by xvy to obtain S' in G — a contradiction.

So we can assume $\delta(G) \geq 3$. If all vertices are of degree 3, then $e(G) = 3n/2 < 2n-2$. If all vertices are of degree at least 4, then $e(G) \geq 2n > 2n - 2$, hence there exists a vertex y of degree 3 adjacent to a vertex x of degree at least 4. Let u, v be the other two neighbors of y, and let $z \neq u, v, y$ be a neighbor of x. If u or v has a neighbor outside these 5 vertices, then we obtain a copy of $S_{2,2,1}$ with center y. If not and $N(x) = \{u, v, y, z\}$, then z must have a neighbor outside these 5 vertices and we obtain a copy of $S_{2,2,1}$ with center x. Finally, if $N(u) \cup N(v) \subseteq \{u, v, x, y, z\}$ and z' is another neighbor of x, then $d_G(z') \geq 3$ implies that z' must have a neighbor outside these 6 vertices, and we obtain a copy of $S_{2,2,1}$ with center x. This contradiction finishes the proof. □

Proof of Theorem 1.7. The assertion is trivial for $n < 7$. For larger n the split graph construction $K_2 + E_{n-2}$ shows that $2n - 3$ is a lower bound.

To derive the same as an upper bound, assume $n > 6$ and consider any $D^*_{2,2}$-free graph G of order n with more than $2n-4$ edges. Then, by Theorem 1.6(2), there is a $D = D_{2,2}$ subgraph in G; let the central edge of D be xy.

If some vertex not in D is adjacent to a leaf of D, then a copy of $D^*_{2,2}$ arises — a contradiction. More generally, there cannot exist any vertex at distance exactly 2 from $\{x, y\}$. By the connectivity of G, it follows that every vertex of G is adjacent to at least one of x and y. On this basis we partition $V(G) - \{x, y\}$, defining

$$X = N(x) - N[y], \qquad Y = N(y) - N[x], \qquad Z = N(x) \cap N(y).$$

Let us assume $|Y| \geq |X|$. Due to the presence of $D_{2,2}$ we know that $|X| + |Z| \geq 2$ holds. Moreover, $|Y| \geq |X|$ with $n \geq 7$ implies $|Y| + |Z| \geq 3$. Hence there cannot be any $X - Y$ edges, moreover $Y \cup Z$ is an independent set, both because G is $D^*_{2,2}$-free. For the same reason, if $|X| + |Z| > 2$, then also $X \cup Z$ is independent. In this case the entire $X \cup Y \cup Z$ is independent and G cannot have more than $2n-3$ edges, yielding just the extremal split graph $K_2 + E_{n-2}$. Otherwise, if $|X| + |Z| = 2$, there can be just one edge inside $X \cup Z$, hence we have 6 edges in the K_4 subgraph induced by $X \cup Z \cup \{x, y\}$, and there are further $n-4$ edges from Y to y. These are altogether $n+2$ edges only, i.e. fewer than the assumed $2n-3$. This contradiction completes the proof. □

Proof of Theorem 1.8. To simplify notation, let $f(n) = \mathrm{ex}_c(n, S_{2,2,2})$. The lower bound for $n \geq 7$ is obtained by the following construction that works for all n. Take a complete graph K_4 on the vertex set $\{v_1, v_2, v_3, v_4\}$ and join all v_i for $i = 5, 6, \ldots, n$ to v_1 and v_2. Equivalently, v_1 and v_2 are universal vertices, supplemented with the single edge v_3v_4. This connected graph with $2n-2$ edges does not contain $S_{2,2,2}$ because it is not possible to delete two vertices from $S_{2,2,2}$ to destroy all but one edges.

The argument for the upper bound applies induction on n, with base cases $n \leq 7$, from which only $n = 7$ is nontrivial. We note here that $n = 5$ and $n = 6$ are the only cases where $2n-2$ is not an upper bound on the formula given for $f(n)$.

For $n = 7$ the assertion is that every connected graph G with 7 vertices and at least 13 edges contains $S_{2,2,2}$ as a subgraph. To prove it, suppose first that G has a cut vertex x, and consider the vertex distribution between the components of $G - x$. If it is $(3, 3)$ — where we unite components if there are more than two, e.g. the distribution $(3, 2, 1)$ is also viewed as $(3, 3)$ — then already 9 nonadjacencies are found, hence G would have at most $21 - 9 = 12$ edges — a contradiction. If the distribution is $(2, 4)$, then it forces 8 nonadjacencies, hence G must be the graph in which the two blocks incident with x are K_3 and K_5. Obviously this graph contains $S_{2,2,2}$. If the distribution is $(1, 5)$, then x has a pendant neighbor, say y, and $G - y$ is a connected graph of order 6, having at least 12 edges. Routine inspection shows that all such graphs G contain $S_{2,2,2}$.

Assume that G is 2-connected. If G has minimum degree 3, then G has a Hamiltonian cycle, say $C = v_1v_2v_3v_4v_5v_6v_7$. (More generally it is well known that a graph of order $2d + 1$ and minimum degree d is non-Hamiltonian if and only if either it is the complete bipartite graph $K_{d,d+1}$ or it has two blocks incident with a cut vertex, both blocks being K_{d+1}; in our case both of them would have only 12 edges.) The presence of any long chord in C, e.g. v_3v_6 immediately creates an $S_{2,2,2}$ with center v_3 and legs $v_3v_2v_1$, $v_3v_4v_5$, $v_3v_6v_7$. Moreover, any three consecutive short chords, e.g. v_2v_4, v_3v_5, v_4v_6 create an $S_{2,2,2}$ with center v_4 and legs $v_4v_2v_1$, $v_4v_3v_5$, $v_4v_6v_7$. And now at least one of these situations holds because in general a cycle of length n without three consecutive short chords and with no other chords at all can have no more than $n + 2n/3 < 2n - 2$ edges if $n \geq 7$.

Hence in the 2-connected case G has minimum degree exactly 2, and if we remove a vertex x of degree 2, we obtain a graph on 6 vertices with at least 11 edges. If it is K_5 with a pendant edge, then the pendant vertex must be adjacent to x and we immediately find $S_{2,2,2}$. Otherwise there can be at most one vertex of degree 2 in $G - x$, hence it contains a C_6, say $v_1v_2v_3v_4v_5v_6$ (as a rather particular corollary of Pósa's theorem). If the two neighbors of x are antipodal in C, e.g. v_3 and v_6, we find $S_{2,2,2}$ with center v_3 and legs v_3xv_6, $v_3v_2v_1$, $v_3v_4v_5$. If the two neighbors of x are consecutive in C, then C extends to C_7 which we already settled. Hence we can assume that the neighbors of x are v_2 and v_4. Since C has at least 5 chords, some of the five chords v_1v_3, v_1v_4, v_2v_5, v_3v_5, v_3v_6 must be present, and each of them creates $S_{2,2,2}$ with x and the edges of C. This completes the proof of $f(7) = 12$.

Turning now to the inductive step, assume that $n \geq 8$ and that the upper bound $2n - 2$ is valid for all smaller orders other than 5 and 6. Depending on the structure of the graph under consideration, we will apply one of the following upper bounds:

$$f(n-1)+2, \qquad f(n-3)+6, \qquad f(n-6)+12.$$

Suppose that G is an $S_{2,2,2}$-free connected graph of order $n \geq 8$, and G is $S_{2,2,2}$-saturated, i.e. the insertion of any new edge inside $V(G)$ would create an $S_{2,2,2}$ subgraph. Under the latter assumption we observe the following.

Claim 3.5. *If x is a vertex of degree 2, say with neighbors y and z, then yz is also an edge of G.*

Proof of Claim 3.5. Otherwise yxz would be an induced path in G. Let then G' be the graph obtained by the insertion of edge yz. By assumption there is an $S = S_{2,2,2}$ subgraph in G', which necessarily contains the edge yz. If yz is a leaf edge of S, then of course the degree-3 center of S cannot be x, it must be another vertex w adjacent to y or to z. But then z or y is a leaf vertex of S, and replacing yz with yx or zx we find another copy of $S_{2,2,2}$ which is a subgraph of G — a contradiction. The other possibility would be that y or z is the degee-3 vertex of S, and the edge yz is continued with a leaf edge zw or yw (allowing also $w = x$). But then x cannot be a mid-vertex of any leg of S since x does not have a neighbor other than y and z. Hence the leg yzw or zyw can be replaced with yxz or zxy, and we would again find a copy of $S_{2,2,2}$ as a subgraph of G. □

As a consequence of Claim 3.5, if G has a vertex of degree 1 or 2, then $|E(G)| \leq f(n-1)+2 \leq 2n-2$ follows by induction, because deleting a vertex of minimum degree the graph remains connected. Hence from now on we may assume that G has minimum degree at least 3.

Let $C = v_1v_2v_3v_4 \dots v_s$ be a longest cycle in G. We have already seen that if $s = n$, then $|E(G)| \leq 5n/3 < 2n - 2$. Next, we observe that if $n > s \geq 5$, then $V(G) \setminus V(C)$ is an independent set. Indeed, if xy is an edge outside C then there is a path P (possibly an edge) from $\{x, y\}$ to C and in this case a copy of $S_{2,2,2}$ is easily found using edges of C, with two edges from $P \cup \{xy\}$. E.g., if v_3x is an edge, then $S_{2,2,2}$ can have center v_3 and legs v_3xy, $v_3v_2v_1$, $v_3v_4v_5$. Thus, every vertex outside of C has at least three neighbors in C. Moreover, no two of those neighbors are consecutive in C, because C is longest. This immediately excludes $s = 5$. But also $s > 5$ is impossible because if e.g. v_2, v_4, v_6 are neighbors of x, then an $S_{2,2,2}$ can have center x and legs xv_2v_1, xv_4v_3, xv_6v_5.

As a consequence, investigations are reduced to $S_{2,2,2}$-free connected graphs with minimum degree at least 3 and without any cycles longer than 4. Such a graph G cannot be 2-connected (because due to Dirac's theorem, 2-connectivity would imply the presence of a cycle longer than 5). Hence G contains at least two endblocks.

Let B be an endblock of G, attached with cut vertex w to the other part of G. We argue that B induces K_4 in G. All vertices of B except w have degree at least 3 inside B, therefore B contains a 4-cycle, say $C' = wxyz$. If there is a vertex u in $V(B) \setminus V(C')$, then 2-connectivity of B and the exclusion of cycles longer than 4 imply that there are exactly two neighbors of u in C', either w and y, or x and z. But then there must exist a third neighbor v of u not in C', and v also has two neighbors in C'; and then a cycle longer than 4 would occur. Thus B is a K_4 indeed.

Now we are in a position to complete the proof of the theorem by induction on n. Consider any maximal $S_{2,2,2}$-free connected graph G of order $n > 7$ that has at least $2n-2$ edges. If G has a vertex of degree at most 2, then apply the upper bound $f(n-1)+2$.

If G has minimum degree at least 3, we know that G is not 2-connected. Then we distinguish cases according to n. If $n = 8$ or $n = 9$, remove all the 6 non-cutting vertices of two K_4 endblocks of G and apply the upper bound $f(n-6)+12$. This yields $|E(G)| \leq 13$ for $n = 8$ and $|E(G)| \leq 15$ for $n = 9$, both are smaller than $2n-2$.

If $n \geq 10$, remove the 3 non-cutting vertices of a K_4 endblock of G and apply the upper bound $f(n-3)+6$. This yields $|E(G)| \leq 2n-2$. $\square$

Remark 3.6. The extremal graphs are not unique if $n \geq 7$. In the graph constructed at the beginning of the proof we can remove three vertices of degree 2 and attach a block K_4 to one of the two high-degree vertices. As another alternative for $n \geq 10$, we can remove six vertices of degree 2 and attach two blocks isomorphic to K_4, one block to each high-degree vertex. A further extremal graph of order 7 can be obtained from K_5 by attaching two pendant edges to a vertex of K_5.

Proof of Theorem 1.9. A lower bound for $n \geq 7$ is the split graph $K_2 + E_{n-2}$ with $2n-3$ edges which does not even contain $S_{2,2,1}$ and hence $S_{3,2,1}$ cannot be a subgraph either.

The proof of the upper bound proceeds by induction on n. The base case $n = 7$ is left to the Reader. Assume G is a minimum connected counterexample with $n \geq 8$ vertices and has at least $2n-2$ edges but no copy of $S_{3,2,1}$. If G contains a vertex v of degree at most 2 such that $H = G - v$ is connected, then, by minimality, $e(H) \leq 2(n-1)-3$ hence $2n-2 \leq e(G) \leq e(H)+2 \leq 2n-3$ — a contradiction.

Next, assume v is a cut vertex with neighbors x and y. Consider the graph H that we obtain from G by deleting v and adding the edge xy. We will show that if H contains $S_{3,2,1}$ then so does G. Let A be the component containing x and B the component containing y. By symmetry we may assume that if H contains a copy S of $S_{3,2,1}$, then its center is in A and so B can contain vertices of at most one leg of S. We consider cases according to the number of vertices in $S \cap B$. If A contains $S_{3,2,1}$ completely, then so does G.

If A contains all of $S_{3,2,1}$ except for a leaf played by y, then the same copy with v replacing y is contained in G. If $S \cap B = \{y, w\}$, then the leg of S ending $x-y-w$ can be replaced in G with $x-v-y$ to obtain a copy S' of $S_{3,2,1}$. If $S \cap B = \{y, w, z\}$, then the leg of S ending $x-y-w-z$ can be replaced in G with $x-v-y-w$ to obtain a copy S' of $S_{3,2,1}$. So, as proved, H must be $S_{3,2,1}$-free, hence $2n-2 \leq e(G) \leq e(H)+1 \leq 2(n-1)-3+1 \leq 2n-4$ — a contradiction.

Therefore, from now on we may assume $\delta(G) \geq 3$. By Theorem 1.6(4), we know that G contains a copy S of $S_{2,2,1}$. Let v be the center of S with legs $v - u$, $v - x - y$, and $v - a - b$. If y or b has a neighbor not in S, then G contains a copy of $S_{3,2,1}$ — a contradiction.

Suppose x (or a) has a neighbor z not in S. Then z cannot be adjacent to any of v, y, a, b as a copy of $S_{3,2,1}$ would appear. Also, z cannot be adjacent to any vertex outside S as again a copy of $S_{3,2,1}$ would appear in G. By $\delta(G) \geq 3$, z must be adjacent to u, x, and a, but then a copy of $S_{3,2,1}$ (this time with center z) would appear in G.

We have shown so far that x, y, a, b cannot have neighbors outside S.

If u has at least two neighbors z and w outside S, then they cannot be adjacent (it would create the leg $v - u - z - w$ of a copy of $S_{3,2,1}$) and none of them can have a neighbor outside S as a copy of $S_{3,2,1}$ would appear in G. As shown above, they cannot be adjacent to any of x, y, a, b hence they have degree at most 2 (with neighbors u and possibly v) contradicting $\delta(G) \geq 3$.

If u has just one neighbor, say z outside S, then z cannot have a neighbor outside S as a copy of $S_{3,2,1}$ would appear, and as before, z cannot be adjacent to any of x, y, a, b hence z can be adjacent to at most u and v but then $d_G(z) \leq 2$ contradicts $\delta(G) \geq 3$.

So the only vertex of S that can have further neighbors outside S is v. We claim that there cannot exist a path $v - w - z$ with $w, z \notin S$. Indeed, if w, z existed, then any of the edges ax, ay would create a copy of $S_{3,2,1}$ with center a. Similarly, any of the edges xa, xb would create a copy of $S_{3,2,1}$ with center b. But then $\delta(G) \geq 3$ implies the presence of ua and ux in G creating a copy of $S_{3,2,1}$ with center u. Therefore all vertices outside S must have degree 1, which case has already been dealt with. This finishes the proof of the induction step. $\square$

Proof of Theorem 1.10. It is enough to prove that if G is a connected n-vertex graph with $\Delta(G) \geq \Delta(T)$, then G contains T or $e(G) \leq \lfloor \frac{(\Delta(T)-1)n}{2} \rfloor$. So fix a vertex v with $d_G(v) = \Delta(G) \geq \Delta(T)$ and consider the partition $\{v\}, N(v), X := V(G) \setminus N[v]$.

If X contains an edge xy, then by connectivity of G, there must exist a path (maybe a single edge) from xy to $N(v)$ and we find a copy of T in G. So we may assume that X is independent, and thus by connectivity of G, every $x \in X$ is adjacent to at least one $u \in N(v)$.

CASE I: $d_G(v) = \Delta(G) > \Delta(T)$.

Then any $x \in X$ is adjacent to exactly one vertex $u \in N(v)$ as if xu, xu' are edges in G, then uxu' can form the long leg of a copy of T with center v and other neighbors of v complete this copy of T. So $d_G(x) = 1$ for all $x \in X$. Let $u, u' \in N(v)$ be two vertices such that at least one of them has a neighbor in X. Then again if uu' is an edge, we find a copy of T. So if $U \subseteq N(v)$ is the set of neighbors of v that are adjacent to a vertex in X and $U' = N(v) \setminus U$, then $e(G) \leq |U \cup X| + e(U')$. If $|U'| \leq \Delta(T) + 1$, then $e(U') \leq \binom{\Delta(T)+1}{2}$ and so $e(G) \leq n - 1 + \binom{\Delta(T)+1}{2} \leq \lfloor \frac{(\Delta(T)-1)n}{2} \rfloor$ as $\Delta(T) - 1 \geq 3$. Finally, if $|U'| \geq \Delta(T) + 2$, then either $G[U']$ is a (partial) matching and thus $e(G) \leq (1 + |U| + |X| - 1) + \frac{3|U'|}{2} \leq \frac{3(n-1)}{2} \leq \lfloor \frac{(\Delta(T)-1)n}{2} \rfloor$ (here we use $\Delta(T) \geq 4$) or $G[U']$ contains a path on 3 vertices, and then by $|U'| \geq \Delta(T) + 2$ we find a copy of T in G.

CASE II: $d_G(v) = \Delta(G) = \Delta(T)$.

As X is independent, we have $e(G) \leq (\Delta(G) + 1)\Delta(G) = (\Delta(T) + 1)\Delta(T) = O(1)$. $\square$

Proof of Theorem 1.11. The lower bound $\lfloor\frac{(k-a)n}{2}\rfloor$ follows from Remark 1.4(1), while, as the diameter of $B(k,a)$ is a, Remark 1.4(2) yields the lower bound $\binom{\lceil\frac{a+1}{2}\rceil}{2}+\lfloor\frac{a-1}{2}\rfloor(n-\lfloor\frac{a+1}{2}\rfloor)$.

To see the upper bound of (2), let $G(V,E)$ be an n-vertex $B(k,a)$-free graph with $a\le k/3$. Assume first that there exists a vertex x with $d_G(x)\ge k-1$. We claim that $G[V\setminus\{x\}]$ does not contain a path on $2a-3$ vertices. Indeed, suppose to the contrary that $y_1,y_2,\dots,y_{2a-3}$ is a path in $G[V\setminus\{x\}]$. Then as G is connected, there exists a path P from x to some y_j that does not contain any other y_i. Then either $x,P,y_j,y_{j-1},\dots,y_1$ or $x,P,y_j,y_{j+1},\dots,y_{2a-3}$ contains at least a vertices. So x and the first $a-1$ of them together with the other neighbors of x form a copy of $B(k,a)$ — a contradiction. Theorem 1.2 implies that if n is large enough, then $e(G)\le n-1+e(G-x)\le n-1+\lfloor\frac{2a-5}{2}\rfloor n\le an\le\lfloor\frac{k-a}{2}n\rfloor$ as $a\le k/3$. This finishes the proof in this case.

Assume finally that $\Delta(G)\le k-2$. Then if n is large enough, every vertex x of G is the endpoint of a path on $a\cdot k$ vertices, since G is connected and have maximum degree at most $k-2$. Suppose towards a contradiction that G contains a vertex x with $d_G(x)=d\ge k-a+1$. Let $z_1,z_2,\dots z_d$ be the neighbors of x and let $x,y_2,y_3,\dots,y_{a\cdot k}$ be a path P. Then y_2 is one of the z_j's, and as $d\le k-2$, there must exist z_j such that $z_j\in P$, say $z_j=y_i$ and either $y_{i-1},y_{i-2},\dots,y_{i-a+2}$ or $y_{i+1},y_{i+2},\dots,y_{i+a-2}$ are not neighbors of x. Then x, these y_is and the neighbors of x form a $B(k,a)$.

We obtained that $\Delta(G)\le k-a$ must hold, which implies $e(G)\le\lfloor\frac{(k-a)n}{2}\rfloor$ as claimed. □

Theorem 1.11 will provide the upper bound of Theorem 1.12. The next statement gives a general lower bound on $\mathrm{ex}_c(n,T)$ and thus will help us obtain the lower bound of Theorem 1.12.

Theorem 3.7. *For any $\varepsilon>0$ there exists a positive integer $k_0=k_0(\varepsilon)$ such that for any tree T on $k\ge k_0$ vertices, we have $\mathrm{ex}_c(n,T)\ge(\frac{k}{6}-\varepsilon)n$ if $k\ge k_0$ and n is large enough.*

Proof. CASE I: $m(T)>\lfloor k/3\rfloor$.

Then by Proposition 1.5(3) we have

$$\mathrm{ex}_c(n,T)\ge n-1+\left\lfloor\frac{n-1}{m(T)-1}\right\rfloor\binom{m(T)-1}{2}\ge(n-1)\left(1+\frac{\lfloor k/3\rfloor-1}{2}\right)$$
$$\ge nk\left(\frac{1}{6}-\varepsilon\right),$$

if k and n are large enough.

CASE II: $m(T)\le\lfloor k/3\rfloor$.

Then $m_2(T)\le 2m(T)\le 2\lfloor\frac{k}{3}\rfloor$, and thus $k-m_2(T)\ge\lceil\frac{k}{3}\rceil$. Proposition 1.5(4) yields

$$\mathrm{ex}_c(n,T)\ge\left\lfloor\frac{n}{\lceil\frac{k}{3}\rceil}\right\rfloor\left(1+\binom{\lceil\frac{k}{3}\rceil}{2}\right)\ge nk\left(\frac{1}{6}-\varepsilon\right),$$

if k and n are large enough. □

Proof of Theorem 1.12. The lower bound follows from Theorem 3.7, the upper bound from Theorem 1.11(2) with taking $a=\lfloor k/3\rfloor$. □

4 Concluding remarks

Theorem 1.12 gave upper and lower bounds on γ. If the lower bound from Theorem 1.11(1) turned out to be (asymptotically) sharp (which we believe to be the case) for $a = (1/2-\varepsilon)k$ or $a = (1/2+\varepsilon)k$, then the upper bound on γ would improve from $2/3$ to $1/2$. Note that a special case of Theorem 1.10 yields $\mathrm{ex}_c(n, S_{3,1,1,1}) = \lfloor \frac{(\Delta(S_{3,1,1,1})-1)n}{2} \rfloor$, so a small case when $a = \lfloor k/2 \rfloor$. We have no evidence to believe that the lower bound of $1/3$ on γ is best possible.

In Remark 1.4 and Proposition 1.5, we enumerated several graph parameters based on which one could define general constructions avoiding trees T for which these parameters have small value. It would be nice to add other parameters to this list, and would be wonderful to prove that it is enough to consider a finite set of parameters to determine the asymptotics of $\mathrm{ex}_c(n, T)$ for all trees T. Of particular interest is the characterization of those trees for which $\mathrm{ex}(n, T) - c(T) \leq \mathrm{ex}_c(n, T) \leq \mathrm{ex}(n, T)$ holds for some constant $c(T)$. As we have seen after Remark 1.4, balanced trees share this property assuming the Erdős-Sós conjecture.

Proposition 1.5 gave constructions that do not contain any tree T on k vertices with given $p(T)$, $\delta_2(T)$, $m(T)$, and $m_2(T)$. It would be interesting to figure out whether these constructions are best possible. For a family $\mathcal{G}$ of graphs, we write $\mathrm{ex}_c(n, \mathcal{G})$ to denote the maximum number of edges in an n-vertex connected graph that does not contain any $G \in \mathcal{G}$ as a subgraph.

Problem 4.1. (1) For any k and p let $\mathcal{T}^0_{k,p}$ denote the set of trees T on k vertices with $p(T) \leq p$. Determine $\mathrm{ex}_c(n, \mathcal{T}^0_{k,p})$.

(2) For any k and $d \geq 3$ let $\mathcal{T}^0_{k,d}$ denote the set of trees T on k vertices with $\delta_2(T) \geq d$. Determine $\mathrm{ex}_c(n, \mathcal{T}^0_{k,d})$.

(3) For any k and m let $\mathcal{T}^1_{k,m}$ denote the set of trees T on k vertices with $m(T) \geq m$. Determine $\mathrm{ex}_c(n, \mathcal{T}^1_{k,m})$.

(4) For any k and m let $\mathcal{T}^2_{k,m}$ denote the set of trees T on k vertices with $m_2(T) \leq m$. Determine $\mathrm{ex}_c(n, \mathcal{T}^2_{k,m})$.

As for special tree classes, one such class that could give some insight is the set of spiders with all legs of at most 2 vertices. For the spider $S = S_{2,2,\ldots,2,1,1,\ldots,1}$ with t legs of two vertices and s legs consisting of a single vertex, we have $|S| = 2t + s + 1$, and

- $\nu(T) = t + 1$ if $s > 0$,
- $\Delta(T) = t + s$,
- $m_2(T) = 4$ if $t \geq 2$.

The construction of Remark 1.4(1) based on maximum degree outperforms the one based on the matching number in Remark 1.4(3) if $s > t$. But the one based on m_2 in Proposition 1.5(4) is better than both previous ones once $s \geq 5$ and $t \geq 2$. It would be interesting to see whether these constructions achieve the asymptotics of $\mathrm{ex}_c(n, S)$.

Classical Turán numbers are monotone with two respects: Firstly, if H is a subgraph of F then $\mathrm{ex}(n, H) \leq \mathrm{ex}(n, F)$. This inequality is preserved for the connected Turán number

$\mathrm{ex}_c(n, F)$ (excluding the small "undefined" cases K_2 and P_3). Secondly, if $m < n$, then $\mathrm{ex}(m, F) \leq \mathrm{ex}(n, F)$. This property is not necessarily preserved by connected Turán numbers for small values of n with respect to $|T|$. There are several examples given by our results, of the following type: $\mathrm{ex}_c(|T| - 1, T) = \binom{|T|-1}{2} > \mathrm{ex}_c(|T|, T)$; see e.g. $T = S_{3,2,1}$.

Problem 4.2. Is it true that there exists a threshold $n_0(F)$ such that $\mathrm{ex}_c(m, F) \leq \mathrm{ex}_c(n, F)$ holds whenever $n_0(F) \leq m < n$?

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On the number of non-isomorphic (simple) k-gonal biembeddings of complete multipartite graphs*

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Abstract

This article aims to provide exponential lower bounds on the number of non-isomorphic k-gonal face-2-colourable embeddings (sometimes called, with abuse of notation, biembeddings) of the complete multipartite graph into orientable surfaces.

For this purpose, we use the concept, introduced by Archdeacon in 2015, of Heffer array and its relations with graph embeddings. In particular we show that, under certain hypotheses, from a single Heffter array, we can obtain an exponential number of distinct graph embeddings. Exploiting this idea starting from the arrays constructed by Cavenagh, Donovan and Yazıcı in 2020, we obtain that, for infinitely many values of k and v, there are at least $k^{\frac{k}{2}+o(k)} \cdot 2^{v \cdot \frac{H(1/4)}{(2k)^2}+o(v)}$ non-isomorphic k-gonal face-2-colourable embeddings of K_v, where $H(\cdot)$ is the binary entropy. Moreover about the embeddings of $K_{\frac{v}{t} \times t}$, for $t \in \{1, 2, k\}$, we provide a construction of $2^{v \cdot \frac{H(1/4)}{2k(k-1)}+o(v,k)}$ non-isomorphic k-gonal face-2-colourable embeddings whenever k is odd and v belongs to a wide infinite family of values.

Keywords: Topological embedding, non-isomorphic embedding, Heffter array.

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1 Introduction

The purpose of this paper is to provide exponential lower bounds on the number of non-isomorphic embeddings of the complete multipartite graph into orientable surfaces that induce faces of a given length k (i.e. we investigate the so-called *k-gonal embeddings*). We first recall some basic definitions, see [28].

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Definition 1.1. Given a graph Γ and a surface Σ, an *embedding* of Γ in Σ is a continuous injective mapping $\psi\colon \Gamma \to \Sigma$, where Γ is viewed with the usual topology as 1-dimensional simplicial complex.

The connected components of $\Sigma \setminus \psi(\Gamma)$ are said ψ-*faces*. Also, with abuse of notation, we say that a closed walk F of Γ is a face (induced by the embedding ψ) if $\psi(F)$ is the boundary of a ψ-face. Then, if each ψ-face is homeomorphic to an open disc, the embedding ψ is called *cellular*. If the boundary of a face is homeomorphic to a circumference (i.e. is a simple cycle), such a face is said to be *simple* and if all the faces are simple we say that the embedding is *circular* (or simple, following the notation of [32]). If moreover, the embedding is *face*-2-*colourable* sometimes, with abuse of notation, we call it a *biembedding*. In this context, we say that two embeddings $\psi\colon \Gamma \to \Sigma$ and $\psi'\colon \Gamma' \to \Sigma'$ are *isomorphic* if and only if there is a graph isomorphism $\sigma\colon \Gamma \to \Gamma'$ such that $\sigma(F)$ is a ψ'-face if and only if F is a ψ-face.

The existence problem of cellular embeddings of a graph Γ into (orientable) surfaces has been widely studied in the case of triangular embeddings, which are the ones whose faces are triangular. This kind of embeddings has been investigated, at first, because their construction was a major step in proving the Map Color Theorem [33]. Among the papers related to this existence problem, we recall [3, 15, 16, 18, 19, 23, 26] where the natural question of the rate growth of the number of non-isomorphic triangular embeddings of complete graphs has been considered too. Moreover, due to the Euler formula, if there exists a triangular embedding ψ from Γ to some surface Σ, ψ minimizes the genus of Σ. For this reason, such kinds of embeddings are called *genus embeddings*. Two naturally related questions are the investigation of the rate of the number of non-isomorphic genus embeddings (see [21, 25]) and that of the k-gonal embeddings (see [17, 22, 24]).

In this paper, we consider the latter question and we study the rate growth of the number of non-isomorphic k-gonal embeddings of the complete multipartite graph with m parts of size t, denoted by $K_{m\times t}$. Here, we provide exponential lower bounds on this number for several infinite classes of parameters k, m and t. Furthermore, our embeddings also realize additional properties: the faces they induce are (in several cases) simple and it is possible to color them within two colors, i.e. these embeddings are 2-face colorable. Finally, in the cases where k is 3, we find new classes of genus embeddings.

The approach we use in this article is purely combinatorial and requires the notion of combinatorial embedding, see [14, 34]. Here, we denote by $D(\Gamma)$ the set of all the oriented edges of the graph Γ and, given a vertex x of Γ, by $N(\Gamma, x)$ the neighborhood of x in Γ.

Definition 1.2. Let Γ be a connected multigraph. A *combinatorial embedding* of Γ (into an orientable surface) is a pair $\Pi = (\Gamma, \rho)$ where $\rho\colon D(\Gamma) \to D(\Gamma)$ satisfies the following properties:

- for any $y \in N(\Gamma, x)$, there exists $y' \in N(\Gamma, x)$ such that $\rho(x, y) = (x, y')$;
- we define ρ_x as the permutation of $N(\Gamma, x)$ such that, given $y \in N(\Gamma, x)$, $\rho(x, y) = (x, \rho_x(y))$. Then the permutation ρ_x is a cycle of order $|N(\Gamma, x)|$.

It is well known that a combinatorial embedding of Γ is equivalent to a cellular embedding of Γ in an orientable surface, see [1, 20, 29]. This observation leads us to study this kind of embedding isomorphisms purely combinatorially. From the combinatorial point of view, the faces are determined using the face-trace algorithm, see [1]. It is easy to see that the faces are closed walks (that is sequences of consecutive vertices and edges, denoted by $v_1, v_2, \dots, v_k$), the *length* of a closed walk is the number of its edges. If the faces are simple then $v_i \neq v_j$ for any $i \neq j$, so the closed walks are indeed cycles with k distinct vertices and k edges. In this context, it is possible to rephrase the definition of embedding isomorphism as done by Korzhik and Voss in [24], see page 61.

Definition 1.3. Let $\Pi := (\Gamma, \rho)$ and $\Pi' := (\Gamma', \rho')$ be two combinatorial embeddings of, respectively, Γ and Γ'. We say that Π is *isomorphic* to Π' if there exists a graph isomorphism $\sigma\colon \Gamma \to \Gamma'$ such that, for any $(x, y) \in D(\Gamma)$, we have either

$$\sigma \circ \rho(x, y) = \rho' \circ \sigma(x, y) \tag{1.1}$$

or

$$\sigma \circ \rho(x, y) = (\rho')^{-1} \circ \sigma(x, y). \tag{1.2}$$

We also say, with abuse of notation, that σ is an *embedding isomorphism* between Π and Π'. Moreover, if Equation (1.1) holds, σ is said to be an *orientation preserving isomorphism* while, if (1.2) holds, σ is said to be an *orientation reversing isomorphism.*

This combinatorial approach has been developed in the literature into two kinds of directions. The first one is the use of recursive constructions and has been applied to construct triangular embeddings of complete graphs from triangular embeddings of complete graphs of a lesser order. Within this method, it was first shown that there are at least $2^{av^2-o(v^2)}$ non-isomorphic face-2-colourable triangular embeddings of the complete graph K_v for several congruence classes modulo 36, 60 and 84 (see [3, 16]) and then that, for an infinite (but rather sparse) family of values of v, there are at least $v^{bv^2-o(v^2)}$ non-isomorphic face-2-colourable triangular embeddings of K_v (see [15, 18, 19]). Another consequence of these kinds of recursive constructions is the existence of $2^{cv^2-o(v^2)}$ non-isomorphic Hamiltonian embeddings of K_v for infinitely many values of v (see [17]).

The second approach uses the current graph technique. Within this method, it was provided the first exponential lower bound (of type 2^{dv}) on the number of non-isomorphic face-2-colourable triangular embeddings of K_v for infinitely many values of v. Then, similar results have been also given in the cases of genus and quadrangular embeddings (see [22, 23, 24, 25]). The approach used in this paper belongs to this second family. The main tool we will use is the concept of Heffter array, introduced by Archdeacon in [1] to provide constructions of current graphs. Section 2 of this paper will be dedicated to introducing this kind of array, to reviewing the literature on this topic and to further investigating the connection with face-2-colourable embeddings. Then, in Section 3, we will deal with the following problem: given a family of embeddings each of which admits $\mathbb{Z}_v$ as a regular automorphism group (i.e. embeddings that are $\mathbb{Z}_v$-regular), how many of its elements can be isomorphic? Proposition 3.4 will provide an upper bound on this number. In the last two sections, we will consider some of the known constructions of Heffter arrays and we will show that, under certain hypotheses, from each of such arrays we can obtain a family of $\mathbb{Z}_v$-regular embeddings that is exponentially big. These families, together with Proposition 3.4, will allow us to achieve the existence of an exponential number of non-isomorphic k-gonal face-2-colourable embeddings of K_v and $K_{\frac{v}{t}\times t}$ in several situations. In particular, in Section 4 we will obtain that, when k is congruent to 3 modulo 4 and v belongs to an infinite family of values, there are $k^{\frac{k}{2}+o(k)} \cdot 2^{g(k)v+o(v)}$ non-isomorphic k-gonal face-2-colourable embeddings of K_v where $g(k)$ is a rational function of k. Finally, in Section 5, we will consider the embeddings of $K_{\frac{v}{t}\times t}$. In this case, for $t\in\{1,2,k\}$, we will provide a construction of $2^{h(k)v+o(v,k)}$ non-isomorphic k-gonal face-2-colourable embeddings whenever k is odd, v belongs to a wide infinite family of values and where $h(k)$ is a rational function of k.

2 Heffter arrays and face-2-colourable embeddings

In this section we introduce the classical concept of Heffter array and its generalizations, showing how these notions are useful tools for getting face-2-colourable embeddings of the complete multipartite graph into an orientable surface.

An $m\times n$ partially filled array on a given set Ω is an $m\times n$ matrix with elements in Ω in which some cells can be empty. Archdeacon [1] introduced a class of partially filled arrays, called *Heffter arrays*, and showed how it is related to several other mathematical concepts such as difference families, graph decompositions, current graphs and face-2-colourable embeddings. These arrays have been then generalized by Costa and al. in [9] as follows.

Definition 2.1. Let $v=2nk+t$ be a positive integer, where t divides $2nk$, and let J be the subgroup of $\mathbb{Z}_v$ of order t. A *Heffter array over* $\mathbb{Z}_v$ *relative to* J, denoted by $\mathrm{H}_t(m,n;h,k)$, is an $m\times n$ partially filled array with elements in $\mathbb{Z}_v$ such that:

(1) each row contains h filled cells and each column contains k filled cells;

(2) for every $x\in\mathbb{Z}_v\setminus J$, either x or $-x$ appears in the array;

(3) the elements in every row and in every column sum to 0 (in $\mathbb{Z}_v$).

Example 2.2. Below we have an $\mathrm{H}_9(11;9)$, say A. Hence the elements of A belongs to $\mathbb{Z}_{207}$ and we avoid the elements of the subgroup of $\mathbb{Z}_{207}$ of order 9.

10	55	101	−90		13	−22		−78	67	−56
−37	−9	45	102	−91		21	−20		−79	68
58	−47	−8	54	103	−81		19	−18		−80
−70	59	−38	−7	44	93	−82		17	−16	
	−71	60	−48	−6	53	94	−83		15	−14
−33		−72	61	−39	11	49	95	−84		12
24	−25		−73	62	−43	4	40	96	−85	
	26	−27		−74	63	−52	3	50	97	−86
−87		28	−29		−75	64	−42	2	41	98
99	−88		30	−31		−76	65	−51	−5	57
36	100	−89		32	−34		−77	66	−35	1

If $t=1$, namely, if J is the trivial subgroup of $\mathbb{Z}_{2nk+1}$, we find the classical Heffter arrays defined by Archdeacon, which are simply denoted by $\mathrm{H}(m,n;h,k)$. It is immediate that if there exists an $\mathrm{H}_t(m,n;h,k)$ then $mh=nk$, $3\le h\le n$ and $3\le k\le m$. Also, $m=n$ implies $k=h$ and an $\mathrm{H}_t(n,n;k,k)$ is simply denoted by $\mathrm{H}_t(n;k)$. The most important result about the existence problem for Heffter arrays is the following, see [2, 5, 13].

Theorem 2.3. *An* $\mathrm{H}(n;k)$ *exists for every* $n\ge k\ge 3$.

For other existence results on classical and generalised Heffter arrays see [32].

In [10] we introduced the further generalization of a *λ-fold Heffter array A over $\mathbb{Z}_v$ relative to* J, denoted by ${}^\lambda\mathrm{H}_t(m,n;h,k)$ replacing property (2) of Definition 2.1 with the following one:

(2') the multiset $\{\pm x \mid x \in A\}$ contains λ times each element of $\mathbb{Z}_v \setminus J$, where $v = \frac{2nk}{\lambda} + t$.

Note that if $\lambda > 1$ then h and k can also be equal to 2.

Example 2.4. The following array A is a ${}^2\mathrm{H}(2,5;5,2)$, in fact the multiset $\{\pm x \mid x \in A\}$ contains 2 times each element of $\mathbb{Z}_{11} \setminus \{0\}$.

1	-2	3	4	5
-1	2	-3	-4	-5

Anyway here we consider the case $\lambda = 1$, since several of our constructions cannot be naturally extended to the case $\lambda > 1$, as it will be underlined in Remark 2.17.

The focus of this paper is not the existence problem of Heffter arrays, but their connection with face-2-colourable embeddings. We point out that there are several papers in which Heffter arrays have been investigated to obtain face-2-colourable embeddings see [1, 4, 6, 8, 10, 11, 12]. To present such a connection, now we have to introduce the concepts of *simple and compatible orderings*.

In the following, given two integers $a \leq b$, by $[a,b]$ we denote the interval containing the integers $\{a, a+1, \ldots, b\}$. If $a > b$, then $[a,b]$ is empty. The rows and the columns of an $m \times n$ array A are denoted by $R_1, \ldots, R_m$ and by $C_1, \ldots, C_n$, respectively. Also we denote by $\mathcal{E}(A)$, $\mathcal{E}(R_i)$, $\mathcal{E}(C_j)$ the list of the elements of the filled cells of A, of the i-th row and of the j-th column, respectively. Given a finite subset T of an abelian group G and an ordering $\omega = (t_1, t_2, \ldots, t_k)$ of the elements of T, for any $i \in [1,k]$ let $s_i = \sum_{j=1}^{i} t_j$ be the i-th partial sum of T. The ordering ω is said to be *simple* if $s_a \neq s_b$ for all $1 \leq a < b \leq k$. We point out that if $s_k = 0$ an ordering ω is simple if no proper subsequence of consecutive elements of ω sums to 0. Note also that, if ω is a simple ordering, then $\omega^{-1} = (t_k, t_{k-1}, \ldots, t_1)$ is simple too. Given an $m \times n$ partially filled array A, by ω_{R_i} and ω_{C_j} we denote an ordering of $\mathcal{E}(R_i)$ and $\mathcal{E}(C_j)$, respectively. If for any $i \in [1,m]$ and for any $j \in [1,n]$, the orderings ω_{R_i} and ω_{C_j} are simple, we define by $\omega_r = \omega_{R_1} \circ \cdots \circ \omega_{R_m}$ the simple ordering for the rows and by $\omega_c = \omega_{C_1} \circ \cdots \circ \omega_{C_n}$ the simple ordering for the columns. Also, by *natural ordering* of a row (column) of A one means the ordering from left to right (from top to bottom).

Definition 2.5. A partially filled array A on an abelian group G is said to be

- *simple* if there exists a simple ordering for each row and each column of A;
- *globally simple* if the natural ordering of each row and each column of A is simple.

It is easy to see that if $k \leq 5$ then every $\mathrm{H}_t(n;k)$ is globally simple. By a direct check one can see that the array of Example 2.2 is globally simple.

Definition 2.6. Given a relative Heffter array A, the orderings ω_r and ω_c are said to be *compatible* if $\omega_c \circ \omega_r$ is a cycle of order $|\mathcal{E}(A)|$.

Reasoning as in [11], we get the following.

Theorem 2.7. *Let A be a relative Heffter array $\mathrm{H}_t(m,n;h,k)$ that admits two compatible orderings ω_r and ω_c. Then there exists a cellular face-2-colourable embedding σ of $K_{\frac{2nk+t}{t}\times t}$, such that every edge is on a face whose boundary has length h and on a face whose boundary has length k, into an orientable surface of genus*

$$g = 1 + \frac{(nk-n-m-1)(2nk+t)}{2}.$$

Moreover, σ is $\mathbb{Z}_{2nk+t}$-regular.

Remark 2.8. As already remarked in the Introduction, in general, in Theorem 2.7, the faces are closed walks, but if the array is simple with respect to the compatible orderings ω_r and ω_c then the faces are cycles. Clearly, in this case the face-2-colourable embedding is circular.

Now we recall the definition of the Archdeacon embedding, see [1]. Let A be an $\mathrm{H}_t(m,n;h,k)$; we consider the permutation ρ_0 on $\pm\mathcal{E}(A) = \mathbb{Z}_{2nk+t} \setminus \frac{2nk+t}{t}\mathbb{Z}_{2nk+t}$, where $\frac{2nk+t}{t}\mathbb{Z}_{2nk+t}$ denotes the subgroup of $\mathbb{Z}_{2nk+t}$ of order t, so defined:

$$\rho_0(a) = \begin{cases} -\omega_r(a) \text{ if } a \in \mathcal{E}(A); \\ \omega_c(-a) \text{ if } a \in -\mathcal{E}(A). \end{cases} \tag{2.1}$$

Note that the complete multipartite graph $K_{\frac{2nk+t}{t}\times t}$ is nothing but the Cayley graph on $\mathbb{Z}_{2nk+t}$ with connection set $\pm\mathcal{E}(A)$, denoted by $Cay[\mathbb{Z}_{2nk+t} : \pm\mathcal{E}(A)]$. Now, we define a map ρ on the set of the oriented edges of this graph as follows:

$$\rho((x, x+a)) = (x, x+\rho_0(a)). \tag{2.2}$$

Since ρ_0 acts cyclically on $\pm\mathcal{E}(A)$, the map ρ is a rotation of $Cay[\mathbb{Z}_{2nk+t} : \pm\mathcal{E}(A)]$.

Example 2.9. Let A be the $\mathrm{H}_9(11;9)$ given in Example 2.2. Consider the following ordering for the rows

$$\begin{aligned} \omega_r = {} & (10,55,101,-90,13,-22,-78,67,-56)(-37,-9,45,102,-91,21,-20,-79,68) \\ & (58,-47,-8,54,103,-81,19,-18,-80)(-70,59,-38,-7,44,93,-82,17,-16) \\ & (-71,60,-48,-6,53,94,-83,15,-14)(-33,-72,61,-39,11,49,95,-84,12) \\ & (24,-25,-73,62,-43,4,40,96,-85)(26,-27,-74,63,-52,3,50,97,-86) \\ & (-87,28,-29,-75,64,-42,2,41,98)(99,-88,30,-31,-76,65,-51,-5,57) \\ & (36,100,-89,32,-34,-77,66,-35,1) \end{aligned}$$

and the following ordering for the columns

$$\begin{aligned} \omega_c = {} & (10,36,99,-87,24,-33,-70,58,-37)(55,-9,-47,59,-71,-25,26,-88,100) \\ & (101,45,-8,-38,60,-72,-27,28,-89)(-90,102,54,-7,-48,61,-73,-29,30) \\ & (-91,103,44,-6,-39,62,-74,-31,32)(13,-81,93,53,11,-43,63,-75,-34) \\ & (-22,21,-82,94,49,4,-52,64,-76)(-20,19,-83,95,40,3,-42,65,-77) \\ & (-78,-18,17,-84,96,50,2,-51,66)(67,-79,-16,15,-85,97,41,-5,-35) \\ & (-56,68,-80,-14,12,-86,98,57,1). \end{aligned}$$

Hence,

$$\begin{aligned} \omega_c \circ \omega_r = {} & (10,-9,-8,-7,-6,11,4,3,2,-5,1,99,100,101,102,103,93,94,95,96,97, \\ & 98,24,26,28,30,32,13,21,19,17,15,12,-70,-71,-72,-73,-74,-75, \\ & -76,-77,-78,-79,-80,-37,-47,-38,-48,-39,-43,-52,-42,-51, \\ & -35,-56,36,55,45,54,44,53,49,40,50,41,57,-87,-89,-91,-82,-84, \\ & -86,-88,-90,-81,-83,-85,-33,-27,-31,-22,-18,-14,-25,-29, \\ & -34,-20,-16,58,59,60,61,62,63,64,65,66,67,68). \end{aligned}$$

So, since $\omega_c \circ \omega_r$ is a cycle of order $99 = |\mathcal{E}(A)|$ the orderings are compatible.

Looking for compatible orderings of a (globally simple) Heffter array leads us to consider the following problem introduced in [7]. Given an $m \times n$ *toroidal* partially filled array A, by r_i we denote the orientation of the i-th row, precisely $r_i = 1$ if it is from left to right and $r_i = -1$ if it is from right to left. Analogously, for the j-th column, if its orientation c_j is from top to bottom then $c_j = 1$ otherwise $c_j = -1$. Assume that an orientation $\mathcal{R} = (r_1, \ldots, r_m)$ and $\mathcal{C} = (c_1, \ldots, c_n)$ is fixed. Given an initial filled cell (i_1, j_1) consider the sequence $L_{\mathcal{R},\mathcal{C}}(i_1, j_1) = ((i_1, j_1), (i_2, j_2), \ldots, (i_\ell, j_\ell), (i_{\ell+1}, j_{\ell+1}), \ldots)$ where $j_{\ell+1}$ is the column index of the filled cell $(i_\ell, j_{\ell+1})$ of the row R_{i_ℓ} next to (i_ℓ, j_ℓ) in the orientation r_{i_ℓ}, and where $i_{\ell+1}$ is the row index of the filled cell of the column $C_{j_{\ell+1}}$ next to $(i_\ell, j_{\ell+1})$ in the orientation $c_{j_{\ell+1}}$. Given an element $(i_k, j_k) \in L_{\mathcal{R},\mathcal{C}}(i_1, j_1)$ we define $S_{\mathcal{R},\mathcal{C}}(i_k, j_k)$ as the element $(i_{k+1}, j_{k+1}) \in L_{\mathcal{R},\mathcal{C}}(i_1, j_1)$. It is easy to see that $S_{\mathcal{R},\mathcal{C}}$ is well defined on the set of the filled cells of A.

The problem proposed in [7] is the following:

Crazy Knight's Tour Problem. Given a toroidal partially filled array A, do there exist $\mathcal{R}$ and $\mathcal{C}$ such that the list $L_{\mathcal{R},\mathcal{C}}$ covers all the filled cells of A?

The Crazy Knight's Tour Problem for a given array A is denoted by $P(A)$, known results can be found in [7, 27]. Also, given a filled cell (i, j), if $L_{\mathcal{R},\mathcal{C}}(i, j)$ covers all the filled positions of A we will say that $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$. The relationship between the Crazy Knight's Tour Problem and (globally simple) relative Heffter arrays is explained in the following result, see [11].

Corollary 2.10. *Let A be a relative Heffter array $\mathrm{H}_t(m, n; h, k)$ such that $P(A)$ admits a solution $(\mathcal{R}, \mathcal{C})$. Then there exists a face-2-colourable embedding of $K_{\frac{2nk+t}{t} \times t}$, such that every edge is on a face whose boundary has length h and on a face whose boundary has length k, into an orientable surface.*

Moreover if A is globally simple, then the face-2-colourable embedding is circular.

Example 2.11. Let A be the $H_9(11; 9)$ of Example 2.2. Let $\mathcal{R} = (1, 1, \ldots, 1)$ and $\mathcal{C} = (-1, 1, 1, \ldots, 1)$. Now we consider $S_{\mathcal{R},\mathcal{C}}(1, 1)$ and, in the following table, in each position we write j if we reach that position after having applied $S_{\mathcal{R},\mathcal{C}}$ to $(1, 1)$ exactly j times.

	$\uparrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
$\rightarrow$	0	56	13	73		27	80		41	97	54
$\rightarrow$	44	1	57	14	68		28	86		42	98
$\rightarrow$	88	45	2	58	15	74		29	81		43
$\rightarrow$	33	89	46	3	59	16	69		30	87	
$\rightarrow$		34	90	47	4	60	17	75		31	82
$\rightarrow$	77		35	91	48	5	61	18	70		32
$\rightarrow$	22	83		36	92	49	6	62	19	76	
$\rightarrow$		23	78		37	93	50	7	63	20	71
$\rightarrow$	66		24	84		38	94	51	8	64	21
$\rightarrow$	11	72		25	79		39	95	52	9	65
$\rightarrow$	55	12	67		26	85		40	96	53	10

Note that $L_{\mathcal{R},\mathcal{C}}(1, 1)$ covers all filled cells of A, hence $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$.

Remark 2.12. The orderings ω_r and ω_c of A described in Example 2.9, correspond to the vectors $\mathcal{R}$ and $\mathcal{C}$ of Example 2.11, respectively. Hence, we also say that $(\mathcal{R}, \mathcal{C})$ induces the cycle $\omega_c \circ \omega_r$.

Clearly, given an array A, a pair $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$ if and only if the induced permutation $\omega_c \circ \omega_r$ is a cycle of order $|\mathcal{E}(A)|$.

Now, to present the results of this section we need some other definitions and notations. By $skel(A)$ we denote the *skeleton* of A, that is the set of the filled positions of A. Given an $n \times n$ partially filled array A, for $i \in [1, n]$ we define the i-th diagonal of A as follows:

$$D_i = \{(i, 1), (i + 1, 2), \ldots, (i - 1, n)\}.$$

Here all the arithmetic on the row and column indices is performed modulo n, where $\{1, 2, \ldots, n\}$ is the set of reduced residues. The diagonals $D_{i+1}, D_{i+2}, \ldots, D_{i+k}$ are called k *consecutive diagonals*. A set of t consecutive diagonals $S = \{D_{i+1}, D_{i+2}, \ldots, D_{i+t}\}$ is said to be an *empty strip of width* t if $D_{i+1}, D_{i+2}, \ldots, D_{i+t}$ are empty diagonals, while D_i and D_{i+t+1} are non-empty diagonals.

Definition 2.13. Let n, k be integers such that $n \geq k \geq 1$. An $n \times n$ partially filled array A is said to be:

- *k-diagonal* if the non-empty cells of A are exactly those of k diagonals;
- *cyclically k-diagonal* if the non-empty cells of A are exactly those of k consecutive diagonals;
- *k-diagonal with width $t_1, t_2, \ldots, t_s$* if it is k-diagonal and has s empty strips with width $t_1, t_2, \ldots, t_s$, respectively;
- *k-diagonal with width t* if it is k-diagonal and all its empty strips have width t.

Clearly a cyclically k-diagonal array of size n is nothing but a k-diagonal array with width $n - k$. Note that the array of Example 2.2 is 9-diagonal with width 1.

Lemma 2.14. *Let A be a partially filled array. If $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$, then also $(-\mathcal{R}, -\mathcal{C})$ is a solution of $P(A)$.*

Proof. By Remark 2.12, if $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$, then the induced cycle $\omega_c \circ \omega_r$ has order $|\mathcal{E}(A)|$. Clearly also $(\omega_c \circ \omega_r)^{-1} = \omega_r^{-1} \circ \omega_c^{-1}$ is a cycle of the same order. The same holds if we consider the conjugate $\omega_r \circ (\omega_r^{-1} \circ \omega_c^{-1}) \circ \omega_r^{-1} = \omega_c^{-1} \circ \omega_r^{-1}$, hence $(-\mathcal{R}, -\mathcal{C})$ is a solution, too. □

Lemma 2.15. *Let A be a cyclically k-diagonal array of size $n \geq k$ and let $\mathcal{R} = (1, 1, \ldots, 1)$. If $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$, then also $(\mathcal{C}, \mathcal{R})$ is a solution of $P(A)$.*

Proof. We can assume, without loss of generality, that $(1, 1)$ is a filled cell of A. If $(\mathcal{R}, \mathcal{C})$ is a solution of $P(A)$, then the induced cycle $\omega_c \circ \omega_r$ has order $|\mathcal{E}(A)|$. Now, since if we commute ω_r and ω_c we still obtain a cycle of order $|\mathcal{E}(A)|$, then $(\mathcal{C}, \mathcal{R})$ is a solution of $P(A^t)$, where by A^t we denote the transposed of A. Note that, in general, A and A^t do not have the same skeleton. Before concluding the proof, we present an example in order to illustrate this fact. Here A is a cyclically 4-diagonal array of size 6 (we put a "•" in the filled cells), $\mathcal{R} = (1, 1, 1, 1, 1, 1)$, as in the hypothesis, and $\mathcal{C} = (1, -1, -1, 1, -1, 1)$.

	$\downarrow$	$\uparrow$	$\uparrow$	$\downarrow$	$\uparrow$	$\downarrow$
$\rightarrow$	$\bullet$			$\bullet$	$\bullet$	$\bullet$
$\rightarrow$	$\bullet$	$\bullet$			$\bullet$	$\bullet$
$\rightarrow$	$\bullet$	$\bullet$	$\bullet$			$\bullet$
$\rightarrow$	$\bullet$	$\bullet$	$\bullet$	$\bullet$		
$\rightarrow$		$\bullet$	$\bullet$	$\bullet$	$\bullet$	
$\rightarrow$			$\bullet$	$\bullet$	$\bullet$	$\bullet$

	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
$\rightarrow$	$\bullet$	$\bullet$	$\bullet$	$\bullet$		
$\leftarrow$		$\bullet$	$\bullet$	$\bullet$	$\bullet$	
$\leftarrow$			$\bullet$	$\bullet$	$\bullet$	$\bullet$
$\rightarrow$	$\bullet$			$\bullet$	$\bullet$	$\bullet$
$\leftarrow$	$\bullet$	$\bullet$			$\bullet$	$\bullet$
$\rightarrow$	$\bullet$	$\bullet$	$\bullet$			$\bullet$

	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
$\rightarrow$	$\bullet$			$\bullet$	$\bullet$	$\bullet$
$\leftarrow$	$\bullet$	$\bullet$			$\bullet$	$\bullet$
$\leftarrow$	$\bullet$	$\bullet$	$\bullet$			$\bullet$
$\rightarrow$	$\bullet$	$\bullet$	$\bullet$	$\bullet$		
$\leftarrow$		$\bullet$	$\bullet$	$\bullet$	$\bullet$	
$\rightarrow$			$\bullet$	$\bullet$	$\bullet$	$\bullet$

Figure 1: Arrays A, A^t and B.

Note that, instead of A^t, we can consider the array B on the right obtained from A^t by a translation on the rows of length $k-1$. We point out that B has the same skeleton of A. We remark that applying $(\mathcal{C},\mathcal{R})$ to A^t is equivalent to apply $(\mathcal{C},\overline{\mathcal{R}})$ to B, where if $\mathcal{R}=(r_1,r_2,\dots,r_n)$, then $\overline{\mathcal{R}}=(r_k,\dots,r_n,r_1,\dots,r_{k-1})$. Since $\mathcal{R}=(1,1,\dots,1)$ then also $\overline{\mathcal{R}}=(1,1,\dots,1)$. Hence $(\mathcal{C},\mathcal{R})$ is a solution of $P(B)$, but $skel(B)=skel(A)$, so $(\mathcal{C},\mathcal{R})$ is a solution of $P(A)$ too. □

Proposition 2.16. *Let A and B be two distinct (globally simple) $\mathrm{H}_t(m,n;h,k)$s such that $\mathcal{E}(A)=\mathcal{E}(B)$. Assume that both A and B admit compatible orderings and denote them, respectively, by (ω_r^A,ω_c^A) and by (ω_r^B,ω_c^B). Then (ω_r^A,ω_c^A) and (ω_r^B,ω_c^B) determine the same (circular) k-gonal face-2-colourable embedding of $K_{\frac{2nk+t}{t}\times t}$ if and only if $\omega_r^A=\omega_r^B$ and $\omega_c^A=\omega_c^B$.*

Proof. Suppose, by contradiction, that there exists $a\in\mathcal{E}(A)=\mathcal{E}(B)$ such that $\omega_r^A(a)\neq\omega_r^B(a)$ or $\omega_c^A(a)\neq\omega_c^B(a)$. In the following we assume, without loss of generality, that the previous condition holds for the rows. Hence, recalling Equations (2.1) and (2.2), from $\omega_r^A(a)\neq\omega_r^B(a)$, it follows that the maps ρ^A and ρ^B are different. Therefore (ω_r^A,ω_c^A) and (ω_r^B,ω_c^B) determine different k-gonal face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$.

Conversely, if we have that $\omega_r^A=\omega_r^B$ and $\omega_c^A=\omega_c^B$ the maps ρ_0^A and ρ_0^B coincide and hence also $\rho^A=\rho^B$. In this case the compatible orderings of A and of B determine the same k-gonal face-2-colourable embedding of $K_{\frac{2nk+t}{t}\times t}$. □

Remark 2.17. Let A be an $\mathrm{H}_t(m,n;h,k)$. It is not hard to see that distinct solutions of $P(A)$ induce distinct orderings ω_r and ω_c of the rows and columns of A, respectively. Also, distinct permutations determine distinct face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$. These facts, in general, do not hold for ${}^\lambda\mathrm{H}_t(m,n;h,k)$ with $\lambda>1$. In the following example we show how two distinct solutions of $P(A)$, where A is a λ-fold Heffter array with $\lambda>1$, induce the same permutations ω_r and ω_c. Moreover, when $\lambda>1$, the definition of the Archdeacon embedding is more complicated since the complete multipartite multigraph ${}^\lambda K_{(\frac{2nk}{\lambda t}+1)\times t}$ has repeated edges, see [10]. In this case, one could show that distinct solutions of $P(A)$ can induce the same face-2-colourable embedding.

Example 2.18. Let A be the ${}^2\mathrm{H}(2,5;5,2)$ of Example 2.4. Set $\mathcal{R}=(1,1)$, $\mathcal{C}_1=(1,1,1,1,1)$, $\mathcal{C}_2=(1,-1,-1,1,-1)$. It is easy to see that $(\mathcal{R},\mathcal{C}_1)$ and $(\mathcal{R},\mathcal{C}_2)$ are two distinct solutions of $P(A)$. Anyway they induce the same permutations:

$$\omega_r=(1,-2,3,4,5)(-1,2,-3,-4,-5),$$
$$\omega_c=(1,-1)(-2,2)(3,-3)(4,-4)(5,-5).$$

Corollary 2.19. *Let A and B be two k-diagonal (globally simple) $\mathrm{H}_t(n;k)$s such that:*

(1) *there exists a non-empty diagonal $D_{\bar{i}}$ where A and B coincide;*

(2) *$\mathcal{E}(A) = \mathcal{E}(B)$ and $skel(A) = skel(B)$;*

(3) *both $P(A)$ and $P(B)$ admit a solution denoted, respectively, by $(\mathcal{R}_A, \mathcal{C}_A)$ and by $(\mathcal{R}_B, \mathcal{C}_B)$.*

Then $(\mathcal{R}_A, \mathcal{C}_A)$ and $(\mathcal{R}_B, \mathcal{C}_B)$ determine the same (circular) k-gonal face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$ if and only if $A = B$ and $(\mathcal{R}_A, \mathcal{C}_A) = (\mathcal{R}_B, \mathcal{C}_B)$.

Proof. Clearly, if $A = B$ and $(\mathcal{R}_A, \mathcal{C}_A) = (\mathcal{R}_B, \mathcal{C}_B)$, we obtain the same face-2-colourable embedding.

Now, assume that $(\mathcal{R}_A, \mathcal{C}_A)$ and $(\mathcal{R}_B, \mathcal{C}_B)$ determine the same k-gonal face-2-colourable embedding of $K_{\frac{2nk+t}{t}\times t}$. We have to prove that $A = B$ and $(\mathcal{R}_A, \mathcal{C}_A) = (\mathcal{R}_B, \mathcal{C}_B)$. At this purpose we will first suppose, by contradiction, that $(\mathcal{R}_A, \mathcal{C}_A) \neq (\mathcal{R}_B, \mathcal{C}_B)$, then we will also consider the possibility that $A \neq B$. Our assumption means that either $\mathcal{R}_A \neq \mathcal{R}_B$ or $\mathcal{C}_A \neq \mathcal{C}_B$.

In the first case, there exists an index ℓ such that $(r_A)_\ell = -(r_B)_\ell$. Moreover, up to translate on the torus the cells of the Heffter arrays A and B, we can assume, without loss of generality that $\ell = \bar{i} = 1$.

Here we set by ω_r^A, ω_c^A the orderings induced by $(\mathcal{R}_A, \mathcal{C}_A)$ on the elements of $\mathcal{E}(A)$ and by ω_r^B, ω_c^B the orderings induced by $(\mathcal{R}_B, \mathcal{C}_B)$ on the elements of $\mathcal{E}(B)$. We also denote the non-empty elements of the first row of A, following the natural ordering, by $(a_{1,1}, a_{1,i_2}, \ldots, a_{1,i_k})$. Then, since $(r_A)_1 = -(r_B)_1$ and since, due to Proposition 2.16, $\omega_r^A = \omega_r^B$, we have that the non-empty elements of the first row of B are, following the natural ordering, $(a_{1,1}, a_{1,i_k}, \ldots, a_{1,i_2})$ where a_{1,i_k} is in the i_2-th column and a_{1,i_2} is in the i_k-th column. Now we consider the element a_{i_2,i_2} in position (i_2, i_2) of A. Since, in the diagonal D_1, the arrays A and B coincide, we have that a_{i_2,i_2} is also the element in position (i_2, i_2) of B. Here we note that, in the array A the elements a_{i_2,i_2} and a_{1,i_2} belong both to the i_2-th column. On the other hand, in the array B they belong to different columns: a_{i_2,i_2} is in the i_2-th and a_{1,i_2} is in the i_k-th. But this implies that the orbits of a_{i_2,i_2} under the action of ω_c^A and ω_c^B are different and hence, due to Proposition 2.16, we would obtain the contradiction that $(\mathcal{R}_A, \mathcal{C}_A)$ and $(\mathcal{R}_B, \mathcal{C}_B)$ determine different face-2-colourable embeddings.

We obtain a similar contradiction also in the case $\mathcal{C}_A \neq \mathcal{C}_B$ and hence we have proved that $(\mathcal{R}_A, \mathcal{C}_A) = (\mathcal{R}_B, \mathcal{C}_B)$.

It is left to prove that $A = B$. At this purpose we suppose, by contradiction, that there is a position (ℓ_1, ℓ_2) where A and B are different and we consider the element a of $D_{\bar{i}}$ that belongs to the ℓ_1-th row. Due to Proposition 2.16 we have that $\omega_r^A(a) = \omega_r^B(a)$ and, inductively, that $(\omega_r^A)^j(a) = (\omega_r^B)^j(a)$ for any $j \in [1, k]$. Since $skel(A) = skel(B)$ and $\mathcal{R}_A = \mathcal{R}_B$, it follows that the ℓ_1-th row of A and that of B are equal. But this would imply that also the elements in position (ℓ_1, ℓ_2) of A and B coincide that contradicts our hypothesis. It follows that $A = B$. □

3 On the maximum number of isomorphic embeddings

Given an embedding Π, we will denote by $\mathrm{Aut}(\Pi)$ the group of all automorphisms of Π and by $\mathrm{Aut}^+(\Pi)$ the group of the orientation preserving automorphisms. Similarly, we will denote by $\mathrm{Aut}_0(\Pi)$ the subgroup of $\mathrm{Aut}(\Pi)$ of the automorphisms that fix 0 and by $\mathrm{Aut}_0^+(\Pi)$ the group of the orientation preserving automorphisms that fix 0. We remark that, since an orientable surface admits exactly two orientations, $\mathrm{Aut}^+(\Pi)$ (resp. $\mathrm{Aut}_0^+(\Pi)$) is a normal subgroup of $\mathrm{Aut}(\Pi)$ (resp. $\mathrm{Aut}_0(\Pi)$) whose index is either 1 or 2. In the following, when we consider a $\mathbb{Z}_v$-regular embedding Π of Γ, we identify the vertex set of Γ with $\mathbb{Z}_v$ and we assume that the translation action is regular. We denote by τ_g the translation by g, i.e. $\tau_g \colon V(\Gamma) = \mathbb{Z}_v \to V(\Gamma) = \mathbb{Z}_v$ is the map such that $\tau_g(x) = x + g$. Applying this convention, we have that $\tau_g \in \mathrm{Aut}(\Pi)$ for any $g \in \mathbb{Z}_v$. Moreover, in the case of the Archdeacon embedding, recalling Equation (2.2), the translations also belong to $\mathrm{Aut}^+(\Pi)$.

Remark 3.1. Let Π and Π' be two isomorphic $\mathbb{Z}_v$-regular embeddings of $K_{m\times t}$, where $v = mt$. Given an embedding isomorphism $\sigma \colon \Pi \to \Pi'$ and $g \in \mathbb{Z}_v$, we define

$$\phi_{\sigma,g} := \sigma \circ \tau_g^{-1} \circ \sigma^{-1} \circ \tau_{\sigma(g)}.$$

Moreover, if $\sigma(0) = 0$ then, since $\phi_{\sigma,g}(0) = 0$, we obtain that:

$$\phi_{\sigma,g} \in \mathrm{Aut}_0(\Pi').$$

Proposition 3.2. *Let* Π_0, Π_1 *and* Π_2 *be* $\mathbb{Z}_v$*-regular embeddings of* $K_{m\times t}$*, where* $v = mt$*. Let us suppose there exist two embedding isomorphisms* $\sigma_1 \colon \Pi_1 \to \Pi_0$ *and* $\sigma_2 \colon \Pi_2 \to \Pi_0$ *such that, considering* σ_1 *and* σ_2 *as maps from* $\mathbb{Z}_v$ *to* $\mathbb{Z}_v$*, the following properties hold:*

(1) $\sigma_1(0) = \sigma_2(0) = 0$*;*

(2) $\sigma_1(1) = \sigma_2(1)$*;*

(3) $\phi_{\sigma_1,1} = \phi_{\sigma_2,1}$.

Then the identity map from Π_1 *to* Π_2 *is an isomorphism.*

Proof. We note that, due to hypothesis (3), we have that:

$$\phi_{\sigma_1,1} = \sigma_1 \circ \tau_1^{-1} \circ \sigma_1^{-1} \circ \tau_{\sigma_1(1)} = \sigma_2 \circ \tau_1^{-1} \circ \sigma_2^{-1} \circ \tau_{\sigma_2(1)} = \phi_{\sigma_2,1}.$$

Since, because of hypothesis (2), $\sigma_1(1) = \sigma_2(1)$ the maps $\tau_{\sigma_1(1)}$ and $\tau_{\sigma_2(1)}$ coincide. Reducing these maps from the composition, we obtain that:

$$\sigma_1 \circ \tau_1^{-1} \circ \sigma_1^{-1} = \sigma_2 \circ \tau_1^{-1} \circ \sigma_2^{-1}. \tag{3.1}$$

Note that Equation (3.1) can be rewritten as:

$$(\sigma_2^{-1} \circ \sigma_1) \circ \tau_1^{-1} = \tau_1^{-1} \circ (\sigma_2^{-1} \circ \sigma_1),$$

hence we have that:

$$\tau_1 \circ (\sigma_2^{-1} \circ \sigma_1) = (\sigma_2^{-1} \circ \sigma_1) \circ \tau_1. \tag{3.2}$$

Setting $\sigma_{1,2} := \sigma_2^{-1} \circ \sigma_1$, by definition of τ_1, it results

$$\tau_1 \circ \sigma_{1,2}(x) = \sigma_{1,2}(x) + 1,$$

and

$$\sigma_{1,2} \circ \tau_1(x) = \sigma_{1,2}(x + 1).$$

Therefore, Equation (3.2) can be written as:

$$\sigma_{1,2}(x+1) = \sigma_{1,2}(x) + 1.$$

Since, for hypothesis (1), $\sigma_1(0) = \sigma_2(0) = 0$ we can prove, inductively, that $\sigma_{1,2}(x) = x$ that is $\sigma_{1,2} = id$. It follows that the identity map from Π_1 to Π_2 is an isomorphism of embeddings. □

Proposition 3.3. *Let* Π *be an embedding of* $K_{m\times t}$ *where* $m \geq 2$. *Then we have that:*

$$|\operatorname{Aut}_0(\Pi)| \leq 2|\operatorname{Aut}_0^+(\Pi)| \leq 2|N(K_{m\times t}, 0)| = 2(m-1)t.$$

Proof. Since $\operatorname{Aut}_0^+(\Pi)$ is a normal subgroup of $\operatorname{Aut}_0(\Pi)$ whose index is at most two, it suffices to prove that $|\operatorname{Aut}_0^+(\Pi)| \leq |N(K_{m\times t}, 0)|$. Because of the definition, $\sigma \in \operatorname{Aut}_0^+(\Pi)$ implies that, for any $x \notin N(K_{m\times t}, 0)$:

$$\sigma \circ \rho(0, x) = \rho \circ \sigma(0, x).$$

Recalling that $\rho(0, x) = (0, \rho_0(x))$ for a suitable map $\rho_0 \colon N(K_{m\times t}, 0) \to N(K_{m\times t}, 0)$, we have that:

$$\sigma \circ \rho(0, x) = (0, \sigma \circ \rho_0(x)) = (0, \rho_0 \circ \sigma(x)) = \rho \circ \sigma(0, x). \tag{3.3}$$

Since $|N(K_{m\times t}, 0)| = (m-1)t$, we can write ρ_0 as the cycle $(x_1 = 1, x_2, x_3, \ldots, x_{(m-1)t})$. Then, setting $\sigma(x_1) = x_i$, Equation (3.3) implies that:

$$(0, \sigma(x_2)) = (0, \rho_0 \circ \sigma(x_1)) = \rho \circ \sigma(0, x_1) = (0, x_{i+1}).$$

Therefore, we can prove, inductively, that:

$$\sigma(x_j) = x_{j+i-1}$$

where the indices are considered modulo $(m-1)t$. This means that $\sigma|_{N(K_{m\times t},0)} = \rho_0^{i-1}$ and that σ is fixed in $N(K_{m\times t}, 0)$ when the image of one element is given. In particular since ρ_0 has order $(m-1)t$, there are at most $|N(K_{m\times t}, 0)|$ possibilities for the map $\sigma|_{N(K_{m\times t},0)}$.

Now we need to prove that, if two automorphisms σ_1 and σ_2 of $\operatorname{Aut}_0(\Pi)$ coincide in $N(K_{m\times t}, 0)$, they coincide everywhere. Set $\sigma_{1,2} = \sigma_2^{-1} \circ \sigma_1$, this is equivalently to prove that $\sigma_{1,2}$ is the identity. Given $x \in N(K_{m\times t}, 0)$ we have that $\sigma_{1,2}(x) = x$ and hence $\sigma_{1,2}$ belongs to the subgroup $\operatorname{Aut}_x^+(\Pi)$ of $\operatorname{Aut}^+(\Pi)$ of the elements that fix x. Proceeding as before we prove that $\sigma_{1,2}|_{N(K_{m\times t},x)}$ is fixed when the image of one element is given. But now we note that $0 \in N(K_{m\times t}, x)$ and we have that $\sigma_{1,2}(0) = 0$. It follows that

$$\sigma_{1,2}|_{N(K_{m\times t},x)} = id.$$

Since σ_1 and σ_2 coincide in $N(K_{m\times t}, 0)$, we also have that

$$\sigma_{1,2}|_{N(K_{m\times t},0)} = id.$$

Now the thesis follows because, for $m \geq 2$,

$$V(K_{m\times t}) = N(K_{m\times t}, 0) \cup N(K_{m\times t}, x).$$

□

Proposition 3.4. *Let $\mathcal{F} = \{\Pi_\alpha : \alpha \in \mathcal{A}\}$ be a family of $\mathbb{Z}_v$-regular distinct embeddings of $K_{m\times t}$ where $v = mt$ and $m \geq 2$. Then, if Π_α is isomorphic to Π_0 for any $\alpha \in \mathcal{A}$, we have that:*

$$|\mathcal{F}| \leq 2|\operatorname{Aut}_0(\Pi_0)| \cdot |N(K_{m\times t}, 0)| \leq 4|N(K_{m\times t}, 0)|^2 = 4((m-1)t)^2.$$

Moreover, if for any $\alpha \in \mathcal{A}$ and any $g \in \mathbb{Z}_v$, the translation τ_g belongs to $\operatorname{Aut}^+(\Pi_\alpha)$, then:

$$|\mathcal{F}| \leq 2|\operatorname{Aut}_0^+(\Pi_0)| \cdot |N(K_{m\times t}, 0)| \leq 2|N(K_{m\times t}, 0)|^2 = 2((m-1)t)^2.$$

Proof. We can assume $\Pi_0 \in \mathcal{F}$ and let us denote by σ_α an isomorphism between Π_α and Π_0 that fixes 0. Note that this isomorphism exists since $\mathcal{F}$ is a family of $\mathbb{Z}_v$-regular embeddings. Let us assume, by contradiction that

$$|\mathcal{F}| > 2|\operatorname{Aut}_0(\Pi_0)| \cdot |N(K_{m\times t}, 0)|.$$

We note that, for any $\alpha \in \mathcal{A}$, $\phi_{\sigma_\alpha,1} \in \operatorname{Aut}_0(\Pi_0)$. Since σ_α is an isomorphism that fixes 0, $\sigma_\alpha(1)$ belongs to $N(K_{m\times t}, 0)$ if and only if 1 belongs to $N(K_{m\times t}, 0)$. It follows that, we have at most

$$\max(|N(K_{m\times t}, 0)|, v - 1 - |N(K_{m\times t}, 0)|) = \max((m-1)t, t-1) = (m-1)t$$

possibilities for $\sigma_\alpha(1)$. Therefore, due to the pigeonhole principle, we would have that there exist Π_1, Π_2 and Π_3 in $\mathcal{F}$ such that:

(1) $\sigma_1(1) = \sigma_2(1) = \sigma_3(1)$;

(2) $\phi_{\sigma_1,1} = \phi_{\sigma_2,1} = \phi_{\sigma_3,1}$.

Hence, due to Proposition 3.2, we would have that the identity is an isomorphism both from $\Pi_1 = (\Gamma_1, \rho_1)$ to $\Pi_2 = (\Gamma_2, \rho_2)$ and from $\Pi_1 = (\Gamma_1, \rho_1)$ to $\Pi_3 = (\Gamma_3, \rho_3)$. It follows from Definition 1.3 that $\Gamma_1 = \Gamma_2 = \Gamma_3$ and $\rho_2, \rho_3 \in \{\rho_1, \rho_1^{-1}\}$. But this means that either $\Pi_1 = \Pi_2$ or $\Pi_1 = \Pi_3$ or $\Pi_2 = \Pi_3$. In each of these cases we would obtain that the elements of $\mathcal{F}$ are not all distinct that contradicts the hypotheses.

We remark that, in case the translations are all elements of $\operatorname{Aut}^+(\Pi_\alpha)$ (for every $\alpha \in \mathcal{A}$), $\phi_{\sigma_\alpha,1}$ would be an element of $\operatorname{Aut}_0^+(\Pi_0)$ and hence we can substitute $\operatorname{Aut}_0(\Pi_0)$ with $\operatorname{Aut}_0^+(\Pi_0)$ in the previous argument. This leads us to obtain:

$$|\mathcal{F}| \leq 2|\operatorname{Aut}_0^+(\Pi_0)| \cdot |N(K_{m\times t}, 0)|.$$

□

Remark 3.5. Clearly if $t = 1$ the complete multipartite graph $K_{m\times t}$ is nothing but the complete graph of order m. Hence the results of Propositions 3.3 and 3.4 hold also for the complete graph.

4 Embeddings from Cavenagh, Donovan and Yazıcı's arrays

We consider now the family of embeddings of K_v obtained by Cavenagh, Donovan, and Yazıcı in [6]. In their constructions, all the face boundaries are cycles of length k.

Set the binary entropy function by $H(p) := -p\log_2 p-(1-p)\log_2(1-p)$ and denoted by $\mathcal{H}(m)$ the cardinality of the derangements on $[0, m-1]$, we will use the following, well known, approximations:

$$m! \approx \sqrt{2m\pi}\left(\frac{m}{e}\right)^m, \tag{4.1}$$

$$\binom{m}{pm} \approx \frac{1}{\sqrt{2m\pi(1-p)p}}2^{mH(p)}, \tag{4.2}$$

$$\mathcal{H}(m) \approx m!/e, \tag{4.3}$$

where the symbol $\approx$ means that the two quantities are asymptotic: their ratio tends to 1 as m tends to infinity. We will also use the simbol $\gtrsim$ in case the $\liminf$ of the ratio between two quantities, as m tends to infinity, is greater than or equal to 1.

Theorem 4.1 (Cavenagh, Donovan and Yazıcı [6])**.** *Let $v = 2nk+1$, $k = 4t+3$ and let $n \equiv 1 \pmod 4$ be either a prime or $n \geq (7k+1)/3$. Moreover, if $n \equiv 0 \pmod 3$, we also assume that $k \equiv 7 \pmod{12}$. Then, the number of distinct circular k-gonal face-2-colourable embeddings of K_v is, at least, of:*

$$(n-2)[\mathcal{H}(t-2)]^2 \approx (n-2)[(t-2)!/e]^2.$$

Also, for all such embeddings and all $g \in \mathbb{Z}_v$, τ_g is an orientation preserving automorphism.

Using Proposition 3.4 and Theorem 4.1, we can prove the following result.

Theorem 4.2. *Let $v = 2nk+1$, $k = 4t+3$ and let $n \equiv 1 \pmod 4$ be either a prime or $n \geq (7k+1)/3$. Moreover, if $n \equiv 0 \pmod 3$, we also assume that $k \equiv 7 \pmod{12}$. Then, the number of non-isomorphic circular k-gonal face-2-colourable embeddings of K_v is, at least, of:*

$$\frac{(n-2)[\mathcal{H}(t-2)]^2}{2(2nk)^2} \approx \frac{\pi(t-2)^{2t-5}}{64e^{2t-2}n} \approx k^{k/2+o(k)}/v.$$

Proof. Let us consider, for given k and v, the distinct circular k-gonal face-2-colourable embeddings of K_v provided in [6]. Let us partition these embeddings into families of isomorphic ones. The thesis easily follows because, due to Proposition 3.4, each of these families has size at most $2(v-1)^2 = 8(nk)^2$. Then the lower bound on the number of non-isomorphic circular k-gonal face-2-colourable embeddings of K_v can be approximated using the Stirling formula for the factorial, that is Equation (4.1), and the approximation (4.3). □

Now we will show that, studying carefully the Crazy Knight's Tour Problem for the Heffter arrays found by Cavenagh, Donovan and Yazıcı it is possible to get many other circular k-gonal face-2-colourable embeddings of K_v.

We consider here a k-diagonal array A of size $n > k$ and vectors $\mathcal{R} = (1, \dots, 1)$ and $\mathcal{C} \in \{-1, 1\}^n$, whose -1 are in positions $E = (e_1, \dots, e_r)$ where $e_1 < e_2 < \dots < e_r$. We state a characterization, obtained with the same proof of Lemma 4.19 of [7], of the solutions of $P(A)$ that have a trivial vector $\mathcal{R}$, i.e. $\mathcal{R} = (1, \dots, 1)$.

Lemma 4.3. *Let $k \geq 3$ be an odd integer and let A be a k-diagonal array of size $n > k$, widths $s_1, s_2, \ldots, s_i$ and with non-empty diagonal D_1. Then the vectors $\mathcal{R} = (1, \ldots, 1)$ and $\mathcal{C} \in \{-1, 1\}^n$, where the positions of each -1 in $\mathcal{C}$ are described by E, are a solution of $P(A)$ if and only if:*

(1) *for any $j \in [1, n]$, the list E covers all the congruence classes modulo d_j, where $d_j = \gcd(n, s_j)$;*

(2) *the list $L_{\mathcal{R},\mathcal{C}}(1, 1)$ covers all the positions of $\{(e, e)|e \in E\}$.*

Proposition 4.4. *Let k be an odd integer, $n > 8k$ be a prime, and let A be a k-diagonal Heffter array $\mathrm{H}(n; k)$ whose filled diagonals are $D_1, D_2, \ldots, D_{k-3}, D_{k-1}, D_k, D_{k+1}$. Then, the number of distinct solutions of $P(A)$ is at least of:*

$$2\binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} \gtrsim \frac{\sqrt{k}}{\sqrt{3\pi n}} 2^{\frac{n}{2k} \cdot H(1/4) + 3}.$$

Proof. Let us consider a subset $E = (e_1, \ldots, e_r)$ of $[1, n]$ where $e_1 < e_2 < \cdots < e_r$ that satisfies the following properties:

(1) the elements $e_1, \ldots, e_r$ of E are integers equivalent to 1 modulo $2k$;

(2) $r = |E|$ is coprime with $k - 2$.

A set E with such properties can be constructed as follows. Let r be a prime in the range $[\frac{n}{8k}, \frac{n}{4k}]$ that exists because of Bertrand's postulate. Then we choose r elements $e_1, \ldots, e_r$ among the $\lceil n/2k \rceil$ integers equivalent to 1 modulo $2k$ contained in $[1, n]$. The number of such choices is at least of

$$\binom{\lceil n/2k \rceil}{r} \geq \binom{\lceil n/2k \rceil}{\lceil n/8k \rceil}.$$

Note that, due to the approximation for the binomial coefficients, see Equation (4.2), this number can be approximated to

$$\binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} \gtrsim \frac{\sqrt{k}}{\sqrt{3\pi n}} 2^{\frac{n}{2k} \cdot H(1/4) + 2}.$$

Hence, in order to obtain the thesis, it suffices to prove that, set $\mathcal{R} = (1, 1, \ldots, 1)$ and $\mathcal{C}_E \in \{-1, 1\}^n$ whose -1 are in positions $E = (e_1, \ldots, e_r)$, $(\mathcal{R}, \mathcal{C}_E)$ is a solution for $P(A)$. Indeed, according to Lemma 2.14, the number of distinct solutions of $P(A)$ would be, at least, of

$$2\binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} \gtrsim \frac{\sqrt{k}}{\sqrt{3\pi n}} 2^{\frac{n}{2k} \cdot H(1/4) + 3}.$$

Since n is a prime, condition (1) of Lemma 4.3 is satisfied. We need to check that also condition (2) of the same lemma holds. At this purpose, we consider an element $(e, e) \in D_1$ with $e \in E$, then there exists a minimum $m \geq 1$ such that $S^m_{\mathcal{R},\mathcal{C}}((e, e)) = (e', e')$ for some $e' \in E$. We define the permutation $\omega_\mathcal{C}$ on E as $\omega_\mathcal{C}(e) = e'$. We need to prove that $\omega_\mathcal{C}$ is a cycle of order r. Given $e \in E$, the second cell of the form (e', e') with $e' \in E$ we meet in the list $L_{\mathcal{R},\mathcal{C}}(e, e)$ is reached after the following moves:

(1) from (e, e) we move backward into the diagonal D_1 with steps of length k until we reach a cell of the form $(e_i + k, e_i + k)$ with $e_i \in E$;

(2) from $S_{\mathcal{R},\mathcal{C}}(e_i + k, e_i + k) = (e_i + (k-1), e_i)$ we move forward into the diagonal D_k with steps of length 1 until we reach the cell $(e_{i+1} - 1 + (k-1), e_{i+1} - 1)$, where the indices are considered modulo r (as for the rest of this proof);

(3) from $S_{\mathcal{R},\mathcal{C}}(e_{i+1} - 1 + (k-1), e_{i+1} - 1) = (e_{i+1} + (k-4), e_{i+1})$ we move forward into the diagonal D_{k-3} with steps of length 1 until we reach the cell $(e_{i+2} - 1 + (k-4), e_{i+2} - 1)$; we reiterate this procedure into the diagonals $D_{k-5}, D_{k-7}, \ldots, D_4$;

(4) since k is odd, we arrive to the cell $(e_{i+(k-3)/2} + 1, e_{i+(k-3)/2}) \in D_2$ from which we move forward with steps of length 1 until we reach the cell $(e_{i+(k-1)/2}, e_{i+(k-1)/2} - 1)$;

(5) from $S_{\mathcal{R},\mathcal{C}}(e_{i+(k-1)/2}, e_{i+(k-1)/2} - 1) = (e_{i+(k-1)/2} + k, e_{i+(k-1)/2})$ we move forward into the diagonal D_{k+1} with steps of length 1 until we reach the cell $(e_{i+(k+1)/2} - 1 + k, e_{i+(k+1)/2} - 1)$; we reiterate this procedure into the diagonals D_{k-1} (here with steps of length 2),$D_{k-4}, \ldots, D_3$;

(6) since k is odd, we arrive to the cell $(e_{i+(k-1)}, e_{i+(k-1)}) \in D_1$ that is the second one of the form $(e', e') \in D_1$ with $e' \in E$ we meet in the list $L_{\mathcal{R},\mathcal{C}}(e, e)$.

We denote by γ the cyclic permutation of the elements of E defined by $(e_1, \ldots, e_r)$. We note that since the distances between elements of E are multiples of k, in the first step of the above procedure we apply the permutation γ^{-1}. Then, from the previous discussion, it follows that $\omega_{\mathcal{C}} = \gamma^{k-1} \circ \gamma^{-1} = \gamma^{k-2}$. Since r is coprime with $k-2$ and γ is a cycle of order r, then $\omega_{\mathcal{C}}$ is also a cycle of order r and hence condition (2) of Lemma 4.3 is satisfied. □

Remark 4.5. We note that, if n is sufficiently large, in the proof of Proposition 4.4, the choice of r could also be done in the range $[\lambda \frac{n}{k}, \frac{n}{4k}]$ where λ is smaller than $1/4$. In fact, if $|\frac{n}{4k} - \lambda \frac{n}{k}| \geq k - 2$, we can find r coprime with $k-2$ also in this range. It follows that, given $\lambda < 1/4$, we can replace the exponent $\frac{n}{2k} \cdot H(1/4)$ of the previous proposition with $\frac{n}{2k} \cdot H(2\lambda)$. However, due to the complications in the notations, we believe it is better to write the statement in the "clearest" case.

Theorem 4.6. *Let $v = 2nk + 1$, $k = 4t + 3$ and let $n \equiv 1 \pmod 4$ be a prime greater than $8k$. Then the number of distinct circular k-gonal face-2-colourable embeddings of K_v is, at least, of:*

$$2(n-2)[\mathcal{H}(t-2)]^2 \binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} \gtrsim \frac{[(t-2)!]^2 \sqrt{(4t+3)n}}{e^2 \sqrt{3\pi}} 2^{\frac{n}{2(4t+3)} \cdot H(1/4) + 3}.$$

Also, for all such embeddings and all $g \in \mathbb{Z}_v$, τ_g is an orientation preserving automorphism.

Proof. We note that, if n is a prime, each array of the family $\mathcal{F}_{n,k} := \{A_i : i \in \mathcal{A}_{n,k}\}$ of globally simple $H(n;k)$s constructed in [6] satisfies (setting $\alpha = 2p + 2$) the hypotheses of Proposition 4.4. Therefore, for each array A_i of $\mathcal{F}_{n,k}$ the number of solutions of $P(A_i)$ is at least of:

$$2 \binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} \gtrsim \frac{\sqrt{k}}{\sqrt{3\pi n}} 2^{\frac{n}{2k} \cdot H(1/4) + 3}.$$

We also recall that, due to Theorem 4.1, the number of such arrays is at least of:

$$(n-2)[\mathcal{H}(t-2)]^2 \approx (n-2)[(t-2)!/e]^2.$$

Now we note that, given n and k, these arrays have all the same entries and skeleton, and coincide in at least 5 diagonals. Therefore, because of Corollary 2.19, however we take $A_i \in \mathcal{F}_i$ and a solution of $P(A_i)$, we determine a different embedding.

It follows that the number of distinct circular k-gonal face-2-colourable embeddings of K_v is, at least, of:

$$2(n-2)[\mathcal{H}(t-2)]^2 \binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} \gtrsim \frac{[(t-2)!]^2\sqrt{kn}}{e^2\sqrt{3\pi}} 2^{\frac{n}{2k}\cdot H(1/4)+3}.$$

□

By Proposition 3.4 and Theorem 4.6, it follows that:

Theorem 4.7. *Let $v = 2nk+1$, $k = 4t+3$ and let $n \equiv 1 \pmod 4$ be a prime greater than $8k$. Then the number of non-isomorphic circular k-gonal face-2-colourable embeddings of K_v is, at least, of:*

$$\begin{aligned}\frac{(n-2)}{(2nk)^2}[\mathcal{H}(t-2)]^2 \binom{\lceil n/2k \rceil}{\lceil n/8k \rceil} &\approx \frac{[(t-2)!]^2}{e^2\sqrt{3\pi(n(4t+3))^3}} 2^{\frac{n}{2(4t+3)}\cdot H(1/4)} \\ &\approx k^{\frac{k}{2}+o(k)} \cdot 2^{v\cdot \frac{H(1/4)}{(2k)^2}+o(v)}.\end{aligned}$$

Proposition 4.8. *Let k be an odd integer, $s_1 \geq 1$, and let A be a k-diagonal Heffter array $\mathrm{H}(n;k)$ whose filled diagonals are $D_1, D_2, \ldots, D_i, D_{i+s_1}, D_{i+s_1+2}, D_{i+s_1+3}, \ldots, D_{k+s_1}$. Assuming that $\gcd(n,2) = \gcd(n,s_1) = \gcd(n,k+s_1-1) = 1$, the number of distinct solutions of $P(A)$ is at least of $2\binom{n}{2}$.*

Proof. Let us consider a subset $E = (e_1, e_2)$ where $e_1 < e_2$ of $[1,n]$. Hence in order to obtain the thesis, it suffices to prove that, set $\mathcal{R} = (1,1,\ldots,1)$ and $\mathcal{C}_E \in \{-1,1\}^n$ whose -1 are in positions $E = (e_1,e_2)$, $(\mathcal{R},\mathcal{C}_E)$ is a solution for $P(A)$. Indeed, due to Lemma 2.14, the number of distinct solutions of $P(A)$ would be, at least, of $2\binom{n}{2}$. Since n is coprime with 2, s_1 and $k+s_1-1$, condition (1) of Lemma 4.3 is satisfied. We need to check that also condition (2) holds. Defined $\omega_{\mathcal{C}}$ and γ as in the proof of Proposition 4.4, we obtain that, also here, $\omega_{\mathcal{C}} = \gamma^{k-2}$. Since γ is a cycle of order 2 and $k-2$ is odd, $\omega_{\mathcal{C}}$ is also a cycle of order 2. Hence condition (2) of Lemma 4.3 is satisfied. □

Theorem 4.9. *Let $v = 2nk+1$, $k = 4t+3$ and let $n \equiv 1 \pmod 4$ be such that $n \geq (7k+1)/3$. Moreover, if $n \equiv 0 \pmod 3$, we also assume that $k \equiv 7 \pmod{12}$. Then the number of distinct circular k-gonal face-2-colourable embeddings of K_v is, at least, of:*

$$2(n-2)\binom{n}{2}[\mathcal{H}(t-2)]^2 \approx \frac{n^3[(t-2)!]^2}{e^2}.$$

Also, for all such embeddings and all $g \in \mathbb{Z}_v$, τ_g is an orientation preserving automorphism.

Proof. The thesis follows from Proposition 4.8 reasoning as in the proof of Theorem 4.6.
□

From Proposition 3.4, it follows that:

Theorem 4.10. *Let* $v = 2nk + 1$, $k = 4t + 3$ *and let* $n \equiv 1 \pmod 4$ *be such that* $n \geq (7k + 1)/3$. *Moreover, if* $n \equiv 0 \pmod 3$, *we also assume that* $k \equiv 7 \pmod{12}$. *Then the number of non-isomorphic circular* k*-gonal face-2-colourable embeddings of* K_v *is, at least, of:*

$$\frac{n-2}{(2nk)^2}\binom{n}{2}[\mathcal{H}(t-2)]^2 \approx \frac{n[(t-2)!]^2}{8((4t+3)e)^2} \approx v \cdot k^{k/2+o(k)}.$$

5 Embeddings from cyclically k-diagonal Heffter arrays

We note that the bounds obtained in Theorems 4.7 and 4.10 grow more than exponentially in k but they have some restrictions on the considered values of n. Furthermore, they grow exponentially in n only when n is a prime. For this reason, in this section, we will provide lower bounds that grow exponentially in n on the number of k-gonal face-2-colourable embeddings not only of complete graphs but also of complete multipartite graphs.

First of all, we need to recall the following existence result reported in [31] (see Corollaries 3.4 and 3.6) on cyclically k-diagonal Heffter arrays.

Lemma 5.1. *Given* $n \geq k \geq 3$, *then there exists a cyclically* k*-diagonal Heffter array* $H_t(n; k)$ *in each of the following cases:*

(1) $t \in \{1, 2\}$ *and* $k \equiv 0 \pmod 4$ [2, 30];

(2) $t \in \{1, 2\}$, $k \equiv 1 \pmod 4$ *and* $n \equiv 3 \pmod 4$ [8, 13];

(3) $t \in \{1, 2\}$, $k \equiv 3 \pmod 4$ *and* $n \equiv 0, 1 \pmod 4$ [2];

(4) $t = k$, $k \equiv 1 \pmod 4$ *and* $n \equiv 3 \pmod 4$ [9];

(5) $t = k$, $k \equiv 3 \pmod 4$ *and* $n \equiv 0, 3 \pmod 4$ [9];

(6) $t \in \{n, 2n\}$, $k = 3$ *and* n *is odd* [11].

Moreover, in [8] and in [11], it is also proved the following existence result on globally simple cyclically k-diagonal Heffter arrays.

Lemma 5.2. *Given* $n \geq k \geq 3$, *then there exists a globally simple, cyclically* k*-diagonal Heffter array* $H_t(n; k)$ *in each of the following cases:*

(1) $t \in \{1, 2\}$, $k \in \{3, 5, 7, 9\}$ *and* $nk \equiv 3 \pmod 4$*;*

(2) $t = k$, $k \in \{3, 5, 7, 9\}$ *and* $n \equiv 3 \pmod 4$*;*

(3) $t \in \{n, 2n\}$, $k = 3$ *and* n *is odd.*

The goal will be now to find an exponential family of solutions of $P(A)$ where A is one of those arrays and then to proceed by using the following remark.

Remark 5.3. Let us assume we have M distinct solutions of $P(A)$ where A is a given (globally simple) cyclically k-diagonal Heffter array $\mathrm{H}_t(n; k)$ and k is an odd integer. In this case we may assume, without loss of generality, that the filled diagonals are D_1,

$D_2, \ldots, D_{(k+1)/2}$ and $D_n, D_{n-1}, \ldots, D_{n-(k-3)/2}$. Then, if we consider A^t, we have that $skel(A) = skel(A^t)$ and hence any solution of $P(A)$ is also a solution of $P(A^t)$. Moreover, A and A^t coincide on D_1 and $\mathcal{E}(A) = \mathcal{E}(A^t)$. Therefore, due to Corollary 2.19, there are at least $2M$ distinct $\mathbb{Z}_{2nk+t}$-regular (circular) k-gonal face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$. Then, because of Proposition 3.4, the number of non-isomorphic (circular) k-gonal face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$ is, at least, of $\frac{M}{(2nk)^2}$.

For a cyclically k-diagonal array A, we recall a characterization, provided in [7], of the solutions of $P(A)$ that have vector $\mathcal{R} = (1, \ldots, 1)$.

We consider here a cyclically k-diagonal array of size $n > k$ and vectors $\mathcal{R} = (1, \ldots, 1)$ and $\mathcal{C} \in \{-1, 1\}^n$, whose -1 are in positions $E = (e_1, \ldots, e_r)$ where $e_1 < e_2 < \cdots < e_r$. We note that, given $e \in E$, there exists a minimum $m \geq 1$ such that $e - m(k-1) \equiv e''$ $\pmod n$ for some $e'' \in E$. We define the permutation $\omega_{1,\mathcal{C}}$ on E as $\omega_{1,\mathcal{C}}(e) = e''$. Finally we define the permutation $\omega_{2,C}$ on $E = (e_1, \ldots, e_r)$ as $\omega_{2,C}(e_i) = e_{i+(k-1)}$ where the indices are considered modulo r. Then, in [7], it is proven that:

Lemma 5.4. *Let $k \geq 3$ be an odd integer and let A be a cyclically k-diagonal array of size $n > k$. Then the vectors $\mathcal{R} := (1, \ldots, 1)$ and $\mathcal{C} \in \{-1, 1\}^n$, whose -1 are in positions $E = (e_1, \ldots, e_r)$ where $e_1 < e_2 < \cdots < e_r$, are a solution of $P(A)$ if and only if:*

(1) *the list E covers all the congruence classes modulo d, where $d = \gcd(n, k-1)$;*

(2) *the permutation $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}}$ on E is a cycle of order $r = |E|$.*

Proposition 5.5. *Let A be a cyclically 3-diagonal Heffter array $\mathrm{H}_t(n; 3)$ where $n \geq 3$ is an odd integer. Then the number of distinct solutions of $P(A)$ is, at least, of $2^{\frac{1}{2}n+2}$.*

Proof. Let us consider a subset $E = (e_1, \ldots, e_r)$ of $[1, n]$ where the elements $e_1, \ldots, e_r$ are odd integers such that $e_1 < e_2 < \cdots < e_r$.

We note that the set O of odd elements in $[1, n]$ has cardinality $\frac{n+1}{2} > \frac{1}{2}n$. The number of subsets of O is then at least of $2^{\frac{1}{2}n}$. It follows that the number of possible choices for E is, at least, of $2^{\frac{1}{2}n}$. Hence, in order to obtain the thesis, it suffices to prove that, set $\mathcal{R} = (1, 1, \ldots, 1)$ and $\mathcal{C}_E \in \{-1, 1\}^n$ whose -1 are in positions $E = (e_1, \ldots, e_r)$, $(\mathcal{R}, \mathcal{C}_E)$ is a solution for $P(A)$. Indeed, due to Lemmas 2.14 and 2.15, the number of distinct solutions of $P(A)$ would be, at least, of $2^{\frac{1}{2}n+2}$.

Here we denote by γ the cyclic permutation of the elements of E defined by $(e_1, \ldots, e_r)$. In this case, since $k - 1 = 2$ we have that $\omega_{2,\mathcal{C}} = \gamma^2$. Similarly, since the elements of E are all odd integers, $\omega_{1,\mathcal{C}} = \gamma^{-1}$. It follows that $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}} = \gamma$. Since n is odd, we also have that $d = \gcd(n, 2) = 1$ and hence both the conditions of Lemma 5.4 are satisfied and $(\mathcal{R}, \mathcal{C}_E)$ is a solution of $P(A)$. $\square$

We can also provide a similar construction for arbitrary odd k. In this case, we still obtain an exponential lower bound to the number of solutions of $P(A)$ but, here, if we consider $k = 3$, the exponent is worse than that of Proposition 5.5.

Proposition 5.6. *Let A be a cyclically k-diagonal Heffter array $\mathrm{H}_t(n; k)$ where $n \geq 4k-3$ and k are odd integers such that $\gcd(n, k-1) = 1$. Then the number of distinct solutions of $P(A)$ is, at least, of*

$$4\binom{\lceil n/(k-1)\rceil}{\lceil n/(4k-4)\rceil} \gtrsim \sqrt{\frac{2(k-1)}{3n\pi}}\, 2^{\frac{n}{k-1}\cdot H(1/4)+3}.$$

Proof. Let us consider a subset $E = (e_1, \ldots, e_r)$ of $[1, n]$, where $e_1 < e_2 < \cdots < e_r$, that satisfies the following properties:

(1) the elements $e_1, \ldots, e_r$ of E are integers equivalent to 1 modulo $k-1$;

(2) $r = |E|$ is an integer coprime with $k-2$.

A set E with such properties can be constructed as follows. Let r be a prime in the range $[\frac{n}{4(k-1)}, \frac{n}{2(k-1)}]$ that exists because of Bertrand's postulate. Then we choose r elements $e_1, \ldots, e_r$ among the $\lceil n/(k-1)\rceil$ integers equivalent to 1 modulo $k-1$ contained in $[1, n]$. The number of such choices is at least of

$$\binom{\lceil n/(k-1)\rceil}{r} \geq \binom{\lceil n/(k-1)\rceil}{\lceil n/(4k-4)\rceil}.$$

Note that, due to the approximation for the binomial coefficients, see Equation (4.2), this number can be so approximated

$$\binom{\lceil n/(k-1)\rceil}{\lceil n/(4k-4)\rceil} \gtrsim \sqrt{\frac{8(k-1)}{3n\pi}}\,2^{\frac{n}{k-1}\cdot H(1/4)}.$$

Hence, also here, in order to obtain the thesis, it suffices to prove that, set $\mathcal{R} = (1, 1, \ldots, 1)$ and $\mathcal{C}_E \in \{-1, 1\}^n$ whose -1 are in positions $E = (e_1, \ldots, e_r)$, $(\mathcal{R}, \mathcal{C}_E)$ is a solution for $P(A)$. Indeed, due to Lemmas 2.14 and 2.15, the number of distinct solutions of $P(A)$ would be, at least, of

$$4\binom{\lceil n/(k-1)\rceil}{\lceil n/(4k-4)\rceil} \gtrsim \sqrt{\frac{2(k-1)}{3n\pi}}\,2^{\frac{n}{k-1}\cdot H(1/4)+3}.$$

Now we proceed as in the proof of Proposition 5.5. We denote by γ the cyclic permutation of the elements of E defined by $(e_1, \ldots, e_r)$. In this case we have that $\omega_{2,\mathcal{C}} = \gamma^{k-1}$. Similarly, since the elements of E are all integers equivalent to 1 modulo $k-1$, $\omega_{1,\mathcal{C}} = \gamma^{-1}$. It follows that $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}} = \gamma^{k-2}$ which is a cyclic permutation on E of order r because r is coprime with $k-2$. Since we have assumed that $d = \gcd(n, k-1) = 1$, both the conditions of Lemma 5.4 are satisfied and hence $(\mathcal{R}, \mathcal{C}_E)$ is a solution of $P(A)$. $\square$

Remark 5.7. As already noted in Remark 4.5, also here, if n is sufficiently large and given $\lambda < 1/2$, we can replace the exponent $\frac{n}{k-1} \cdot H(1/4)$ of the previous proposition with $\frac{n}{k-1} \cdot H(\lambda)$. However, also in this case, we believe it is better to write the statement in the "clearest" case.

Proposition 5.8. *Let A be a cyclically 7-diagonal Heffter array $\mathrm{H}_t(n; 7)$ where $n > 120$ is an odd integer. Then the number of distinct solutions of $P(A)$ is, at least, of*

$$4\binom{\lfloor n/6\rfloor}{\lfloor n/24\rfloor} \gtrsim \frac{1}{\sqrt{n\pi}}\,2^{\lfloor \frac{n}{6}\rfloor\cdot H(1/4)+4}.$$

Proof. We divide the proof in two cases. If $gcd(n, 6) = 1$, the thesis follows from Proposition 5.6. In fact, in this case, the number of distinct solutions of $P(A)$ is, at least, of

$$4\binom{\lceil n/6\rceil}{\lceil n/24\rceil} \geq 4\binom{\lfloor n/6\rfloor}{\lfloor n/24\rfloor}.$$

Otherwise, we have that $gcd(n, 6) = 3$. In this case we consider a subset $E = (e_1, \ldots, e_r)$ of $[1, n]$, where $e_1 < e_2 < \cdots < e_r$, that satisfies the following properties:

(1) $e_1 = 1$ and $e_2 = 2$;

(2) the elements $e_3, \dots, e_r$ of E are integers equivalent to 3 modulo 6;

(3) $r = |E|$ is equivalent to 4 modulo 5.

We note that the number of integers equivalent to 3 modulo 6 in $[1, n]$ is $\lfloor \frac{n+3}{6} \rfloor \geq \lfloor \frac{n}{6} \rfloor$. Now, we fix $r \equiv 4 \pmod 5$ in $[\frac{n}{24}, \frac{n}{12}]$. Then the number of possible choices for a set E of cardinality r among the integers equivalent to 3 modulo 6 is, at least, of

$$\binom{\lfloor n/6 \rfloor}{\lceil n/24 \rceil} \geq \binom{\lfloor n/6 \rfloor}{\lfloor n/24 \rfloor} \gtrsim \frac{1}{\sqrt{n\pi}} 2^{\lfloor \frac{n}{6} \rfloor \cdot H(1/4)+2}.$$

As usual, we denote by γ the cyclic permutation of the elements of E defined by $(e_1, \dots, e_r)$. Here we have that $\omega_{2,\mathcal{C}} = \gamma^6$ and that, for $x \notin \{e_1, e_2, e_3\}$, $\omega_{1,\mathcal{C}} = \gamma^{-1}$. It follows that, if $x \notin \{e_1, e_2, e_3\}$, $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}} = \gamma^5$, that is $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}}(e_i) = e_{i+5}$ for $i \notin \{1, 2, 3\}$ and where the indices are considered modulo r. Due to the definition, we also have that $\omega_{1,\mathcal{C}}(e_1) = e_1$, $\omega_{1,\mathcal{C}}(e_2) = e_2$ and $\omega_{1,\mathcal{C}}(e_3) = e_r$. It means that $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}}(e_1) = \gamma^6(e_1) = e_7$, $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}}(e_2) = \gamma^6(e_2) = e_8$ and $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}}(e_3) = e_6$.

Since $r \equiv 4 \pmod 5$, we have that:

$$\gamma^5 = (e_1, e_6, e_{6+5}, \dots, e_{r-3}, e_2, e_7, \dots, e_{r-2}, e_3, e_{3+5}, \dots, e_{r-1}, e_4, \dots, e_r, \\ e_5, \dots, e_{r-4}).$$

It follows that $\omega_{2,\mathcal{C}} \circ \omega_{1,\mathcal{C}}$ is the cycle of order r given by:

$$(e_1, e_7, \dots, e_{r-2}, e_3, e_6, e_{6+5}, \dots, e_{r-3}, e_2, e_8, \dots, e_{r-1}, e_4, \dots, e_r, e_5, \dots, e_{r-4}).$$

Moreover, since E covers all the congruence classes modulo 3 in $[1, n]$, both the conditions of Lemma 5.4 are satisfied and $(\mathcal{R}, \mathcal{C}_E)$ is a solution of $P(A)$. Finally, the thesis follows because, due to Lemmas 2.14 and 2.15, from each such solution $(\mathcal{R}, \mathcal{C}_E)$ we obtain four different solutions of $P(A)$. □

Theorem 5.9. *Let $n \geq 3$ and t be such that either $t \in \{1, 2\}$ and $n \equiv 1 \pmod 4$ or $t = 3$ and $n \equiv 3 \pmod 4$ or $t \in \{n, 2n\}$ and n is odd. Then, set $v = 6n + t$, the number of non-isomorphic circular 3-gonal face-2-colourable embeddings of $K_{\frac{6n+t}{t} \times t}$ is, at least, of:*

$$\frac{2^{n/2}}{9n^2} \approx \begin{cases} 2^{v/12+o(v)} & \text{if } t \in \{1, 2, 3\}; \\ 2^{v/14+o(v)} & \text{if } t = n; \\ 2^{v/16+o(v)} & \text{if } t = 2n. \end{cases}$$

Proof. For these sets of parameters n and t, Lemma 5.2 assures the existence of a cyclically k-diagonal $\mathrm{H}_t(n; 3)$, say A. Then, due to Proposition 5.5, the problem $P(A)$ admits at least $2^{n/2+2}$ solutions. The thesis follows from Remark 5.3. □

Remark 5.10. If $t = 1$, namely if we are considering the complete graph K_{6n+1}, the lower bound of Theorem 5.9 is surely worse than the ones already obtained in the literature (see [3, 15, 16, 18, 19]). On the other hand, we want to underline that our result is still exponential in v and holds also for other values of t.

Theorem 5.11. *Let $k \in \{5,7,9\}$, let $n \geq 120$ and t be such that either $t \in \{1,2\}$ and $nk \equiv 3 \pmod 4$ or $t = k$ and $n \equiv 3 \pmod 4$. Then, set $v = 2nk + t$, the number of non-isomorphic circular k-gonal face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$ is, at least, of:*

$$\frac{\binom{\lfloor n/(k-1)\rfloor}{\lfloor n/(4k-4)\rfloor}}{(nk)^2} \gtrsim \frac{\sqrt{\frac{2(k-1)}{3n\pi}}2^{\lfloor \frac{n}{k-1}\rfloor \cdot H(1/4)+1}}{(nk)^2} \approx 2^{v\cdot \frac{H(1/4)}{2k(k-1)}+o(v,k)}.$$

Proof. We proceed as in the proof of Theorem 5.9 by using Propositions 5.6 and 5.8 instead of Proposition 5.5. □

Theorem 5.12. *Let $k > 9$ be odd, let $n \geq 4k-3$ and t be such that either $t \in \{1,2\}$ and $nk \equiv 3 \pmod 4$ or $t = k$ and $n \equiv 3 \pmod 4$. Assume also that $\gcd(n, k-1) = 1$ and set $v = 2nk + t$. Then the number of non-isomorphic, non necessarily circular, k-gonal face-2-colourable embeddings of $K_{\frac{2nk+t}{t}\times t}$ is, at least, of:*

$$\frac{\binom{\lceil n/(k-1)\rceil}{\lceil n/(4k-4)\rceil}}{(nk)^2} \gtrsim \frac{\sqrt{\frac{2(k-1)}{3n\pi}}2^{\frac{n}{k-1}\cdot H(1/4)+1}}{(nk)^2} \approx 2^{v\cdot \frac{H(1/4)}{2k(k-1)}+o(v,k)}.$$

Proof. We proceed as in the proof of Theorem 5.9 by using Lemma 5.1 instead of Lemma 5.2 and Proposition 5.6 instead of Proposition 5.5. □

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Complete resolution of the circulant nut graph order–degree existence problem

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Abstract

A circulant nut graph is a non-trivial simple graph such that its adjacency matrix is a circulant matrix whose null space is spanned by a single vector without zero elements. Regarding these graphs, the order–degree existence problem can be thought of as the mathematical problem of determining all the possible pairs (n, d) for which there exists a d-regular circulant nut graph of order n. This problem was initiated by Bašić et al. and the first major results were obtained by Damnjanović and Stevanović, who proved that for each odd $t \geq 3$ such that $t \not\equiv_{10} 1$ and $t \not\equiv_{18} 15$, there exists a $4t$-regular circulant nut graph of order n for each even $n \geq 4t + 4$. Afterwards, Damnjanović improved these results by showing that there necessarily exists a $4t$-regular circulant nut graph of order n whenever t is odd, n is even, and $n \geq 4t + 4$ holds, or whenever t is even, n is such that $n \equiv_4 2$, and $n \geq 4t + 6$ holds. In this paper, we extend the aforementioned results by completely resolving the circulant nut graph order–degree existence problem. In other words, we fully determine all the possible pairs (n, d) for which there exists a d-regular circulant nut graph of order n.

Keywords: Circulant graph, nut graph, graph spectrum, graph eigenvalue, cyclotomic polynomial.

Math. Subj. Class. (2020): 05C50, 11C08, 12D05, 13P05

1 Introduction

In this paper we will consider all graphs to be undirected, finite, simple and non-null. Thus, every graph will have at least one vertex and there shall be no loops or multiple

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edges. Also, for convenience, we will take that each graph of order n has the vertex set $\{0, 1, 2, \ldots, n-1\}$.

A graph G is considered to be a circulant graph if its adjacency matrix A has the form

$$A = \begin{bmatrix} a_0 & a_1 & a_2 & \cdots & a_{n-1} \\ a_{n-1} & a_0 & a_1 & \cdots & a_{n-2} \\ a_{n-2} & a_{n-1} & a_0 & \cdots & a_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_1 & a_2 & a_3 & \ldots & a_0 \end{bmatrix}.$$

Here, we clearly have $a_0 = 0$, as well as $a_j = a_{n-j}$ for all $j = \overline{1, n-1}$. A concise way of describing a circulant graph is by taking into consideration the set of all the values $1 \le j \le \frac{n}{2}$ such that $a_j = a_{n-j} = 1$. We shall refer to this set as the generator set of a circulant graph and we will use $\mathrm{Circ}(n, S)$ to denote the circulant graph of order n whose generator set is S.

A nut graph is a non-trivial graph whose adjacency matrix has nullity one and is such that its non-zero null space vectors have no zero elements, as first described by Sciriha in [10]. Bearing this in mind, a circulant nut graph is simply a nut graph whose adjacency matrix additionally represents a circulant matrix. The study of regular nut graphs was initiated by Gauci et al. [7], who proved that there exists a cubic nut graph of order n if and only if $n = 12$ or $2 \mid n$, $n \ge 18$ and that there exists a quartic nut graph of order n if and only if $n \in \{8, 10, 12\}$ or $n \ge 14$. These results were later extended by Fowler et al. [6, Theorem 7], who determined all the orders that a d-regular nut graph can have for any $5 \le d \le 11$. In the aforementioned paper, the following question was also asked regarding the existence of vertex-transitive nut graphs.

Problem 1.1 (Fowler et al. [6, Question 9])**.** For what pairs (n, d) does a vertex-transitive nut graph of order n and degree d exist?

The necessary conditions for the existence of a d-regular vertex-transitive nut graph of order n were further derived in the form of the next theorem.

Theorem 1.2 (Fowler et al. [6, Theorem 10])**.** *Let G be a vertex-transitive nut graph on n vertices, of degree d. Then n and d satisfy the following conditions. Either $d \equiv_4 0$, and $n \equiv_2 0$ and $n \ge d + 4$; or $d \equiv_4 2$, and $n \equiv_4 0$ and $n \ge d + 6$.*

Afterwards, Bašić et al. [2] demonstrated that there exists a 12-regular nut graph of order n if and only if $n \ge 16$. While doing so, the study of circulant nut graphs was initiated and several results concerning these graphs were disclosed, alongside the following conjecture.

Conjecture 1.3 (Bašić et al. [2])**.** *For every d, where $d \equiv_4 0$, and for every even n, $n \ge d + 4$, there exists a circulant nut graph $\mathrm{Circ}(n, \{s_1, s_2, s_3, \ldots, s_{\frac{d}{2}}\})$ of degree d.*

Damnjanović and Stevanović [4, Lemma 18] quickly disproved Conjecture 1.3 by showing that for each d such that $8 \mid d$, a d-regular circulant nut graph cannot have an order that is below $d + 6$. However, Conjecture 1.3 did indirectly bring up an interesting question which represents a natural follow-up of Question 1.1 and of an earlier question regarding the existence of regular nut graphs [7, Problem 13]:

Problem 1.4. What are all the pairs (n, d) for which there exists a d-regular circulant nut graph of order n?

Henceforth, we shall refer to Question 1.4 as the circulant nut graph order–degree existence problem, and we will use $\mathcal{N}_d$ to denote the set of all the orders that a d-regular circulant nut graph can have, for each $d \in \mathbb{N}_0$. Regarding the aforementioned problem, there are several basic facts that can quickly be noticed, as demonstrated by Damnjanović and Stevanović [4]. First of all, it is easy to show that every d-regular circulant nut graph of order n must satisfy $4 \mid d$ and $2 \mid n$. Moreover, for any odd $t \in \mathbb{N}$, a $4t$-regular circulant nut graph cannot have an order below $4t+4$, while for any even $t \in \mathbb{N}$, such a graph cannot have an order smaller than $4t + 6$, as already discussed.

Furthermore, Damnjanović and Stevanović [4] have managed to construct a $4t$-regular circulant nut graph of order n for each even $n \geq 4t + 4$, provided t is odd, $t \not\equiv_{10} 1$ and $t \not\equiv_{18} 15$. This result is disclosed in the following theorem.

Theorem 1.5 (Damnjanović and Stevanović [4])**.** *For each odd $t \geq 3$ such that $t \not\equiv_{10} 1$ and $t \not\equiv_{18} 15$, the circulant graph $\mathrm{Circ}(n, \{1, 2, 3, \ldots, 2t + 1\} \setminus \{t\})$ is a nut graph for each even $n \geq 4t + 4$.*

Thus, Theorem 1.5 fully determines $\mathcal{N}_{4t}$ for infinitely many odd values of t. On top of that, Damnjanović and Stevanović [4, Proposition 19] have also found the set

$$\mathcal{N}_8 = \{14\} \cup \{n \in \mathbb{N} \colon 2 \mid n \wedge n \geq 18\}. \tag{1.1}$$

In this scenario, it is interesting to notice that a surprising "irregularity" exists due to the absence of an 8-regular circulant nut graph of order 16.

Afterwards, Damnjanović [3] succeeded in improving the previously disclosed results by finding the set $\mathcal{N}_{4t}$ for each odd $t \in \mathbb{N}$:

$$\mathcal{N}_{4t} = \{n \in \mathbb{N} \colon 2 \mid n \wedge n \geq 4t + 4\} \qquad (\forall t \in \mathbb{N},\ 2 \nmid t).$$

This result is an immediate corollary of the next two theorems.

Theorem 1.6 (Damnjanović [3])**.** *For each odd $t \in \mathbb{N}$ and $n \geq 4t + 4$ such that $4 \mid n$, the circulant graph*

$$\mathrm{Circ}\left(n, \{1, 2, \ldots, t-1\} \cup \left\{\frac{n}{4}, \frac{n}{4} + 1\right\} \cup \left\{\frac{n}{2} - (t-1), \ldots, \frac{n}{2} - 2, \frac{n}{2} - 1\right\}\right)$$

must be a $4t$-regular nut graph of order n.

Theorem 1.7 (Damnjanović [3])**.** *For each $t \in \mathbb{N}$ and $n \geq 4t + 6$ such that $n \equiv_4 2$, the circulant graph*

$$\mathrm{Circ}\left(n, \{1, 2, \ldots, t-1\} \cup \left\{\frac{n+2}{4}, \frac{n+6}{4}\right\} \cup \left\{\frac{n}{2} - (t-1), \ldots, \frac{n}{2} - 2, \frac{n}{2} - 1\right\}\right)$$

must be a $4t$-regular nut graph of order n.

In this paper, we fully resolve the circulant nut graph order–degree existence problem by finding $\mathcal{N}_d$ for each $d \in \mathbb{N}_0$. The main result is given in the following theorem.

Theorem 1.8 (Circulant nut graph order–degree existence theorem)**.** *For each* $d \in \mathbb{N}_0$*, the set* $\mathcal{N}_d$ *can be determined via the following expression:*

$$\mathcal{N}_d = \begin{cases} \varnothing, & d = 0 \lor 4 \nmid d, \\ \{n \in \mathbb{N} \colon 2 \mid n \land n \geq d + 4\}, & d \equiv_8 4, \\ \{14\} \cup \{n \in \mathbb{N} \colon 2 \mid n \land n \geq 18\}, & d = 8, \\ \{n \in \mathbb{N} \colon 2 \mid n \land n \geq d + 6\}, & 8 \mid d \land d \geq 16. \end{cases} \tag{1.2}$$

The result given in the case $d = 0 \lor 4 \nmid d$ of Equation (1.2) is straightforward to see, while the expression corresponding to the case $d = 8$ follows directly from Equation (1.1). Given the fact that the case $d \equiv_8 4$ represents an immediate corollary of Theorems 1.6 and 1.7, as we have already mentioned, the only remaining case left to be proved is when $8 \mid d \land d \geq 16$. However, Theorem 1.7 tells us that for each such d, there does exist a circulant nut graph of every order n such that $n \equiv_4 2$ and $n \geq d + 6$. Thus, taking everything into consideration, in order to complete the proof of Theorem 1.8, it only remains to be shown that for each even $t \geq 4$, there must exist a $4t$-regular circulant nut graph of each order n such that $4 \mid n$ and $n \geq 4t + 8$. This is precisely the task that the remainder of the paper will solve.

The structure of the paper shall be organized in the following manner. After Section 1, which is the introduction, Section 2 will serve to preview certain theoretical facts regarding the circulant matrices, circulant nut graphs and cyclotomic polynomials which are required to successfully finalize the proof of Theorem 1.8. Afterwards, we shall use three separate constructions in order to show the existence of all the required circulant nut graphs. In Section 3 we will construct a $4t$-regular circulant nut graph of order $4t + 8$, for each even $t \geq 4$, thereby showing that such a graph necessarily exists. After that, Section 4 will be used to show that, for any even $t \geq 4$, there exists a $4t$-regular circulant nut graph of order n for each $n \geq 4t + 16$ such that $8 \mid n$. Subsequently, Section 5 will demonstrate the existence of a $4t$-regular circulant nut graph of order n for each $n \geq 4t + 12$ such that $n \equiv_8 4$, where $t \geq 4$ is an arbitrarily chosen even integer. Finally, Section 6 shall provide a brief conclusion regarding all the obtained results and give two additional problems to be examined in the future.

2 Preliminaries

It is known from elementary linear algebra theory (see, for example, [8, Section 3.1]) that the circulant matrix

$$A = \begin{bmatrix} a_0 & a_1 & a_2 & \cdots & a_{n-1} \\ a_{n-1} & a_0 & a_1 & \cdots & a_{n-2} \\ a_{n-2} & a_{n-1} & a_0 & \cdots & a_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_1 & a_2 & a_3 & \ldots & a_0 \end{bmatrix}$$

must have the eigenvalues

$$P(1), P(\omega), P(\omega^2), \ldots, P(\omega^{n-1}),$$

where $\omega = e^{i\frac{2\pi}{n}}$ is an n-th root of unity, and

$$P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1}.$$

Starting from the aforementioned result, Damnjanović and Stevanović [4] have managed to give the necessary and sufficient conditions for a circulant graph to be a nut graph in the form of the following lemma.

Lemma 2.1 (Damnjanović and Stevanović [4]). *Let $G = \mathrm{Circ}(n, S)$ where $n \ge 2$. The graph G is a nut graph if and only if all of the following conditions hold:*

- $2 \mid n$*;*
- *S consists of t odd and t even integers from $\{1, 2, 3, \dots, \frac{n}{2} - 1\}$, for some $t \ge 1$;*
- *$P(\omega^j) \neq 0$ for each $j \in \{1, 2, 3, \dots, \frac{n}{2} - 1\}$.*

Suppose that we are given an arbitrary circulant graph of even order n whose generator set is non-empty and contains equally many odd and even integers, all of which are positive integers smaller than $\frac{n}{2}$. Taking into consideration Lemma 2.1, it becomes apparent that in order to show that such a graph is a nut graph, it is sufficient to prove that it satisfies the third condition given in the lemma. In other words, it is enough to demonstrate that, for this graph, the polynomial $P(x) \in \mathbb{Z}[x]$ has no n-th roots of unity among its roots, except potentially -1 or 1.

Furthermore, it is clear that $\zeta^{n-j} = \frac{1}{\zeta^j}$ for each $j = \overline{1, n-1}$ and each n-th root of unity $\zeta \in \mathbb{C}$. Bearing this in mind, we quickly obtain that

$$P(\zeta) = \left(\zeta^{s_0} + \frac{1}{\zeta^{s_0}}\right) + \left(\zeta^{s_1} + \frac{1}{\zeta^{s_1}}\right) + \dots + \left(\zeta^{s_{k-1}} + \frac{1}{\zeta^{s_{k-1}}}\right) \tag{2.1}$$

for an arbitrary n-th root of unity ζ and circulant graph $G = \mathrm{Circ}(n, S)$, where $S = \{s_0, s_1, s_2, \dots, s_{k-1}\}$, provided all the generator set elements are lower than $\frac{n}{2}$. Sections 3, 4 and 5 will all heavily rely on Equation (2.1), as well as Lemma 2.1, whilst proving that the soon-to-be constructed circulant graphs are indeed nut graphs.

Last but not least, it is crucial to point out that the cyclotomic polynomials shall play a key role in demonstrating whether or not certain polynomials of interest contain the given roots of unity among their roots. The cyclotomic polynomial $\Phi_b(x)$ can be defined for each $b \in \mathbb{N}$ via

$$\Phi_b(x) = \prod_{\xi} (x - \xi),$$

where ξ ranges over the primitive b-th roots of unity. It is known that these polynomials have integer coefficients and that they are all irreducible in $\mathbb{Q}[x]$ (see, for example, [1]). Hence, an arbitrary polynomial in $\mathbb{Q}[x]$ has a primitive b-th root of unity among its roots if and only if it is divisible by $\Phi_b(x)$.

While inspecting whether certain integer polynomials are divisible by cyclotomic polynomials, we will strongly rely on the following theorem on the divisibility of lacunary polynomials by cyclotomic polynomials.

Theorem 2.2 (Filaseta and Schinzel [5]). *Let $P(x) \in \mathbb{Z}[x]$ have N nonzero terms and let $\Phi_b(x) \mid P(x)$. Suppose that $p_1, p_2, \dots, p_k$ are distinct primes such that*

$$\sum_{j=1}^{k} (p_j - 2) > N - 2.$$

Let e_j be the largest exponent such that $p_j^{e_j} \mid b$. Then for at least one j, $1 \le j \le k$, we have that $\Phi_{b'}(x) \mid P(x)$, where $b' = \frac{b}{p_j^{e_j}}$.

3 Construction for $n = 4t + 8$

In this section, we will demonstrate that for each even $t \geq 4$ there does exist a $4t$-regular circulant nut graph of order $4t + 8$. In order to achieve this, we shall provide a concrete example of such a graph, for each even $t \geq 4$, and then prove that the given graph is indeed a circulant nut graph. While constructing these graphs, we will rely on two different construction patterns. One pattern will be used for the scenario when $4 \mid t$, while the second will give us our desired result provided $t \equiv_4 2$. In the rest of the section we present the two according lemmas.

Lemma 3.1. *For each $t \geq 4$ such that $4 \mid t$, the circulant graph*

$$\mathrm{Circ}(4t + 8, \{1, 2, 3, \dots, 2t + 3\} \setminus \{t + 1, t + 3, t + 4\})$$

must be a $4t$-regular circulant nut graph of order $4t + 8$.

Proof. Let $n = 4t+8$. First of all, we know that $t+1$ and $t+3$ are odd, while $t+4$ is even, which directly tells us that the given circulant graph does have a non-empty generator set that contains equally many odd and even integers, all of which are positive, but smaller than $\frac{n}{2}$. Thus, by virtue of Lemma 2.1, in order to prove the given lemma, it is sufficient to show that the polynomial $P(x)$ has no n-th roots of unity among its roots, except potentially 1 or -1.

Let $\zeta \in \mathbb{C}$ be an arbitrary n-th root of unity that is different from both 1 and -1. By implementing Equation (2.1), we swiftly obtain

$$P(\zeta) = \sum_{j=1}^{2t+3} \left(\zeta^j + \zeta^{-j}\right) - \left(\zeta^{t+1} + \zeta^{-t-1}\right) - \left(\zeta^{t+3} + \zeta^{-t-3}\right) - \left(\zeta^{t+4} + \zeta^{-t-4}\right).$$

However, since $\zeta \neq 1$, we know that

$$\begin{aligned}
& & \sum_{j=0}^{n-1} \zeta^j &= 0 \\
&\implies & \zeta^{-2t-3} \sum_{j=0}^{4t+7} \zeta^j &= 0 \\
&\implies & \sum_{j=-2t-3}^{2t+4} \zeta^j &= 0 \\
&\implies & \zeta^{2t+4} + 1 + \sum_{j=1}^{2t+3} \left(\zeta^j + \zeta^{-j}\right) &= 0 \\
&\implies & \sum_{j=1}^{2t+3} \left(\zeta^j + \zeta^{-j}\right) &= -1 - \zeta^{2t+4}.
\end{aligned}$$

Thus, the condition $P(\zeta) = 0$ quickly becomes equivalent to

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & -1 - \zeta^{2t+4} - \zeta^{t+1} - \zeta^{-t-1} - \zeta^{t+3} - \zeta^{-t-3} - \zeta^{t+4} - \zeta^{-t-4} = 0 \\ \iff \quad & -\zeta^{t+4}(-1 - \zeta^{2t+4} - \zeta^{t+1} - \zeta^{-t-1} - \zeta^{t+3} - \zeta^{-t-3} - \zeta^{t+4} - \zeta^{-t-4}) = 0 \\ \iff \quad & \zeta^{3t+8} + \zeta^{2t+8} + \zeta^{2t+7} + \zeta^{2t+5} + \zeta^{t+4} + \zeta^3 + \zeta + 1 = 0. \end{aligned} \tag{3.1}$$

We will finish the proof of the lemma by dividing the problem into two cases depending on the value of $\zeta^{\frac{n}{2}}$.

Case $\zeta^{\frac{n}{2}} = -1$. In this case, we have $\zeta^{2t+4} = -1$, hence $\zeta^{3t+8} = -\zeta^{t+4}$, which means that Equation (3.1) leads us to

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & \zeta^{2t+8} + \zeta^{2t+7} + \zeta^{2t+5} + \zeta^3 + \zeta + 1 = 0 \\ \iff \quad & -\zeta^4 - \zeta^3 - \zeta + \zeta^3 + \zeta + 1 = 0 \\ \iff \quad & 1 - \zeta^4 = 0 \\ \iff \quad & \zeta^4 = 1. \end{aligned}$$

However, $\zeta^4 = 1$ cannot possibly hold. Moreover, $\zeta \neq 1, -1$ by definition, while i and $-i$ do not satisfy the conditions $i^{\frac{n}{2}} = -1$ and $(-i)^{\frac{n}{2}} = -1$ due to the fact that $4 \mid 2t+4$. Thus, $P(\zeta) = 0$ does not hold for any n-th root of unity ζ that is different from both 1 and -1 and such that $\zeta^{\frac{n}{2}} = -1$.

Case $\zeta^{\frac{n}{2}} = 1$. In this scenario, we immediately see that $\zeta^{3t+8} = \zeta^{t+4}$, which further helps us obtain from Equation (3.1)

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & \zeta^{2t+8} + \zeta^{2t+7} + \zeta^{2t+5} + 2\zeta^{t+4} + \zeta^3 + \zeta + 1 = 0 \\ \iff \quad & \zeta^4 + \zeta^3 + \zeta + 2\zeta^{t+4} + \zeta^3 + \zeta + 1 = 0 \\ \iff \quad & 2\zeta^{t+4} + \zeta^4 + 2\zeta^3 + 2\zeta + 1 = 0. \end{aligned} \tag{3.2}$$

We now divide the problem into two subcases depending on the value of $\zeta^{\frac{n}{4}}$.

Subcase $\zeta^{\frac{n}{4}} = -1$. Here, it is clear that $\zeta^{t+4} = -\zeta^2$, which means that Equation (3.2) directly transforms to

$$P(\zeta) = 0 \quad \iff \quad \zeta^4 + 2\zeta^3 - 2\zeta^2 + 2\zeta + 1 = 0.$$

However, the polynomial $x^4 + 2x^3 - 2x^2 + 2x + 1 \in \mathbb{Q}[x]$ has no roots of unity among its roots, as demonstrated in Appendix D. This means that $P(\zeta) = 0$ cannot possibly hold for any ζ that is an n-th root of unity, as desired.

Subcase $\zeta^{\frac{n}{4}} = 1$. In this subcase, we obtain $\zeta^{t+4} = \zeta^2$. Thus, Equation (3.2) gives us

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & \zeta^4 + 2\zeta^3 + 2\zeta^2 + 2\zeta + 1 = 0 \\ \iff \quad & (\zeta^2 + 1)(\zeta + 1)^2 = 0 \\ \iff \quad & \zeta^2 + 1 = 0. \end{aligned}$$

Now, by taking into consideration that $i^{\frac{n}{4}} = (-i)^{\frac{n}{4}} = -1$ due to the fact that $\frac{n}{4} = t+2 \equiv_4 2$, we clearly see that for any n-th root of unity $\zeta \in \mathbb{C}$ different from 1 and -1 and such that $\zeta^{\frac{n}{4}} = 1$, the equality $\zeta^2 + 1 = 0$ truly cannot hold. Hence, we reach $P(\zeta) \neq 0$ once again. □

Lemma 3.2. *For each $t \geq 6$ such that $t \equiv_4 2$, the circulant graph*

$$\mathrm{Circ}(4t + 8, \{1, 2, 3 \ldots, 2t + 3\} \setminus \{t - 2, t + 1, t + 3\})$$

must be a $4t$-regular circulant nut graph of order $4t + 8$.

Proof. Let $n = 4t + 8$. It is clear that $t - 2$ is even, while $t + 1$ and $t + 3$ are odd, which implies that the given circulant graph has a non-empty generator set that contains equally many odd and even integers, all of which are positive and lower than $\frac{n}{2}$. By relying on Lemma 2.1, we know that in order to finalize the proof of the lemma, it is enough to demonstrate that the polynomial $P(x)$ has no n-th roots of unity among its roots, except potentially 1 or -1.

We will use a very similar strategy to complete the proof as it was done in Lemma 3.1. Let $\zeta \in \mathbb{C}$ be an arbitrary n-th root of unity such that $\zeta \neq 1, -1$. By using Equation (2.1), we immediately get

$$P(\zeta) = \sum_{j=1}^{2t+3} \left(\zeta^j + \zeta^{-j}\right) - \left(\zeta^{t-2} + \zeta^{-t+2}\right) - \left(\zeta^{t+1} + \zeta^{-t-1}\right) - \left(\zeta^{t+3} + \zeta^{-t-3}\right).$$

Now, we can use the same equality $\sum_{j=0}^{2t+3} \left(\zeta^j + \zeta^{-j}\right) = -1 - \zeta^{2t+4}$ that was proved in Lemma 3.1 in order to conclude that

$$\begin{aligned} && P(\zeta) = 0 \\ \iff && -1 - \zeta^{2t+4} - \zeta^{t-2} - \zeta^{-t+2} - \zeta^{t+1} - \zeta^{-t-1} - \zeta^{t+3} - \zeta^{-t-3} = 0 \\ \iff && -\zeta^{t+3}(-1 - \zeta^{2t+4} - \zeta^{t-2} - \zeta^{-t+2} - \zeta^{t+1} - \zeta^{-t-1} - \zeta^{t+3} - \zeta^{-t-3}) = 0 \\ \iff && \zeta^{3t+7} + \zeta^{2t+6} + \zeta^{2t+4} + \zeta^{2t+1} + \zeta^{t+3} + \zeta^5 + \zeta^2 + 1 = 0. \end{aligned} \tag{3.3}$$

We shall finish the proof by dividing the problem into two cases depending on the value of $\zeta^{\frac{n}{2}}$.

Case $\zeta^{\frac{n}{2}} = -1$. Here, we see that $\zeta^{2t+4} = -1$, hence $\zeta^{3t+7} = -\zeta^{t+3}$. On behalf of Equation (3.3), $P(\zeta) = 0$ becomes further equivalent to

$$\begin{aligned} && P(\zeta) = 0 \\ \iff && \zeta^{2t+6} + \zeta^{2t+4} + \zeta^{2t+1} + \zeta^5 + \zeta^2 + 1 = 0 \\ \iff && -\zeta^2 - 1 - \frac{1}{\zeta^3} + \zeta^5 + \zeta^2 + 1 = 0 \\ \iff && \zeta^5 - \frac{1}{\zeta^3} = 0 \\ \iff && \zeta^8 = 1. \end{aligned}$$

However, $\frac{n}{2} = 2t + 4$, where $t \equiv_4 2$, which means that $8 \mid \frac{n}{2}$. This implies that whenever some eighth root of unity is raised to the power of $\frac{n}{2}$, it yields 1, not -1. Hence, the equality $\zeta^8 = 1$ cannot possibly hold for any n-th root of unity $\zeta \in \mathbb{C}$ such that $\zeta^{\frac{n}{2}} = -1$. Thus, we obtain $P(\zeta) \neq 0$, as desired.

Case $\zeta^{\frac{n}{2}} = 1$. In this case, it is clear that $\zeta^{3t+7} = \zeta^{t+3}$, which allows us to implement Equation (3.3) in order to reach

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & \zeta^{2t+6} + \zeta^{2t+4} + \zeta^{2t+1} + 2\zeta^{t+3} + \zeta^5 + \zeta^2 + 1 = 0 \\ \iff \quad & \zeta^2 + 1 + \frac{1}{\zeta^3} + 2\zeta^{t+3} + \zeta^5 + \zeta^2 + 1 = 0 \\ \iff \quad & \zeta^3 \left(2\zeta^{t+3} + \zeta^5 + 2\zeta^2 + 2 + \frac{1}{\zeta^3} \right) = 0 \\ \iff \quad & 2\zeta^{t+6} + \zeta^8 + 2\zeta^5 + 2\zeta^3 + 1 = 0. \end{aligned} \tag{3.4}$$

We now divide the problem into two subcases depending on the value of $\zeta^{\frac{n}{4}}$.

Subcase $\zeta^{\frac{n}{4}} = -1$. In this subcase, we know that $\zeta^{t+6} = -\zeta^4$, hence Equation (3.4) quickly implies

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & \zeta^8 + 2\zeta^5 - 2\zeta^4 + 2\zeta^3 + 1 = 0 \\ \iff \quad & (\zeta^2 + 1)(\zeta^6 - \zeta^4 + 2\zeta^3 - \zeta^2 + 1) = 0. \end{aligned}$$

Furthermore, we have $i^{\frac{n}{4}} = (-i)^{\frac{n}{4}} = 1$ due to the fact that $\frac{n}{4} = t + 2 \equiv_4 0$, which means that $\zeta^2 + 1 \neq 0$. This leads us to

$$P(\zeta) = 0 \quad \iff \quad \zeta^6 - \zeta^4 + 2\zeta^3 - \zeta^2 + 1 = 0.$$

However, the polynomial $x^6 - x^4 + 2x^3 - x^2 + 1 \in \mathbb{Q}[x]$ has no roots of unity among its roots, as shown in Appendix D. This implies that $P(\zeta) \neq 0$ for any n-th root of unity ζ such that $\zeta \neq 1, -1$ and $\zeta^{\frac{n}{4}} = -1$.

Subcase $\zeta^{\frac{n}{4}} = 1$. Here, we get $\zeta^{t+6} = \zeta^4$, which enables us to use Equation (3.4) to swiftly obtain

$$\begin{aligned} & P(\zeta) = 0 \\ \iff \quad & \zeta^8 + 2\zeta^5 + 2\zeta^4 + 2\zeta^3 + 1 = 0 \\ \iff \quad & (\zeta + 1)^2(\zeta^6 - 2\zeta^5 + 3\zeta^4 - 2\zeta^3 + 3\zeta^2 - 2\zeta + 1) = 0 \\ \iff \quad & \zeta^6 - 2\zeta^5 + 3\zeta^4 - 2\zeta^3 + 3\zeta^2 - 2\zeta + 1 = 0. \end{aligned}$$

The polynomial $x^6 - 2x^5 + 3x^4 - 2x^3 + 3x^2 - 2x + 1 \in \mathbb{Q}[x]$ has no roots of unity among its roots, as demonstrated in Appendix D. This clearly shows that $P(\zeta) = 0$ cannot hold, as desired. □

4 Construction for $8 \mid n \wedge n \geq 4t + 16$

In this section we will give a constructive proof of the existence of a $4t$-regular circulant nut graph of any order $n \in \mathbb{N}$ such that $n \geq 4t + 16$ and $8 \mid n$, for any even $t \geq 4$. In order to achieve this, we will prove the following theorem.

Theorem 4.1. *For any even $t \geq 4$ and any $n \geq 4t+16$ such that $8 \mid n$, the circulant graph $\mathrm{Circ}(n, S'_{t,n})$ where*

$$S'_{t,n} = \{1, 2, \dots, t-3\} \cup \{t-1, t\} \cup \left\{\frac{n}{4}, \frac{n}{4}+2\right\} \cup \left\{\frac{n}{2}-t, \frac{n}{2}-(t-1)\right\} \cup \left\{\frac{n}{2}-(t-3), \dots, \frac{n}{2}-2, \frac{n}{2}-1\right\}$$

must be a $4t$-regular circulant nut graph of order n.

For starters, it is clear that the set $S'_{t,n}$ is well defined, given the fact that $t < \frac{n}{4}$ and $\frac{n}{4}+2 < \frac{n}{2}-t$ for each even $t \geq 4$ and each $n \geq 4t+16$ such that $8 \mid n$. Moreover, it is not difficult to see that this set necessarily contains equally many odd and even integers, all of which are positive and smaller than $\frac{n}{2}$. By virtue of Lemma 2.1, in order to prove Theorem 4.1, it is sufficient to show that $P(x)$ has no n-th roots of unity among its roots, except potentially 1 or -1.

The proof of Theorem 4.1 will be carried out in a fashion that is very similar to the strategy used by Damnjanović [3]. Thus, we will rely on a few auxiliary lemmas which will be used in order to finalize the proof in a more concise manner. We start off by defining the following two polynomials

$$\begin{aligned}
Q_t(x) &= 2x^{2t+1} - 2x^{2t-1} + 2x^{2t-2} + x^{t+3} - x^{t+2} + x^{t-1} - x^{t-2} - 2x^3 + 2x^2 - 2,\\
R_t(x) &= 2x^{2t+1} - 2x^{2t-1} + 2x^{2t-2} - x^{t+3} + x^{t+2} - 4x^{t+1}\\
&\qquad + 4x^t - x^{t-1} + x^{t-2} - 2x^3 + 2x^2 - 2,
\end{aligned}$$

for each even $t \geq 6$. Now, since it is clear that $3 < t-2$ and $t+3 < 2t-2$ hold for any even $t \geq 6$, we see that $Q_t(x)$ must have exactly 10 non-zero terms, while $R_t(x)$ surely has exactly 12 non-zero terms. Let L'_t and L''_t be the sets containing the powers of these terms, respectively, i.e.

$$\begin{aligned}
L'_t &= \{0, 2, 3, t-2, t-1, t+2, t+3, 2t-2, 2t-1, 2t+1\},\\
L''_t &= \{0, 2, 3, t-2, t-1, t, t+1, t+2, t+3, 2t-2, 2t-1, 2t+1\},
\end{aligned}$$

for each even $t \geq 6$. In the next lemma we will show one valuable property regarding these two sets.

Lemma 4.2. *For each even $t \geq 6$ and each $\beta \in \mathbb{N}$, $\beta \geq 10$, L'_t must contain an element whose remainder modulo β is unique within the set. Also, for each even $t \geq 6$ and each $\beta \in \mathbb{N}$, $\beta \geq 7$ such that $\beta \nmid t$, L''_t necessarily contains an element whose remainder modulo β is unique within the set.*

Proof. It is clear that, for any $\beta \geq 7$, the elements $t-2, t-1, t, t+1, t+2, t+3$ must all have mutually distinct remainders modulo β. If the element $t-1$ were to have a distinct remainder modulo β from all the remainders of the elements $0, 2, 3, 2t-2, 2t-1, 2t+1$, then this value would represent an element of the set L'_t, as well as the set L''_t, which has a unique remainder modulo β inside the said set. The lemma statement would swiftly follow from here. Now, suppose otherwise, i.e. that the value $t-1$ does have the same remainder modulo β as some number from the set $\{0, 2, 3, 2t-2, 2t-1, 2t+1\}$. We will finish the proof off by showing that the lemma statement holds in this scenario as well. For convenience, we will divide the problem into six corresponding cases.

	$t \equiv_\beta -2$	$t \equiv_\beta 0$	$t \equiv_\beta 1$	$t \equiv_\beta 3$	$t \equiv_\beta 4$
$0 \equiv_\beta$	0	0	0	0	0
$2 \equiv_\beta$	2	2	2	2	2
$3 \equiv_\beta$	3	3	3	3	3
$t-2 \equiv_\beta$	-4	-2	-1	1	2
$t-1 \equiv_\beta$	-3	-1	0	2	3
$t \equiv_\beta$	-2	0	1	3	4
$t+1 \equiv_\beta$	-1	1	2	4	5
$t+2 \equiv_\beta$	0	2	3	5	6
$t+3 \equiv_\beta$	1	3	4	6	7
$2t-2 \equiv_\beta$	-6	-2	0	4	6
$2t-1 \equiv_\beta$	-5	-1	1	5	7
$2t+1 \equiv_\beta$	-3	1	3	7	9

Table 1: The elements of the sets L'_t and L''_t modulo β, for certain values of $t \bmod \beta$.

Case $t-1 \equiv_\beta 0$. In this case we obtain $t \equiv_\beta 1$. From Table 1 it is now clear that the element $t-2$ must have a unique remainder modulo β in both L'_t and L''_t.

Case $t-1 \equiv_\beta 2$. In this case we get $t \equiv_\beta 3$. Once again, Table 1 tells us that the element $t-2$ must have a unique remainder modulo β in both L'_t and L''_t.

Case $t-1 \equiv_\beta 3$. Here, we conclude that $t \equiv_\beta 4$. According to Table 1, we see that the element t necessarily has a unique remainder modulo β in L''_t, whenever $\beta \geq 7$. On the other hand, if $\beta \geq 10$, then the element 0 certainly has a unique remainder modulo β within the set L'_t.

Case $t-1 \equiv_\beta 2t-2$. In this scenario we get $t \equiv_\beta 1$, hence this case is solved in absolutely the same way as the previous case $t-1 \equiv_\beta 0$.

Case $t-1 \equiv_\beta 2t-1$. Here, we immediately get $t \equiv_\beta 0$. By virtue of Table 1, we see that the element 0 has a unique remainder modulo β in the set L'_t. On the other hand, the set L''_t contains no element with a unique remainder modulo β. In fact, we can group the elements of L''_t into six equivalence pairs according to their remainders modulo β. We will rely on this fact later on.

Case $t-1 \equiv_\beta 2t+1$. In this case, we obtain $t \equiv_\beta -2$. It is easy to see from Table 1 that whenever $\beta \geq 10$, the element $t-2$ must have a unique remainder modulo β within the set L'_t. Similarly, if $\beta \geq 7$, then the element $t+1$ surely has a unique remainder modulo β inside the set L''_t. □

Now, by implementing Lemma 4.2, we are able to prove the following lemma regarding the divisibility of $Q_t(x)$ and $R_t(x)$ polynomials by certain polynomials that shall be of later use to us.

Lemma 4.3. *For any even $t \geq 6$ and each $\beta \geq 10$, the polynomial $Q_t(x)$ cannot be divisible by a polynomial $V(x) \in \mathbb{Q}[x]$ with at least two non-zero terms such that all of its terms have powers divisible by β. Similarly, for any even $t \geq 6$ and each $\beta \geq 7$, the polynomial $R_t(x)$ also cannot be divisible by any such $V(x)$.*

Proof. Let $t \geq 6$ be an arbitrarily chosen even integer and let $\beta \geq 10$ be any positive integer. Suppose that the polynomial $Q_t(x)$ is divisible by a $V(x)$ with at least two non-zero terms such that all of its terms have powers divisible by β. Now, we will use $Q_t^{(\beta,j)}(x)$

to denote the polynomial composed of all the terms of $Q_t(x)$ whose powers are congruent to j modulo β, for each $j = \overline{0, \beta - 1}$. If we write

$$Q_t(x) = V(x)\, V_1(x)$$

and use the notation $V_1^{(\beta,j)}(x)$ in a manner analogous to the previously stated $Q_t^{(\beta,j)}(x)$, it becomes easy to notice that

$$Q_t^{(\beta,j)}(x) = V(x)\, V_1^{(\beta,j)}(x)$$

must hold for each $j = \overline{0, \beta - 1}$. Hence, we obtain that $V(x) \mid Q_t^{(\beta,j)}(x)$ is true for each $j = \overline{0, \beta - 1}$. However, by virtue of Lemma 4.2, we know that there exists an element of L'_t that has a unique remainder modulo β within the set. This implies that there exists a j such that $Q_t^{(\beta,j)}(x)$ has the form $c\, x^a$ for some $c \in \mathbb{Z} \setminus \{0\}$ and $a \in \mathbb{N}_0$. By taking this into consideration, we get that $V(x) \mid c\, x^a$, which further implies that $V(x)$ cannot have more than one non-zero term, thus yielding a contradiction.

Now, let $t \geq 6$ be any even integer and let $\beta \geq 7$ be some positive integer. Suppose that $R_t(x)$ is divisible by a $V(x)$ with at least two non-zero terms such that all of its terms have powers divisible by β. If $\beta \nmid t$, then we can obtain a contradiction by applying Lemma 4.2 in a manner that is entirely analogous to the technique previously used while dealing with the $Q_t(x)$ polynomial. Thus, we choose to omit the proof details of this case and focus solely on the remaining scenario when $\beta \mid t$ holds.

By taking into consideration the remainders given in Table 1, we see that for $\beta \geq 7$ and $\beta \mid t$, the divisibility $V(x) \mid R_t(x)$ further implies

$$\begin{aligned} &V(x) \mid 4x^t - 2, \\ &V(x) \mid x^{t+2} + 2x^2, \end{aligned}$$

from which we swiftly obtain

$$\begin{aligned} & V(x) \mid x^2\,(4x^t - 2) + (x^{t+2} + 2x^2) \\ \implies \quad & V(x) \mid 5x^{t+2}, \end{aligned}$$

thus yielding a contradiction once more, as desired. □

We now turn our attention to the cyclotomic polynomials and investigate the divisibility of $Q_t(x)$ and $R_t(x)$ by these polynomials, for all possible even values $t \geq 6$. By taking into consideration that each cyclotomic polynomial $\Phi_b(x)$ must have at least two non-zero terms, it becomes apparent that Lemma 4.3 will play a big role in our analysis to come. In fact, its usage is immediately demonstrated within the next lemma.

Lemma 4.4. *For each even $t \geq 6$, the divisibility $\Phi_b(x) \mid Q_t(x)$ for some $b \in \mathbb{N}$ implies*

- *$p^2 \nmid b$ for any prime number $p \geq 11$;*
- *$7^3 \nmid b$, $5^3 \nmid b$, $3^4 \nmid b$, $2^2 \nmid b$.*

Also, for each even $t \geq 6$, the divisibility $\Phi_b(x) \mid R_t(x)$ for some $b \in \mathbb{N}$ implies

- *$p^2 \nmid b$ for any prime number $p \geq 7$;*
- *$5^3 \nmid b$, $3^3 \nmid b$, $2^2 \nmid b$.*

Proof. Let $b \in \mathbb{N}$ be such that $p^2 \mid b$ for some prime number p. In this case, $\frac{b}{p}$ is a positive integer divisible by p, hence we get that $\Phi_b(x) = \Phi_{\frac{b}{p}}(x^p)$ (see, for example, [9, page 160]). Similarly, if $p^k \mid b$ for some $k \geq 2$, we inductively obtain that $\Phi_b(x) = \Phi_{\frac{b}{p^{k-1}}}(x^{p^{k-1}})$. We will now implement this observation in order to complete the proof of the lemma by dividing it into two separate cases for $Q_t(x)$ and $R_t(x)$.

Case $Q_t(x)$. Suppose that $\Phi_b(x) \mid Q_t(x)$ for some even $t \geq 6$ and some $b \in \mathbb{N}$. If $p^2 \mid b$ for some prime number $p \geq 11$, we then get that $\Phi_b(x) = \Phi_{\frac{b}{p}}(x^p)$, hence all the terms of $\Phi_b(x)$ must have powers divisible by $p \geq 11$. By virtue of Lemma 4.3, the divisibility $\Phi_b(x) \mid Q_t(x)$ cannot hold, hence we obtain a contradiction.

If we suppose that $7^3 \mid b$ or $5^3 \mid b$ or $3^4 \mid b$, we get that all the terms of $\Phi_b(x)$ must have powers divisible by 49 or 25 or 27, respectively. In each of these cases, Lemma 4.3 tells us that the divisibility $\Phi_b(x) \mid Q_t(x)$ does not hold, thus yielding a contradiction. In order to prove the part of the lemma regarding the $Q_t(x)$ polynomial, it becomes sufficient to show that $4 \mid b$ cannot be true.

Now, suppose that $4 \mid b$ holds. In this case, we immediately get that $\Phi_b(x)$ contains only terms whose powers are even. By taking into consideration that the numbers $0, 2, t-2, t+2, 2t-2$ are even, while $3, t-1, t+3, 2t-1, 2t+1$ are odd, we conclude that

$$\begin{aligned}
&\Phi_b(x) \mid 2x^{2t-2} - x^{t+2} - x^{t-2} + 2x^2 - 2,\\
&\Phi_b(x) \mid 2x^{2t+1} - 2x^{2t-1} + x^{t+3} + x^{t-1} - 2x^3.
\end{aligned}$$

If we denote

$$\begin{aligned}
A(x) &= 2x^{2t-2} - x^{t+2} - x^{t-2} + 2x^2 - 2,\\
B(x) &= 2x^{2t+1} - 2x^{2t-1} + x^{t+3} + x^{t-1} - 2x^3,\\
C(x) &= x^{t+7} - x^{t+5} + x^{t+3} - x^{t+1} + \frac{1}{2}x^9 + 2x^7 - 3x^5 + 4x^3 - \frac{3}{2}x,\\
D(x) &= -x^{t+4} - x^t + \frac{1}{2}x^8 - x^4 + 2x^2 - \frac{3}{2},
\end{aligned}$$

then it can be further obtained that

$$\begin{aligned}
&\Phi_b(x) \mid A(x)\,C(x) + B(x)\,D(x)\\
\implies\quad &\Phi_b(x) \mid 3x^9 - 8x^7 + 10x^5 - 8x^3 + 3x\\
\implies\quad &\Phi_b(x) \mid x(x-1)^2(x+1)^2(3x^4 - 2x^2 + 3)\\
\implies\quad &\Phi_b(x) \mid 3x^4 - 2x^2 + 3.
\end{aligned}$$

However, the polynomial $3x^4 - 2x^2 + 3 \in \mathbb{Q}[x]$ has no roots of unity among its roots, as demonstrated in Appendix D, thus yielding a contradiction. This means that $4 \mid b$ cannot possibly be true, as desired.

Case $R_t(x)$. Suppose that $\Phi_b(x) \mid R_t(x)$ for some even $t \geq 6$ and some $b \in \mathbb{N}$. It can be shown that $p^2 \nmid b$ for any prime $p \geq 7$, as well as $5^3 \nmid b$ and $3^3 \nmid b$, by implementing Lemma 4.3 in a completely analogous manner as done in the proof of the previous case. For this reason, we choose to leave out the according details. Thus, in order to finalize the proof, it is enough to show that $4 \nmid b$.

Suppose that $4 \mid b$ does hold. Similarly as in the previous case, we conclude that $\Phi_b(x)$ contains only terms whose powers are even. Besides that, the numbers $0, 2, t-2, t, t+2, 2t-2$ are even, while $3, t-1, t+1, t+3, 2t-1, 2t+1$ are odd. Bearing this in mind, we get

$$\Phi(b) \mid 2x^{2t-2} + x^{t+2} + 4x^t + x^{t-2} + 2x^2 - 2,$$
$$\Phi(b) \mid 2x^{2t+1} - 2x^{2t-1} - x^{t+3} - 4x^{t+1} - x^{t-1} - 2x^3.$$

Now, if we denote

$$\begin{aligned}
A(x) &= 2x^{2t-2} + x^{t+2} + 4x^t + x^{t-2} + 2x^2 - 2,\\
B(x) &= 2x^{2t+1} - 2x^{2t-1} - x^{t+3} - 4x^{t+1} - x^{t-1} - 2x^3,\\
C(x) &= -x^{t+7} - 3x^{t+5} + 3x^{t+3} + x^{t+1} + \frac{1}{2}x^9 + 6x^7 + 5x^5 + 8x^3 - \frac{3}{2}x,\\
D(x) &= x^{t+4} + 4x^{t+2} + x^t + \frac{1}{2}x^8 + 4x^6 + 7x^4 + 6x^2 - \frac{3}{2},
\end{aligned}$$

it is clear that

$$\begin{aligned}
& \Phi_b(x) \mid A(x)\,C(x) + B(x)\,D(x)\\
\implies\quad & \Phi_b(x) \mid 3x^9 - 16x^7 - 6x^5 - 16x^3 + 3x\\
\implies\quad & \Phi_b(x) \mid x(x^2 - 2x - 1)(x^2 + 2x - 1)(3x^4 + 2x^2 + 3)\\
\implies\quad & \Phi_b(x) \mid (x^2 - 2x - 1)(x^2 + 2x - 1)(3x^4 + 2x^2 + 3).
\end{aligned}$$

However, neither of the polynomials $x^2 - 2x - 1, x^2 + 2x - 1, 3x^4 + 2x^2 + 3$ contains a root that represents a root of unity, which immediately leads us to a contradiction. Thus, we reach $4 \nmid b$. □

Lemma 4.4 indicates that the cyclotomic polynomials which divide $Q_t(x)$ and $R_t(x)$ are very specific. Moreover, it can be shown that for any $b \geq 3$, the cyclotomic polynomial $\Phi_b(x)$ can divide neither $Q_t(x)$ nor $R_t(x)$. In fact, our next step shall be to prove this exact statement. In order to do this, we will need the following two short auxiliary lemmas.

Lemma 4.5. *For each even $t \geq 6$ and each prime number $p \geq 11$, $Q_t(x)$ cannot be divisible by $\Phi_p(x)$ or $\Phi_{2p}(x)$. Similarly, for any even $t \geq 6$ and any prime number $p \geq 13$, $R_t(x)$ cannot be divisible by $\Phi_p(x)$ or $\Phi_{2p}(x)$.*

Proof. The lemma statement about the $Q_t(x)$ polynomial can be proved in a fairly analogous manner as the part regarding $R_t(x)$. In fact, the proof of $\Phi_p(x) \nmid R_t(x)$ and $\Phi_{2p}(x) \nmid R_t(x)$ is slightly more difficult to perform due to the existence of one additional edge case which does not exist when we are dealing with $Q_t(x)$. For this reason, we choose to leave out the proof details for $\Phi_p(x) \nmid Q_t(x)$ and $\Phi_{2p}(x) \nmid Q_t(x)$ and focus solely on the $R_t(x)$ polynomial.

Now, let $t \geq 6$ be an arbitrary even integer and let $p \geq 11$ be some prime number. By noticing that

$$\Phi_p(x) = \sum_{j=0}^{p-1} x^j, \qquad \Phi_{2p}(x) = \sum_{j=0}^{p-1} (-1)^j x^j,$$

we immediately see that $\deg \Phi_p = \deg \Phi_{2p} = p - 1$. We will finalize the proof by splitting the problem into two cases depending on whether we are dealing with $\Phi_p(x)$ or $\Phi_{2p}(x)$.

Case $\Phi_p(x)$. Let $R_t^{\bmod p}(x)$ be the following polynomial:

$$\begin{aligned} R_t^{\bmod p}(x) = 2x^{(2t+1) \bmod p} &- 2x^{(2t-1) \bmod p} + 2x^{(2t-2) \bmod p} - x^{(t+3) \bmod p} \\ &+ x^{(t+2) \bmod p} - 4x^{(t+1) \bmod p} + 4x^{t \bmod p} \\ &- x^{(t-1) \bmod p} + x^{(t-2) \bmod p} - 2x^3 + 2x^2 - 2. \end{aligned}$$

It is clear that $\Phi_p(x) \mid R_t(x)$ holds if and only if $\Phi_p(x) \mid R_t^{\bmod p}(x)$ does, too. If we suppose that $\Phi_p(x) \mid R_t(x)$ is true and take into consideration that

$$\deg R_t^{\bmod p} \le p - 1 = \deg \Phi_p,$$

we quickly obtain two possibilities:

- $R_t^{\bmod p}(x) \equiv 0$;
- $R_t^{\bmod p}(x) = c\,\Phi_p(x)$ for some $c \in \mathbb{Q} \setminus \{0\}$.

It is not difficult to see that $R_t^{\bmod p}(x) \equiv 0$ cannot hold. If $p \nmid t$, then Lemma 4.2 dictates that there exists an element of L_t'' that has a unique remainder modulo p within that set. Hence, $R_t^{\bmod p}(x)$ must have at least one term corresponding to that element. On the other hand, if $p \mid t$, then according to Table 1, in order for $R_t^{\bmod p}(x) \equiv 0$ to be true, we would need $4x^{t \bmod p} - 2 = 0$ to hold, which clearly does not. It is worth pointing out that while performing the analogous proof for $Q_t(x)$, the edge case $p \mid t$ does not exist, which can immediately be noticed in the formulation itself of Lemma 4.2.

Now, suppose that $R_t^{\bmod p}(x) = c\,\Phi_p(x)$ holds for some $c \in \mathbb{Q} \setminus \{0\}$. The polynomial $\Phi_p(x)$ has p non-zero terms, which means that $R_t^{\bmod p}(x)$ needs to have exactly p non-zero terms as well. This is obviously not possible whenever $p \ge 13$, since $R_t^{\bmod p}(x)$ can have at most 12 non-zero terms.

Case $\Phi_{2p}(x)$. Let $\hat{R}_t^{\bmod p}(x)$ be the following polynomial:

$$\begin{aligned} \hat{R}_t^{\bmod p}(x) = 2(-1)^{\lfloor \frac{2t+1}{p} \rfloor} x^{(2t+1) \bmod p} &- 2(-1)^{\lfloor \frac{2t-1}{p} \rfloor} x^{(2t-1) \bmod p} \\ + 2(-1)^{\lfloor \frac{2t-2}{p} \rfloor} x^{(2t-2) \bmod p} &- (-1)^{\lfloor \frac{t+3}{p} \rfloor} x^{(t+3) \bmod p} \\ + (-1)^{\lfloor \frac{t+2}{p} \rfloor} x^{(t+2) \bmod p} &- 4(-1)^{\lfloor \frac{t+1}{p} \rfloor} x^{(t+1) \bmod p} \\ + 4(-1)^{\lfloor \frac{t}{p} \rfloor} x^{t \bmod p} &- (-1)^{\lfloor \frac{t-1}{p} \rfloor} x^{(t-1) \bmod p} \\ + (-1)^{\lfloor \frac{t-2}{p} \rfloor} x^{(t-2) \bmod p} &- 2x^3 + 2x^2 - 2. \end{aligned}$$

We know that each primitive $2p$-th root of unity gives -1 when raised to the power of p. For this reason, it is not difficult to conclude that $\Phi_{2p}(x) \mid R_t(x)$ is equivalent to $\Phi_{2p}(x) \mid \hat{R}_t^{\bmod p}(x)$. Now, if we suppose that $\Phi_{2p}(x) \mid R_t(x)$ holds and bear in mind that

$$\deg \hat{R}_t^{\bmod p} \le p - 1 = \deg \Phi_{2p},$$

we reach the same two possibilities as in the previous case:

- $\hat{R}_t^{\bmod p}(x) \equiv 0$;
- $\hat{R}_t^{\bmod p}(x) = c\,\Phi_p(x)$ for some $c \in \mathbb{Q} \setminus \{0\}$.

The rest of the proof can be carried out in a manner analogous to the previous case. Thus, we choose to omit it. □

Lemma 4.6. *For each even $t \geq 6$, $Q_t(x)$ cannot be divisible by a cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$ is a positive integer such that*

- *it does not have any prime factors outside of the set $\{2, 3, 5, 7\}$;*
- *it does not contain all the prime factors from the set $\{3, 5, 7\}$;*
- $2^2 \nmid b$, $3^4 \nmid b$, $5^3 \nmid b$, $7^3 \nmid b$.

Also, for any even $t \geq 6$, $R_t(x)$ cannot be divisible by a cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$ is a positive integer such that

- *it does not have any prime factors outside of the set $\{2, 3, 5, 7, 11\}$;*
- *it does not contain both prime factors from the set $\{7, 11\}$ or from the set $\{5, 11\}$;*
- $2^2 \nmid b$, $3^3 \nmid b$, $5^3 \nmid b$, $7^2 \nmid b$, $11^2 \nmid b$.

Proof. Let $Q_t^{\bmod b}(x)$ and $R_t^{\bmod b}(x)$ be the next two polynomials:

$$\begin{aligned} Q_t^{\bmod b}(x) = {} & 2x^{(2t+1) \bmod b} - 2x^{(2t-1) \bmod b} + 2x^{(2t-2) \bmod b} + x^{(t+3) \bmod b} \\ & - x^{(t+2) \bmod b} + x^{(t-1) \bmod b} - x^{(t-2) \bmod b} \\ & - 2x^{3 \bmod b} + 2x^{2 \bmod b} - 2, \\ R_t^{\bmod b}(x) = {} & 2x^{(2t+1) \bmod b} - 2x^{(2t-1) \bmod b} + 2x^{(2t-2) \bmod b} - x^{(t+3) \bmod b} \\ & + x^{(t+2) \bmod b} - 4x^{(t+1) \bmod b} + 4x^{t \bmod b} - x^{(t-1) \bmod b} \\ & + x^{(t-2) \bmod b} - 2x^{3 \bmod b} + 2x^{2 \bmod b} - 2. \end{aligned}$$

Here, it is crucial to point out that $\Phi_b(x) \mid Q_t(x) \iff \Phi_b(x) \mid Q_t^{\bmod b}(x)$ and $\Phi_b(x) \mid R_t(x) \iff \Phi_b(x) \mid R_t^{\bmod b}(x)$. However, for a fixed value of $b \in \mathbb{N}$, it is clear that there exist only finitely many polynomials $Q_t^{\bmod b}(x)$ and $R_t^{\bmod b}(x)$ as t ranges over the even integers greater than or equal to 6. Thus, if we show that $\Phi_b(x)$ divides none of these concrete $Q_t^{\bmod b}(x)$ polynomials, this is sufficient to prove that $\Phi_b(x)$ does not divide $Q_t(x)$. The same can be said regarding $R_t(x)$.

In order to prove the lemma, it is enough to demonstrate that $\Phi_b(x) \nmid Q_t^{\bmod b}(x)$ and $\Phi_b(x) \nmid R_t^{\bmod b}(x)$ for all the required values of b and for all the possible remainders $t \bmod b$. However, the lemma formulation specifies only a finite set of b values corresponding to $Q_t(x)$ and to $R_t(x)$. For this reason, it is trivial to perform the proof of the lemma via computer. The required computational results are disclosed in Appendices A and B. □

We now proceed to prove the aforementioned statement regarding the divisibility of $Q_t(x)$ and $R_t(x)$ polynomials by cyclotomic polynomials. In order to do this, we shall heavily rely on Theorem 2.2. The reason why this theorem is so convenient to use is clear — it is due to the sheer fact that the $Q_t(x)$ and $R_t(x)$ polynomials have very few non-zero terms.

Lemma 4.7. *For each even $t \geq 6$, $Q_t(x)$ is not divisible by any cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$.*

Proof. Suppose that $\Phi_b(x) \mid Q_t(x)$ for some even $t \geq 6$ and some $b \geq 3$. We now divide the problem into two cases depending on whether b is divisible by some prime number from the set $\{3, 5, 7\}$.

Case $3 \nmid b \wedge 5 \nmid b \wedge 7 \nmid b$. In this case, it is clear that b has at least one prime factor greater than 7, since $b \notin \{1, 2\}$ and $2^2 \nmid b$, according to Lemma 4.4. Now, since $Q_t(x)$ has exactly 10 non-zero terms, and $p - 2 \geq 10 - 2$ for any prime $p \geq 11$, we are able to repeatedly apply Theorem 2.2 in order to cancel out any additional prime divisor of b greater than 7, until exactly one is left. This leads us to

$$\Phi_{b'}(x) \mid Q_t(x),$$

where b' has a single prime divisor greater than 7, and is potentially divisible by two as well. Taking into consideration Lemma 4.4, we conclude that b' must either be equal to some prime $p \geq 11$ or have the form $2p$, where $p \geq 11$ is a prime number. Either way, Lemma 4.5 tells us that such a $\Phi_{b'}(x)$ cannot possibly divide $Q_t(x)$, hence we obtain a contradiction.

Case $3 \mid b \vee 5 \mid b \vee 7 \mid b$. In this scenario, we can apply Theorem 2.2 in a similar fashion in order to cancel out any potential prime divisor of b greater than 7 until we reach

$$\Phi_{b'}(x) \mid Q_t(x),$$

where $b' \geq 3$ is such that all of its prime factors belong to the set $\{2, 3, 5, 7\}$, and $2^2 \nmid b'$, $3^4 \nmid b'$, $5^3 \nmid b'$, $7^3 \nmid b'$, by virtue of Lemma 4.4. Furthermore, we know that $(3 - 2) + (5 - 2) + (7 - 2) > 10 - 2$, hence we can suppose without loss of generality that b' is not divisible by at least one prime number from the set $\{3, 5, 7\}$, in accordance with Theorem 2.2. However, Lemma 4.6 dictates that such a $\Phi_{b'}(x)$ cannot divide $Q_t(x)$, yielding a contradiction. □

Lemma 4.8. *For each even $t \geq 6$, $R_t(x)$ is not divisible by any cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$.*

Proof. Suppose that $\Phi_b(x) \mid R_t(x)$ for some even $t \geq 6$ and some $b \geq 3$. We proceed by dividing the problem into two cases depending on whether b is divisible by some prime number from $\{3, 5, 7, 11\}$.

Case $3 \nmid b \wedge 5 \nmid b \wedge 7 \nmid b \wedge 11 \nmid b$. Due to the fact that $b \notin \{1, 2\}$ and $2^2 \nmid b$, by virtue of Lemma 4.4, we deduce that b has at least one prime factor greater than 11. Since $R_t(x)$ has exactly 12 non-zero terms and $p - 2 > 12 - 2$ for any prime $p \geq 13$, we can implement Theorem 2.2 and Lemma 4.4 in an analogous fashion as in Lemma 4.7 in order to reach

$$\Phi_{b'}(x) \mid R_t(x),$$

for some b' that is either equal to a prime $p \geq 13$ or has the form $2p$, for some prime number $p \geq 13$. Once again, Lemma 4.5 tells us that such a divisibility cannot hold, leading to a contradiction.

Case $3 \mid b \vee 5 \mid b \vee 7 \mid b \vee 11 \mid b$. In this case, we apply Theorem 2.2 once more in order to cancel out any potential prime divisor of b greater than 11 until we get

$$\Phi_{b'}(x) \mid R_t(x),$$

where $b' \geq 3$ is such that all of its prime factors belong to the set $\{2, 3, 5, 7, 11\}$, and $2^2 \nmid b'$, $3^3 \nmid b'$, $5^3 \nmid b'$, $7^2 \nmid b'$, $11^2 \nmid b'$ due to Lemma 4.4. Besides that, it is clear that $(7-2)+(11-2) > 12-2$ and $(5-2)+(11-2) > 12-2$, which means that it is safe to suppose that b' is not divisible by both elements from $\{7, 11\}$ or from $\{5, 11\}$. Bearing this in mind, it is easy to reach a contradiction by taking into consideration Lemma 4.6. □

Finally, we are able to put all the pieces of the puzzle together and complete the proof of Theorem 4.1.

Proof of Theorem 4.1. From Equation (2.1) we immediately obtain

$$P(\zeta) = \left(\zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}}\right) + \left(\zeta^{\frac{n}{4}+2} + \frac{1}{\zeta^{\frac{n}{4}+2}}\right) + \sum_{\substack{j=1,\\ j\neq t-2}}^{t} \left(\zeta^j + \frac{1}{\zeta^j}\right) + \sum_{\substack{j=\frac{n}{2}-t,\\ j\neq \frac{n}{2}-t+2}}^{\frac{n}{2}-1} \left(\zeta^j + \frac{1}{\zeta^j}\right),$$

where ζ is an arbitrarily chosen n-th root of unity different from 1 and -1. It is easy to further conclude that

$$P(\zeta) = \left(\zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}}\right) + \left(\zeta^{\frac{n}{4}+2} + \frac{1}{\zeta^{\frac{n}{4}+2}}\right) + \sum_{\substack{j=1,\\ j\neq t-2}}^{t} \left(\zeta^j + \frac{1}{\zeta^j} + \zeta^{\frac{n}{2}-j} + \frac{1}{\zeta^{\frac{n}{2}-j}}\right). \quad (4.1)$$

We will finish the proof by showing that $P(\zeta) \neq 0$ must necessarily hold. For the purpose of making the proof easier to follow, we shall divide it into two cases depending on whether $\zeta^{\frac{n}{2}}$ is equal to 1 or -1.

Case $\zeta^{\frac{n}{2}} = -1$. It is straightforward to see that $\zeta^{\frac{n}{2}-j} = -\frac{1}{\zeta^j}$ and $\frac{1}{\zeta^{\frac{n}{2}-j}} = -\zeta^j$, which swiftly gives

$$\zeta^j + \frac{1}{\zeta^j} + \zeta^{\frac{n}{2}-j} + \frac{1}{\zeta^{\frac{n}{2}-j}} = 0$$

for any $j = \overline{1, t}$. Thus, Equation (4.1) simplifies to

$$P(\zeta) = \zeta^{\frac{n}{4}+2} + \zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}} + \frac{1}{\zeta^{\frac{n}{4}+2}}.$$

The condition $P(\zeta) = 0$ now becomes equivalent to

$$\begin{aligned} & & P(\zeta) &= 0 \\ &\iff & \zeta^{\frac{n}{4}+2}\left(\zeta^{\frac{n}{4}+2} + \zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}} + \frac{1}{\zeta^{\frac{n}{4}+2}}\right) &= 0 \\ &\iff & \zeta^{\frac{n}{2}+4} + \zeta^{\frac{n}{2}+2} + \zeta^2 + 1 &= 0 \\ &\iff & -\zeta^4 - \zeta^2 + \zeta^2 + 1 &= 0 \\ &\iff & \zeta^4 &= 1. \end{aligned}$$

However, due to the fact that $4 \mid \frac{n}{2}$, it is evident that each fourth root of unity among ζ cannot satisfy $\zeta^{\frac{n}{2}} = -1$. Thus, provided $\zeta^{\frac{n}{2}} = -1$, $\zeta^4 \neq 1$ cannot be true, from which we immediately obtain $P(\zeta) \neq 0$, as desired.

Case $\zeta^{\frac{n}{2}} = 1$. Here, we swiftly obtain $\zeta^{\frac{n}{2}-j} = \frac{1}{\zeta^j}$ and $\frac{1}{\zeta^{\frac{n}{2}-j}} = \zeta^j$. This immediately implies

$$\zeta^j + \frac{1}{\zeta^j} + \zeta^{\frac{n}{2}-j} + \frac{1}{\zeta^{\frac{n}{2}-j}} = 2\left(\zeta^j + \frac{1}{\zeta^j}\right)$$

for any $j = \overline{1, t}$. By applying Equation (4.1), it is now clear that $P(\zeta) = 0$ is equivalent to

$$\begin{aligned}
& P(\zeta) = 0 \\
\iff \quad & \left(\zeta^{\frac{n}{4}+2} + \zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}} + \frac{1}{\zeta^{\frac{n}{4}+2}}\right) + 2\sum_{\substack{j=1,\\ j\neq t-2}}^{t}\left(\zeta^j + \frac{1}{\zeta^j}\right) = 0 \\
\iff \quad & \left(\zeta^{\frac{n}{4}+2} + \zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}} + \frac{1}{\zeta^{\frac{n}{4}+2}}\right) - 2 - 2\zeta^{t-2} - \frac{2}{\zeta^{t-2}} + 2\sum_{j=-t}^{t}\zeta^j = 0 \\
\iff \quad & \zeta^t\left(\zeta^{\frac{n}{4}+2} + \zeta^{\frac{n}{4}} + \frac{1}{\zeta^{\frac{n}{4}}} + \frac{1}{\zeta^{\frac{n}{4}+2}} - 2 - 2\zeta^{t-2} - \frac{2}{\zeta^{t-2}} + 2\sum_{j=-t}^{t}\zeta^j\right) = 0 \\
\iff \quad & \zeta^{t+\frac{n}{4}+2} + \zeta^{t+\frac{n}{4}} + \zeta^{t-\frac{n}{4}} + \zeta^{t-\frac{n}{4}-2} - 2\zeta^t - 2\zeta^{2t-2} - 2\zeta^2 + 2\sum_{j=0}^{2t}\zeta^j = 0.
\end{aligned}$$

Given the fact that

$$\begin{aligned}
(\zeta - 1)&\left(\zeta^{t+\frac{n}{4}+2} + \zeta^{t+\frac{n}{4}} + \zeta^{t-\frac{n}{4}} + \zeta^{t-\frac{n}{4}-2} - 2\zeta^t - 2\zeta^{2t-2} - 2\zeta^2 + 2\sum_{j=0}^{2t}\zeta^j\right) = \\
&= \zeta^{t+\frac{n}{4}+3} - \zeta^{t+\frac{n}{4}+2} + \zeta^{t+\frac{n}{4}+1} - \zeta^{t+\frac{n}{4}} + \zeta^{t-\frac{n}{4}+1} - \zeta^{t-\frac{n}{4}} + \zeta^{t-\frac{n}{4}-1} - \zeta^{t-\frac{n}{4}-2} \\
&\quad - 2\zeta^{t+1} + 2\zeta^t - 2\zeta^{2t-1} + 2\zeta^{2t-2} - 2\zeta^3 + 2\zeta^2 + 2\zeta^{2t+1} - 2 \\
&= \zeta^{t+\frac{n}{4}+3} - \zeta^{t+\frac{n}{4}+2} + 2\zeta^{t+\frac{n}{4}+1} - 2\zeta^{t+\frac{n}{4}} + \zeta^{t+\frac{n}{4}-1} - \zeta^{t+\frac{n}{4}-2} \\
&\quad + 2\zeta^{2t+1} - 2\zeta^{2t-1} + 2\zeta^{2t-2} - 2\zeta^{t+1} + 2\zeta^t - 2\zeta^3 + 2\zeta^2 - 2,
\end{aligned}$$

it is straightforward to see that $P(\zeta) = 0$ is further equivalent to

$$\begin{aligned}
&\zeta^{t+\frac{n}{4}+3} - \zeta^{t+\frac{n}{4}+2} + 2\zeta^{t+\frac{n}{4}+1} - 2\zeta^{t+\frac{n}{4}} + \zeta^{t+\frac{n}{4}-1} - \zeta^{t+\frac{n}{4}-2} \\
&\quad + 2\zeta^{2t+1} - 2\zeta^{2t-1} + 2\zeta^{2t-2} - 2\zeta^{t+1} + 2\zeta^t - 2\zeta^3 + 2\zeta^2 - 2 = 0.
\end{aligned} \tag{4.2}$$

We now divide the problem into two separate subcases depending on whether $\zeta^{\frac{n}{4}}$ is equal to 1 or -1.

Subcase $\zeta^{\frac{n}{4}} = 1$. In this subcase, it can be easily noticed from Equation (4.2) that $P(\zeta) = 0$ is equivalent to

$$\begin{aligned}
&\zeta^{t+3} - \zeta^{t+2} + 2\zeta^{t+1} - 2\zeta^t + \zeta^{t-1} - \zeta^{t-2} \\
&\quad + 2\zeta^{2t+1} - 2\zeta^{2t-1} + 2\zeta^{2t-2} - 2\zeta^{t+1} + 2\zeta^t - 2\zeta^3 + 2\zeta^2 - 2 = 0,
\end{aligned}$$

that is

$$2\zeta^{2t+1} - 2\zeta^{2t-1} + 2\zeta^{2t-2} + \zeta^{t+3} - \zeta^{t+2} + \zeta^{t-1} - \zeta^{t-2} - 2\zeta^3 + 2\zeta^2 - 2 = 0. \tag{4.3}$$

Suppose that $P(\zeta) = 0$ does hold for some n-th root of unity ζ different from 1 and -1. For $t = 4$, Equation (4.3) simplifies to

$$\begin{aligned} & 2\zeta^9 - \zeta^7 + \zeta^6 - \zeta^3 + \zeta^2 - 2 = 0 \\ \iff\quad & (\zeta - 1)(\zeta + 1)^2(2\zeta^6 - 2\zeta^5 + 3\zeta^4 - 2\zeta^3 + 3\zeta^2 - 2\zeta + 2) = 0 \\ \iff\quad & 2\zeta^6 - 2\zeta^5 + 3\zeta^4 - 2\zeta^3 + 3\zeta^2 - 2\zeta + 2 = 0. \end{aligned}$$

However, the polynomial $2x^6 - 2x^5 + 3x^4 - 2x^3 + 3x^2 - 2x + 2 \in \mathbb{Q}[x]$ has no roots of unity among its roots, as shown in Appendix D. Thus, we reach a contradiction. On the other hand, if $t \geq 6$, then Equation (4.3) is equivalent to $Q_t(\zeta) = 0$, which immediately implies that the polynomial $Q_t(x)$ must be divisible by a cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$. However, by virtue of Lemma 4.7, this is not possible, yielding a contradiction once more.

Subcase $\zeta^{\frac{n}{4}} = -1$. Here, implementing Equation (4.2) means that $P(\zeta) = 0$ is equivalent to

$$\begin{aligned} & -\zeta^{t+3} + \zeta^{t+2} - 2\zeta^{t+1} + 2\zeta^t - \zeta^{t-1} + \zeta^{t-2} \\ & \quad + 2\zeta^{2t+1} - 2\zeta^{2t-1} + 2\zeta^{2t-2} - 2\zeta^{t+1} + 2\zeta^t - 2\zeta^3 + 2\zeta^2 - 2 = 0, \end{aligned}$$

that is

$$\begin{aligned} & 2\zeta^{2t+1} - 2\zeta^{2t-1} + 2\zeta^{2t-2} - \zeta^{t+3} + \zeta^{t+2} \\ & \quad - 4\zeta^{t+1} + 4\zeta^t - \zeta^{t-1} + \zeta^{t-2} - 2\zeta^3 + 2\zeta^2 - 2 = 0. \end{aligned} \tag{4.4}$$

Now, suppose that $P(\zeta) = 0$ is true for some n-th root of unity $\zeta \neq 1, -1$. If $t = 4$, then Equation (4.4) transforms to

$$\begin{aligned} & 2\zeta^9 - 3\zeta^7 + 3\zeta^6 - 4\zeta^5 + 4\zeta^4 - 3\zeta^3 + 3\zeta^2 - 2 = 0 \\ \iff\quad & (\zeta - 1)(2\zeta^8 + 2\zeta^7 - \zeta^6 + 2\zeta^5 - 2\zeta^4 + 2\zeta^3 - \zeta^2 + 2\zeta + 2) = 0 \\ \iff\quad & 2\zeta^8 + 2\zeta^7 - \zeta^6 + 2\zeta^5 - 2\zeta^4 + 2\zeta^3 - \zeta^2 + 2\zeta + 2 = 0. \end{aligned}$$

However, the polynomial $2x^8 + 2x^7 - x^6 + 2x^5 - 2x^4 + 2x^3 - x^2 + 2x + 2 \in \mathbb{Q}[x]$ has no roots of unity among its roots, as demonstrated in Appendix D, hence $P(\zeta) = 0$ leads to a contradiction, as desired. On the other hand, whenever $t \geq 6$, Equation (4.4) becomes equivalent to $R_t(\zeta) = 0$, which further implies that $R_t(x)$ is divisible by some cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$. However, Lemma 4.8 dictates that this is impossible, hence we reach a contradiction yet again. □

5 Construction for $n \equiv_8 4 \wedge n \geq 4t + 12$

In this section we shall give a constructive proof of the existence of a $4t$-regular circulant nut graph of any order $n \in \mathbb{N}$ such that $n \geq 4t + 12$ and $n \equiv_8 4$, for any even $t \geq 4$. The proof will be given in the form of the next theorem.

Theorem 5.1. *For any even $t \geq 4$ and any $n \geq 4t + 12$ such that $n \equiv_8 4$, the circulant graph* $\mathrm{Circ}(n, S''_{t,n})$ *where*

$$S''_{t,n} = \{1, 2, \dots, t-1\} \cup \left\{\frac{n}{4} - 1, \frac{n}{4} + 3\right\} \cup \left\{\frac{n}{2} - (t-1), \dots, \frac{n}{2} - 2, \frac{n}{2} - 1\right\}$$

must be a $4t$-regular circulant nut graph of order n.

We will show that Theorem 5.1 holds by using a similar strategy as with Theorem 4.1. To begin with, it can be easily deduced that the set $S''_{t,n}$ is well defined, since $t - 1 < \frac{n}{4} - 1$ and $\frac{n}{4} + 3 < \frac{n}{2} - (t-1)$ for each even $t \geq 4$ and each $n \geq 4t + 12$ such that $n \equiv_8 4$. Besides that, the set $S''_{t,n}$ certainly contains equally many odd and even integers, all of which are positive and smaller than $\frac{n}{2}$. This means that, by implementing Lemma 2.1, we can prove Theorem 5.1 if we simply show that $P(x)$ has no n-th roots of unity among its roots, except potentially 1 or -1.

To begin with, we shall define the following two polynomials

$$\begin{aligned} U_t(x) &= 2x^{2t-1} + x^{t+3} - x^{t+2} + x^{t+1} - 3x^t + 3x^{t-1} - x^{t-2} + x^{t-3} - x^{t-4} - 2, \\ W_t(x) &= 2x^{2t-1} - x^{t+3} + x^{t+2} - x^{t+1} - x^t + x^{t-1} + x^{t-2} - x^{t-3} + x^{t-4} - 2, \end{aligned}$$

for each even $t \geq 4$. Now, for $t \geq 6$ we have $2t - 1 > t + 3$ and $t - 4 > 0$, while the equalities $2t - 1 = t + 3$ and $t - 4 = 0$ hold for $t = 4$. This means that the polynomials $U_t(x)$ and $W_t(x)$ have exactly 10 non-zero terms for any even $t \geq 6$, and 8 non-zero terms in case $t = 4$. We will use M_t to denote the set containing the powers of these terms, i.e.

$$M_t = \{0, t-4, t-3, t-2, t-1, t, t+1, t+2, t+3, 2t-1\},$$

for each even $t \geq 4$. We are now able to present the following lemma that demonstrates a property of M_t similar to the one displayed in Lemma 4.2 regarding the sets L'_t and L''_t.

Lemma 5.2. *For each even $t \geq 4$ and each $\beta \in \mathbb{N}$, $\beta \geq 6$, M_t must contain an element whose remainder modulo β is unique within the set.*

Proof. It is clear that the six consecutive integers $t-3, t-2, t-1, t, t+1, t+2$ must all have mutually distinct remainders modulo β for any $\beta \geq 6$. Regardless of whether $t = 4$ or $t \geq 6$, it is easy to establish that at least two of these integers must have a distinct remainder modulo β from all the elements of the set $\{0, t-4, t+3, 2t-1\}$. Hence, these integers must have a unique remainder modulo β within M_t and the lemma statement follows swiftly from here. $\square$

By relying on Lemma 5.2, we can now prove another lemma regarding the divisibility of $U_t(x)$ and $W_t(x)$ polynomials that is analogous to Lemma 4.3.

Lemma 5.3. *For any even $t \geq 4$ and each $\beta \geq 6$, neither $U_t(x)$ nor $W_t(x)$ can be divisible by a polynomial $V(x) \in \mathbb{Q}[x]$ with at least two non-zero terms such that all of its terms have powers divisible by β.*

Proof. This lemma can be proved in an absolutely analogous manner as Lemma 4.3. The only difference is that Lemma 5.2 is implemented in place of Lemma 4.2. For this reason, we choose to omit the proof details. $\square$

In a similar manner as done so in Section 4, we now investigate the divisibility of $U_t(x)$ and $W_t(x)$ polynomials by cyclotomic polynomials. By directly implementing Lemma 5.3, we are able to prove the following result.

Lemma 5.4. *For each even $t \geq 4$, if $\Phi_b(x) \mid U_t(x)$ or $\Phi_b(x) \mid W_t(x)$ hold for some $b \geq 3$, we then necessarily have*

- *$p^2 \nmid b$ for any prime number $p \geq 7$;*
- *$5^3 \nmid b$, $3^3 \nmid b$;*
- *if $2^2 \mid b$, then $b \in \{4, 8\}$.*

Proof. The proof of this lemma can be carried out in a manner that is almost entirely analogous to the proof of Lemma 4.4. To be more precise, the results $p^2 \nmid b$ for any prime $p \geq 7$, $5^3 \nmid b$ and $3^3 \nmid b$ can all be shown by simply implementing Lemma 5.3 together with the same idea used in the aforementioned proof of Lemma 4.4. Thus, we decide to leave out this part of the proof and focus solely on demonstrating $4 \mid b \implies b \in \{4, 8\}$. We will do this separately for $U_t(x)$ and $W_t(x)$ by splitting the remaining piece of the problem into two corresponding cases.

Case $U_t(x)$. For a given even $t \geq 4$, suppose that $\Phi_b(x) \mid U_t(x)$ for some $b \in \mathbb{N}$ such that $4 \mid b$. Since the integers $2t-1, t+3, t+1, t-1, t-3$ are odd, while $t+2, t, t-2, t-4, 0$ are even, it is easy to use the same logic displayed in the proof of Lemma 4.4 in order to deduce that

$$\begin{aligned}
&\Phi_b(x) \mid 2x^{2t-1} + x^{t+3} + x^{t+1} + 3x^{t-1} + x^{t-3},\\
&\Phi_b(x) \mid -x^{t+2} - 3x^t - x^{t-2} - x^{t-4} - 2.
\end{aligned}$$

If we denote

$$\begin{aligned}
A(x) &= 2x^{2t-1} + x^{t+3} + x^{t+1} + 3x^{t-1} + x^{t-3},\\
B(x) &= -x^{t+2} - 3x^t - x^{t-2} - x^{t-4} - 2,
\end{aligned}$$

we immediately obtain

$$\begin{aligned}
&\Phi_b(x) \mid (x^6 + 3x^4 + x^2 + 1)\, A(x) + 2x^{t+3}\, B(x)\\
\implies \quad &\Phi_b(x) \mid x^{t+9} + 4x^{t+7} + 7x^{t+5} + 8x^{t+3} + 7x^{t+1} + 4x^{t-1} + x^{t-3}\\
\implies \quad &\Phi_b(x) \mid x^{t-3}\, (x^2+1)^4 (x^4+1)\\
\implies \quad &\Phi_b(x) \mid (x^2+1)^4 (x^4+1).
\end{aligned}$$

From here, it follows that any b-th primitive root of unity must also be a root of at least one of the two polynomials $x^2 + 1, x^4 + 1 \in \mathbb{Q}[x]$. Hence, $b \in \{4, 8\}$.

Case $W_t(x)$. In this case, let $t \geq 4$ be some even integer and let $\Phi_b(x) \mid W_t(x)$ be true for some $b \in \mathbb{N}$ such that $4 \mid b$. In an absolutely analogous way as in the previous case, we conclude that

$$\begin{aligned}
&\Phi_b(x) \mid 2x^{2t-1} - x^{t+3} - x^{t+1} + x^{t-1} - x^{t-3},\\
&\Phi_b(x) \mid x^{t+2} - x^t + x^{t-2} + x^{t-4} - 2.
\end{aligned}$$

By denoting

$$A(x) = 2x^{2t-1} - x^{t+3} - x^{t+1} + x^{t-1} - x^{t-3},$$
$$B(x) = x^{t+2} - x^t + x^{t-2} + x^{t-4} - 2,$$

we swiftly get

$$\begin{aligned} & \Phi_b(x) \mid (-x^6 + x^4 - x^2 - 1)\, A(x) + 2x^{t+3}\, B(x) \\ \implies \quad & \Phi_b(x) \mid x^{t+9} - x^{t+5} - x^{t+1} + x^{t-3} \\ \implies \quad & \Phi_b(x) \mid x^{t-3}\,(x-1)^2(x+1)^2(x^2+1)^2(x^4+1) \\ \implies \quad & \Phi_b(x) \mid (x^2+1)^2(x^4+1). \end{aligned}$$

Thus, once again we see that any b-th primitive root of unity must also be a root of at least one of the two polynomials $x^2 + 1, x^4 + 1 \in \mathbb{Q}[x]$, from which we quickly obtain $b \in \{4, 8\}$, as desired. □

Lemma 5.4 tells us that only certain cyclotomic polynomials could divide the $U_t(x)$ and $W_t(x)$ polynomials. In fact, except potentially the four polynomials $\Phi_1(x), \Phi_2(x), \Phi_4(x), \Phi_8(x)$, no other cyclotomic polynomial can divide $U_t(x)$ or $W_t(x)$, for each even $t \geq 4$. We shall now prove this claim by strongly relying on the next two auxiliary lemmas that greatly resemble the previously disclosed Lemmas 4.5 and 4.6.

Lemma 5.5. *For each even $t \geq 4$ and each prime number $p \geq 11$, neither $U_t(x)$ nor $W_t(x)$ can be divisible by $\Phi_p(x)$ or $\Phi_{2p}(x)$.*

Proof. This lemma can be proved in an absolutely analogous manner as Lemma 4.5, the only difference being that Lemma 5.2 is used in place of Lemma 4.2. For this reason, we choose to omit the proof details. □

Lemma 5.6. *For each even $t \geq 4$, neither $U_t(x)$ nor $W_t(x)$ can be divisible by a cyclotomic polynomial $\Phi_b(x)$ where $b \geq 3$ is a positive integer such that*

- *it does not have any prime factors outside of the set $\{2, 3, 5, 7\}$;*
- *it does not contain all the prime factors from the set $\{3, 5, 7\}$;*
- $2^2 \nmid b$, $3^3 \nmid b$, $5^3 \nmid b$, $7^2 \nmid b$.

Proof. This lemma can be proved in an absolutely analogous manner as Lemma 4.6, hence we choose the leave out the proof details. The corresponding computational results can be found in Appendix C. □

We will now prove the previously mentioned statement regarding the divisibility of $U_t(x)$ and $W_t(x)$ polynomials by cyclotomic polynomials. In order to accomplish this, we shall strongly rely on Theorem 2.2 in a similar way as we have already done so while proving Lemmas 4.7 and 4.8.

Lemma 5.7. *For each even $t \geq 4$ and each positive integer $b \in \mathbb{N}$ such that $b \notin \{1, 2, 4, 8\}$, neither $U_t(x)$ nor $W_t(x)$ are divisible by $\Phi_b(x)$.*

Proof. Suppose that $\Phi_b(x) \mid U_t(x)$ or $\Phi_b(x) \mid W_t(x)$ for some even $t \geq 4$ and some $b \notin \{1, 2, 4, 8\}$. We will now finalize the proof via contradiction by splitting the problem into two separate cases depending on whether b is divisible by a prime number from the set $\{3, 5, 7\}$.

Case $3 \nmid b \wedge 5 \nmid b \wedge 7 \nmid b$. By implementing Lemma 5.4, it becomes evident that b has at least one prime factor greater than 7, given the fact that $b \notin \{1, 2, 4, 8\}$. Further on, we see that both $U_t(x)$ and $W_t(x)$ have at most 10 non-zero terms, which means that Theorem 2.2 can be applied to any prime $p \geq 11$ in an analogous manner as it was done in the proof of Lemma 4.7. By cancelling out every single prime divisor of b greater than 7 until exactly one is left, we conclude that

$$\Phi_{b'}(x) \mid U_t(x) \quad \vee \quad \Phi_{b'}(x) \mid W_t(x)$$

where b' has a single prime divisor greater than 7, and is potentially divisible by two as well, but not by four. By virtue of Lemma 5.4, it is not difficult to deduce that b' must either represent a prime number $p \geq 11$ or have the form $2p$ for some prime $p \geq 11$. Either way, Lemma 5.5 swiftly leads us to a contradiction.

Case $3 \mid b \vee 5 \mid b \vee 7 \mid b$. In this case, Theorem 2.2 can be applied in an analogous manner in order to cancel out any potential prime divisor of b greater than 7 until we obtain

$$\Phi_{b'}(x) \mid U_t(x) \quad \vee \quad \Phi_{b'}(x) \mid W_t(x)$$

for some $b' \in \mathbb{N}$ such that all of its prime factors belong to the set $\{2, 3, 5, 7\}$ and $3 \mid b' \vee 5 \mid b' \vee 7 \mid b'$. It is clear that $b' \geq 3$. By using Lemma 5.4, we now see that $7^2 \nmid b'$, $5^3 \nmid b'$, $3^3 \nmid b'$, as well as $2^2 \nmid b'$. By virtue of Theorem 2.2, we can suppose without loss of generality that b' is not divisible by all the elements from the set $\{3, 5, 7\}$, due to the fact that $(3 - 2) + (5 - 2) + (7 - 2) > 10 - 2$. Taking everything into consideration, we conclude that b' must satisfy the criteria given in Lemma 5.6, which immediately yields a contradiction once more. $\square$

We shall now implement Lemma 5.7 in order to finalize the proof of Theorem 5.1 in a similar manner as we have done so with Theorem 4.1.

Proof of Theorem 5.1. Equation (2.1) directly gives us

$$P(\zeta) = \left(\zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}}\right) + \left(\zeta^{\frac{n}{4}+3} + \frac{1}{\zeta^{\frac{n}{4}+3}}\right) + \sum_{j=1}^{t-1} \left(\zeta^j + \frac{1}{\zeta^j}\right) + \sum_{j=\frac{n}{2}-t+1}^{\frac{n}{2}-1} \left(\zeta^j + \frac{1}{\zeta^j}\right),$$

where ζ is an arbitrarily chosen n-th root of unity different from 1 and -1. From here, we immediately get

$$P(\zeta) = \left(\zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}}\right) + \left(\zeta^{\frac{n}{4}+3} + \frac{1}{\zeta^{\frac{n}{4}+3}}\right) + \sum_{j=1}^{t-1} \left(\zeta^j + \frac{1}{\zeta^j} + \zeta^{\frac{n}{2}-j} + \frac{1}{\zeta^{\frac{n}{2}-j}}\right). \tag{5.1}$$

We now divide the problem into two cases depending on whether $\zeta^{\frac{n}{2}}$ is equal to 1 or -1. We shall finalize the proof by showing that $P(\zeta) \neq 0$ is certainly true in both cases.

Case $\zeta^{\frac{n}{2}} = -1$. It is obvious that $\zeta^{\frac{n}{2}-j} = -\frac{1}{\zeta^j}$ and $\frac{1}{\zeta^{\frac{n}{2}-j}} = -\zeta^j$, from which we get

$$\zeta^j + \frac{1}{\zeta^j} + \zeta^{\frac{n}{2}-j} + \frac{1}{\zeta^{\frac{n}{2}-j}} = 0$$

for any $j = \overline{1, t-1}$. For this reason, Equation (5.1) simplifies to

$$P(\zeta) = \zeta^{\frac{n}{4}+3} + \zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}} + \frac{1}{\zeta^{\frac{n}{4}+3}}.$$

The condition $P(\zeta) = 0$ now becomes equivalent to

$$\begin{aligned} & & P(\zeta) &= 0 \\ \iff & & \zeta^{\frac{n}{4}+3}\left(\zeta^{\frac{n}{4}+3} + \zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}} + \frac{1}{\zeta^{\frac{n}{4}+3}}\right) &= 0 \\ \iff & & \zeta^{\frac{n}{2}+6} + \zeta^{\frac{n}{2}+2} + \zeta^4 + 1 &= 0 \\ \iff & & -\zeta^6 - \zeta^2 + \zeta^4 + 1 &= 0 \\ \iff & & -(\zeta-1)(\zeta+1)(\zeta^4+1) &= 0 \\ \iff & & \zeta^4 &= -1. \end{aligned}$$

Thus, $P(\zeta) = 0$ holds if and only if ζ is a primitive eighth root of unity. However, $8 \nmid n$, hence no n-th root of unity can be a primitive eighth root of unity. Thus, $P(\zeta) \neq 0$, as desired.

Case $\zeta^{\frac{n}{2}} = 1$. In this case, it is clear that $\zeta^{\frac{n}{2}-j} = \frac{1}{\zeta^j}$ and $\frac{1}{\zeta^{\frac{n}{2}-j}} = \zeta^j$, which immediately leads us to

$$\zeta^j + \frac{1}{\zeta^j} + \zeta^{\frac{n}{2}-j} + \frac{1}{\zeta^{\frac{n}{2}-j}} = 2\left(\zeta^j + \frac{1}{\zeta^j}\right)$$

for any $j = \overline{1, t-1}$. Bearing this in mind, it is straightforward to see that

$$\begin{aligned} & & P(\zeta) &= 0 \\ \iff & & \left(\zeta^{\frac{n}{4}+3} + \zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}} + \frac{1}{\zeta^{\frac{n}{4}+3}}\right) + 2\sum_{j=1}^{t-1}\left(\zeta^j + \frac{1}{\zeta^j}\right) &= 0 \\ \iff & & \left(\zeta^{\frac{n}{4}+3} + \zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}} + \frac{1}{\zeta^{\frac{n}{4}+3}}\right) - 2 + 2\sum_{j=-t+1}^{t-1}\zeta^j &= 0 \\ \iff & & \zeta^{t-1}\left(\zeta^{\frac{n}{4}+3} + \zeta^{\frac{n}{4}-1} + \frac{1}{\zeta^{\frac{n}{4}-1}} + \frac{1}{\zeta^{\frac{n}{4}+3}} - 2 + 2\sum_{j=-t+1}^{t-1}\zeta^j\right) &= 0 \\ \iff & & \zeta^{t+\frac{n}{4}+2} + \zeta^{t+\frac{n}{4}-2} + \zeta^{t-\frac{n}{4}} + \zeta^{t-\frac{n}{4}-4} - 2\zeta^{t-1} + 2\sum_{j=0}^{2t-2}\zeta^j &= 0 \\ \iff & (\zeta-1) & \left(\zeta^{t+\frac{n}{4}+2} + \zeta^{t+\frac{n}{4}-2} + \zeta^{t-\frac{n}{4}} + \zeta^{t-\frac{n}{4}-4} - 2\zeta^{t-1} + 2\sum_{j=0}^{2t-2}\zeta^j\right) &= 0, \end{aligned}$$

which finally means that $P(\zeta) = 0$ must be equivalent to

$$\begin{aligned}\zeta^{t+\frac{n}{4}+3} - \zeta^{t+\frac{n}{4}+2} + \zeta^{t+\frac{n}{4}-1} - \zeta^{t+\frac{n}{4}-2} + \zeta^{t-\frac{n}{4}+1} - \zeta^{t-\frac{n}{4}} + \zeta^{t-\frac{n}{4}-3} - \zeta^{t-\frac{n}{4}-4} \\ + 2\zeta^{2t-1} - 2\zeta^{t} + 2\zeta^{t-1} - 2 = 0.\end{aligned} \tag{5.2}$$

We now split the problem into two separate subcases depending on whether $\zeta^{\frac{n}{4}}$ is equal to 1 or -1.

Subcase $\zeta^{\frac{n}{4}} = 1$. In this subcase, the implementation of Equation (5.2) directly gives that $P(\zeta) = 0$ is further equivalent to

$$\begin{aligned}\zeta^{t+3} - \zeta^{t+2} + \zeta^{t-1} - \zeta^{t-2} + \zeta^{t+1} - \zeta^{t} + \zeta^{t-3} - \zeta^{t-4} \\ + 2\zeta^{2t-1} - 2\zeta^{t} + 2\zeta^{t-1} - 2 = 0,\end{aligned}$$

that is

$$2\zeta^{2t-1} + \zeta^{t+3} - \zeta^{t+2} + \zeta^{t+1} - 3\zeta^{t} + 3\zeta^{t-1} - \zeta^{t-2} + \zeta^{t-3} - \zeta^{t-4} - 2 = 0.$$

In other words, $P(\zeta) = 0$ is equivalent to ζ being a root of $U_t(x)$. Now, we know that $\zeta \neq 1, -1$ and that ζ cannot be a primitive eighth root of unity, as discussed earlier. On top of that, $\zeta \neq i, -i$ given the fact that $\frac{n}{2} \equiv_4 2$, hence $i^{\frac{n}{2}} = (-i)^{\frac{n}{2}} = -1$. Bearing this in mind, it is clear that if were $P(\zeta) = 0$ were to hold, then $U_t(x)$ would be divisible by some cyclotomic polynomial $\Phi_b(x)$ where $b \notin \{1, 2, 4, 8\}$. However, this is not possible according to Lemma 5.7. For this reason, $P(\zeta) \neq 0$ must hold.

Subcase $\zeta^{\frac{n}{4}} = -1$. In this scenario, Equation (5.2) can be quickly simplified to

$$\begin{aligned}-\zeta^{t+3} + \zeta^{t+2} - \zeta^{t-1} + \zeta^{t-2} - \zeta^{t+1} + \zeta^{t} - \zeta^{t-3} + \zeta^{t-4} \\ + 2\zeta^{2t-1} - 2\zeta^{t} + 2\zeta^{t-1} - 2 = 0,\end{aligned}$$

that is

$$2\zeta^{2t-1} - \zeta^{t+3} + \zeta^{t+2} - \zeta^{t+1} - \zeta^{t} + \zeta^{t-1} + \zeta^{t-2} - \zeta^{t-3} + \zeta^{t-4} - 2 = 0.$$

Thus, we get that $P(\zeta) = 0$ is equivalent to ζ being a root of $W_t(x)$. By using the analogous logic as in the previous subcase, it is easy to establish that $P(\zeta) = 0$ would imply that $W_t(x)$ is divisible by some cyclotomic polynomial $\Phi_b(x)$ where $b \notin \{1, 2, 4, 8\}$, which is again impossible due to Lemma 5.7. Hence, $P(\zeta) = 0$ cannot be true, which completes the proof. □

6 Conclusion

Theorem 1.8 provides the full answer to Question 1.4 posed by the circulant nut graph order–degree existence problem. It is evident that there exists a clear and rich pattern that the orders and degrees of circulant nut graphs must follow, with the sole exception being the case $(n, d) = (16, 8)$. Bearing this in mind, it now becomes possible to explore other types of nut graphs more easily.

For example, it is clear that each circulant graph is necessarily a Cayley graph, which is, in turn, surely a vertex-transitive graph. For this reason, if we are trying to investigate the existence of Cayley nut graphs or vertex-transitive nut graphs, Theorem 1.8 provides a solid starting point. Taking all the aforementioned facts into consideration, we are able to disclose the following corollary.

Corollary 6.1. *Let $d \in \mathbb{N}$ be such that $4 \mid d$, and let $n \in \mathbb{N}$ be such that $2 \mid n$ and*

- $n \geq d + 4$ *if* $8 \nmid d$;
- $n \geq d + 6$ *if* $8 \mid d$;
- $(n, d) \neq (16, 8)$.

There necessarily exists a d-regular Cayley nut graph of order n, as well as a d-regular vertex-transitive nut graph of order n.

It becomes clear that Corollary 6.1 gives a partial answer to Question 1.1. One of the possible ways of extending the research concerning the vertex-transitive nut graphs is by providing a full answer to the aforementioned question. Another possibility is to consider the order–degree existence problem regarding the Cayley nut graphs, whose conditions are also less restrictive than those corresponding to the circulant nut graphs. Bearing this in mind, we end the paper with the following open problem.

Problem 6.2. What are all the pairs (n, d) for which there exists a d-regular Cayley nut graph of order n?

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Appendices

A Inspection for $\Phi_b(x) \nmid Q_t(x)$

In this appendix section, we will disclose the computational results that demonstrate $\Phi_b(x) \nmid Q_t(x)$ for all the required values of $b \geq 3$, as stated in Lemma 4.6. First of all, the set of all such values of b can be obtained in a plethora of ways. For example, the following short Python script can be used.

```
import numpy as np


def main():
    part_1 = np.multiply.outer([1, 2], [1, 3, 9, 27]).reshape(-1)
    part_2 = np.multiply.outer([1, 5, 25], [1, 7, 49]).reshape(-1)

    all_of_them = np.multiply.outer(part_1, part_2).reshape(-1)
    all_of_them.sort()
    all_of_them = all_of_them.tolist()

    result = list(filter(lambda item: item % 105 != 0, all_of_them))
    result = list(filter(lambda item: item >= 3, result))

    print(len(result))
    print(result)


if __name__ == "__main__":
    main()
```

The said script quickly finds that there exist exactly 46 values of b that satisfy the given criteria:

$$\{3, 5, 6, 7, 9, 10, 14, 15, 18, 21, 25, 27, 30, 35, 42, 45, 49, 50, 54, 63,$$
$$70, 75, 90, 98, 126, 135, 147, 150, 175, 189, 225, 245, 270, 294,$$
$$350, 378, 441, 450, 490, 675, 882, 1225, 1323, 1350, 2450, 2646\}.$$

For each of these values, it can be determined that $\Phi_b(x) \nmid Q_t^{\text{mod } b}(x)$ for any possible remainder $t \bmod b$. In order to achieve this, we can use, for example, the following Mathematica command.

```
Min[Table[
  Min[Table[
    Length[CoefficientRules[
      PolynomialRemainder[
       2 x^Mod[2 t + 1, b] - 2 x^Mod[2 t - 1, b] +
        2 x^Mod[2 t - 2, b] + x^Mod[t + 3, b] - x^Mod[t + 2, b] +
        x^Mod[t - 1, b] - x^Mod[t - 2, b] - 2 x^3 + 2 x^2 - 2,
```

```
      Cyclotomic[b, x], x]]], {t, 0, b - 1}]], {b, {3, 5, 6, 7, 9,
    10, 14, 15, 18, 21, 25, 27, 30, 35, 42, 45, 49, 50, 54, 63, 70,
    75, 90, 98, 126, 135, 147, 150, 175, 189, 225, 245, 270, 294, 350,
     378, 441, 450, 490, 675, 882, 1225, 1323, 1350, 2450, 2646}}]]
```

This command yields the minimum possible number of non-zero terms that the polynomial $Q_t^{\text{mod } b}(x) \bmod \Phi_b(x)$ can have, as b ranges through all the necessary values and $t \bmod b$ varies through all the possible remainders. It can be promptly checked that this number is equal to one, which immediately means that the remainder $Q_t^{\text{mod } b}(x) \bmod \Phi_b(x)$ is never equal to the zero polynomial. From here, we quickly obtain our desired result.

B Inspection for $\Phi_b(x) \nmid R_t(x)$

Here, we elaborate the computational results showing that $\Phi_b(x) \nmid R_t(x)$ for all the values of $b \geq 3$ given in Lemma 4.6. For starters, the set of all such values of b can be computed, for example, by using the following Python script.

```python
import numpy as np


def main():
    part_1 = np.multiply.outer([1, 2], [1, 7, 11, 77]).reshape(-1)
    part_2 = np.multiply.outer([1, 3, 9], [1, 5, 25]).reshape(-1)

    all_of_them = np.multiply.outer(part_1, part_2).reshape(-1)
    all_of_them.sort()
    all_of_them = all_of_them.tolist()

    result = list(filter(lambda item: item % 77 != 0, all_of_them))
    result = list(filter(lambda item: item % 55 != 0, result))
    result = list(filter(lambda item: item >= 3, result))

    print(len(result))
    print(result)


if __name__ == "__main__":
    main()
```

The Python script easily concludes that there exist exactly 40 values of b that satisfy the given criteria:

$$\{3, 5, 6, 7, 9, 10, 11, 14, 15, 18, 21, 22, 25, 30, 33, 35, 42,\\ 45, 50, 63, 66, 70, 75, 90, 99, 105, 126, 150, 175, 198,\\ 210, 225, 315, 350, 450, 525, 630, 1050, 1575, 3150\}.$$

For each of these values, it can be determined that $\Phi_b(x) \nmid R_t^{\text{mod } b}(x)$ regardless of what the remainder $t \bmod b$ is. This can be done, for example, by using the next Mathematica command.

```
Min[Table[
  Min[Table[
    Length[CoefficientRules[
```

```
      PolynomialRemainder[
       2 x^Mod[2 t + 1, b] - 2 x^Mod[2 t - 1, b] +
        2 x^Mod[2 t - 2, b] - x^Mod[t + 3, b] + x^Mod[t + 2, b] -
        4 x^Mod[t + 1, b] + 4 x^Mod[t, b] - x^Mod[t - 1, b] +
        x^Mod[t - 2, b] - 2 x^3 + 2 x^2 - 2, Cyclotomic[b, x],
       x]]], {t, 0, b - 1}]], {b, {3, 5, 6, 7, 9, 10, 11, 14, 15, 18,
    21, 22, 25, 30, 33, 35, 42, 45, 50, 63, 66, 70, 75, 90, 99, 105,
    126, 150, 175, 198, 210, 225, 315, 350, 450, 525, 630, 1050, 1575,
     3150}}]]
```

The said command computes the minimum possible number of non-zero terms that the polynomial $R_t^{\bmod b}(x) \bmod \Phi_b(x)$ can have, as b ranges through all the required values and $t \bmod b$ varies through all the possible remainders. The computation output is equal to one, hence we obtain our desired result in the same way as in Appendix A.

C Inspection for $\Phi_b(x) \nmid U_t(x)$ and $\Phi_b(x) \nmid W_t(x)$

We can use an analogous mechanism to disclose the computational results that demonstrate $\Phi_b(x) \nmid U_t(x)$, as well as $\Phi_b(x) \nmid W_t(x)$, for all the values of $b \geq 3$ stated in Lemma 5.6. The set of all the required values of b can be determined, for example, by using the following Python script.

```
import numpy as np


def main():
    part_1 = np.multiply.outer([1, 2], [1, 3, 9]).reshape(-1)
    part_2 = np.multiply.outer([1, 5, 25], [1, 7]).reshape(-1)

    all_of_them = np.multiply.outer(part_1, part_2).reshape(-1)
    all_of_them.sort()
    all_of_them = all_of_them.tolist()

    result = list(filter(lambda item: item % 105 != 0, all_of_them))
    result = list(filter(lambda item: item >= 3, result))

    print(len(result))
    print(result)


if __name__ == "__main__":
    main()
```

The given Python script finds that there exist exactly 26 values of b that satisfy the given criteria:

$$\{3, 5, 6, 7, 9, 10, 14, 15, 18, 21, 25, 30, 35, 42, 45,$$
$$50, 63, 70, 75, 90, 126, 150, 175, 225, 350, 450\}.$$

For each of these values, it can be promptly shown that $\Phi_b(x) \nmid U_t^{\bmod b}(x)$ and $\Phi_b(x) \nmid W_t^{\bmod b}(x)$ for any possible remainder $t \bmod b$. This can be accomplished, for example, by using the following two Mathematica commands.

```
Min[Table[
  Min[Table[
    Length[CoefficientRules[
      PolynomialRemainder[
        2 x^Mod[2 t - 1, b] + x^Mod[t + 3, b] - x^Mod[t + 2, b] +
         x^Mod[t + 1, b] - 3 x^Mod[t, b] + 3 x^Mod[t - 1, b] -
         x^Mod[t - 2, b] + x^Mod[t - 3, b] - x^Mod[t - 4, b] - 2,
        Cyclotomic[b, x], x]]], {t, 0, b - 1}]], {b, {3, 5, 6, 7, 9,
    10, 14, 15, 18, 21, 25, 30, 35, 42, 45, 50, 63, 70, 75, 90, 126,
    150, 175, 225, 350, 450}}]]
```

```
Min[Table[
  Min[Table[
    Length[CoefficientRules[
      PolynomialRemainder[
        2 x^Mod[2 t - 1, b] - x^Mod[t + 3, b] + x^Mod[t + 2, b] -
         x^Mod[t + 1, b] - x^Mod[t, b] + x^Mod[t - 1, b] +
         x^Mod[t - 2, b] - x^Mod[t - 3, b] + x^Mod[t - 4, b] - 2,
        Cyclotomic[b, x], x]]], {t, 0, b - 1}]], {b, {3, 5, 6, 7, 9,
    10, 14, 15, 18, 21, 25, 30, 35, 42, 45, 50, 63, 70, 75, 90, 126,
    150, 175, 225, 350, 450}}]]
```

The given two commands yield the minimum possible number of non-zero terms that the polynomials ${U_t}^{\bmod b}(x)$ and ${W_t}^{\bmod b}(x)$ can have, respectively, as b ranges through all the required values and $t \bmod b$ takes on any possible value. Both computation outputs are equal to one, which means that none of the aforementioned remainders are equal to the zero polynomial, as desired.

D Roots of certain polynomials

In this appendix section, we will demonstrate that none of the following polynomials

$$\begin{aligned}
Z_1(x) &= x^4 + 2x^3 - 2x^2 + 2x + 1,\\
Z_2(x) &= x^6 - x^4 + 2x^3 - x^2 + 1,\\
Z_3(x) &= x^6 - 2x^5 + 3x^4 - 2x^3 + 3x^2 - 2x + 1,\\
Z_4(x) &= 3x^4 - 2x^2 + 3,\\
Z_5(x) &= x^2 - 2x - 1,\\
Z_6(x) &= x^2 + 2x - 1,\\
Z_7(x) &= 3x^4 + 2x^2 + 3,\\
Z_8(x) &= 2x^6 - 2x^5 + 3x^4 - 2x^3 + 3x^2 - 2x + 2,\\
Z_9(x) &= 2x^8 + 2x^7 - x^6 + 2x^5 - 2x^4 + 2x^3 - x^2 + 2x + 2,
\end{aligned}$$

contain a root of unity among its roots. This can be swiftly achieved by simply showing that none of them are divisible by any cyclotomic polynomial $\Phi_b(x)$. In fact, it is clear that, for each $j = \overline{1, 9}$, the polynomial $Z_j(x)$ cannot be divisible by a $\Phi_b(x)$ such that $\deg \Phi_b > \deg Z_j$. Thus, in order to prove the desired result, it is sufficient to show that each given polynomial is not divisible by the corresponding cyclotomic polynomials whose degrees do not exceed its own. This is trivial to accomplish via computer.

For starters, it is not difficult to determine all 18 cyclotomic polynomials whose degree is not above 8:

$$\begin{aligned}
\Phi_1(x) &= x - 1, & \Phi_7(x) &= x^6 + x^5 + x^4 + x^3 + x^2 + x + 1,\\
\Phi_2(x) &= x + 1, & \Phi_9(x) &= x^6 + x^3 + 1,\\
\Phi_3(x) &= x^2 + x + 1, & \Phi_{14}(x) &= x^6 - x^5 + x^4 - x^3 + x^2 - x + 1,\\
\Phi_4(x) &= x^2 + 1, & \Phi_{18}(x) &= x^6 - x^3 + 1,\\
\Phi_6(x) &= x^2 - x + 1, & \Phi_{15}(x) &= x^8 - x^7 + x^5 - x^4 + x^3 - x + 1,\\
\Phi_5(x) &= x^4 + x^3 + x^2 + x + 1, & \Phi_{16}(x) &= x^8 + 1,\\
\Phi_8(x) &= x^4 + 1, & \Phi_{20}(x) &= x^8 - x^6 + x^4 - x^2 + 1,\\
\Phi_{10}(x) &= x^4 - x^3 + x^2 - x + 1, & \Phi_{24}(x) &= x^8 - x^4 + 1,\\
\Phi_{12}(x) &= x^4 - x^2 + 1, & \Phi_{30}(x) &= x^8 + x^7 - x^5 - x^4 - x^3 + x + 1.
\end{aligned}$$

The necessary computational results can be found on Tables 2, 3, 4 and 5. The disclosed remainders clearly indicate that no given polynomial can be divisible by any cyclotomic polynomial of interest, as desired.

b	$Z_5(x) \bmod \Phi_b(x)$	$Z_6(x) \bmod \Phi_b(x)$
1	-2	2
2	2	-2
3	$-2-3x$	$-2+x$
4	$-2-2x$	$-2+2x$
6	$-2-x$	$-2+3x$

Table 2: The required remainders of $Z_5(x)$ and $Z_6(x)$.

b	$Z_1(x) \bmod \Phi_b(x)$	$Z_4(x) \bmod \Phi_b(x)$	$Z_7(x) \bmod \Phi_b(x)$
1	4	4	8
2	-4	4	8
3	$5+5x$	$5+5x$	$1+x$
4	4	8	4
6	$1-x$	$5-5x$	$1-x$
5	$x-3x^2+x^3$	$-3x-5x^2-3x^3$	$-3x-x^2-3x^3$
8	$2x-2x^2+2x^3$	$-2x^2$	$2x^2$
10	$3x-3x^2+3x^3$	$3x-5x^2+3x^3$	$3x-x^2+3x^3$
12	$2x-x^2+2x^3$	x^2	$5x^2$

Table 3: The required remainders of $Z_1(x)$, $Z_4(x)$ and $Z_7(x)$.

b	$Z_2(x) \bmod \Phi_b(x)$	$Z_3(x) \bmod \Phi_b(x)$	$Z_8(x) \bmod \Phi_b(x)$
1	2	2	4
2	-2	14	16
3	5	-1	1
4	$-2x$	$-2x$	$-2x$
6	1	-1	1
5	$2 + 2x + 3x^3$	$-4 - 4x - 5x^3$	$-3 - 3x - 5x^3$
8	$2 - 2x^2 + 2x^3$	$-2 + 2x^2 - 2x^3$	$-1 + x^2 - 2x^3$
10	$2 - 2x + x^3$	x^3	$1 - x + x^3$
12	$1 - 2x^2 + 2x^3$	$-3 + 6x^2 - 4x^3$	$-3 + 6x^2 - 4x^3$
7	$-x - 2x^2 + x^3 - 2x^4 - x^5$	$-3x + 2x^2 - 3x^3 + 2x^4 - 3x^5$	$-4x + x^2 - 4x^3 + x^4 - 4x^5$
9	$-x^2 + x^3 - x^4$	$-2x + 3x^2 - 3x^3 + 3x^4 - 2x^5$	$-2x + 3x^2 - 4x^3 + 3x^4 - 2x^5$
14	$x - 2x^2 + 3x^3 - 2x^4 + x^5$	$-x + 2x^2 - x^3 + 2x^4 - x^5$	$x^2 + x^4$
18	$-x^2 + 3x^3 - x^4$	$-2x + 3x^2 - x^3 + 3x^4 - 2x^5$	$-2x + 3x^2 + 3x^4 - 2x^5$

Table 4: The required remainders of $Z_2(x)$, $Z_3(x)$ and $Z_8(x)$.

b	$Z_9(x) \bmod \Phi_b(x)$
1	8
2	-8
3	$-x$
4	4
6	$5x$
5	$6 + 3x + 3x^2 + 6x^3$
8	6
10	$2 + x - x^2 - 2x^3$
12	$5 - 2x - 5x^2 + 4x^3$
7	$5 + 5x + 3x^3 - x^4 + 3x^5$
9	$3 - 3x^2 + 3x^3 - 4x^4$
14	$1 - x + x^3 - x^4 + x^5$
18	$3 - 3x^2 + x^3 + 4x^5$
15	$4x - x^2 - x^6 + 4x^7$
16	$2x - x^2 + 2x^3 - 2x^4 + 2x^5 - x^6 + 2x^7$
20	$2x + x^2 + 2x^3 - 4x^4 + 2x^5 + x^6 + 2x^7$
24	$2x - x^2 + 2x^3 + 2x^5 - x^6 + 2x^7$
30	$-x^2 + 4x^3 + 4x^5 - x^6$

Table 5: The required remainders of $Z_9(x)$.

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$\mathbb{Z}_3^8$ is not a CI-group

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Abstract

A Cayley graph $\mathrm{Cay}(G, S)$ has the CI (Cayley Isomorphism) property if for every isomorphic graph $\mathrm{Cay}(G, T)$, there is a group automorphism α of G such that $S^\alpha = T$. The DCI (Directed Cayley Isomorphism) property is defined analogously on digraphs. A group G is a CI-group if every Cayley graph on G has the CI property, and is a DCI-group if every Cayley digraph on G has the DCI property. Since a graph is a special type of digraph, this means that every DCI-group is a CI-group, and if a group is not a CI-group then it is not a DCI-group.

In 2009, Spiga showed that $\mathbb{Z}_3^8$ is not a DCI-group, by producing a digraph that does not have the DCI property. He also showed that $\mathbb{Z}_3^5$ is a DCI-group (and therefore also a CI-group). Until recently the question of whether there are elementary abelian 3-groups that are not CI-groups remained open. In a recent preprint with Dave Witte Morris, we showed that $\mathbb{Z}_3^{10}$ is not a CI-group. In this paper we show that with slight modifications, the underlying undirected graph of order 3^8 described by Spiga is does not have the CI property, so $\mathbb{Z}_3^8$ is not a CI-group.

Keywords: Cayley graphs, elementary abelian groups, CI graphs, CI groups, isomorphism.

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1 Introduction

Let G be a group, and $S \subseteq G$. The Cayley digraph $\mathrm{Cay}(G, S)$ is the digraph whose vertices are the elements of the group G, with an arc from g to h if and only if $h - g \in S$ (we are using additive notation in this paper, but Cayley graphs can be defined similarly on nonabelian groups). If $S = -S$ then for any arc from g to h there is a paired arc from h to g; we replace these two arcs with a single undirected edge and call the resulting structure

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the Cayley graph $\mathrm{Cay}(G, S)$. It is well-known that Γ is isomorphic to a Cayley graph on G if and only if $\mathrm{Aut}(\Gamma)$ has a regular subgroup isomorphic to G. Typically we abuse notation by ignoring the isomorphism and simply saying that Γ is a Cayley graph on G in this event.

The Cayley graph $\mathrm{Cay}(G, S)$ has the CI (Cayley Isomorphism) property if for every isomorphic graph $\mathrm{Cay}(G, T)$, there is a group automorphism α of G such that $S^\alpha = T$. Note that whenever α is an automorphism of G, it induces a graph isomorphism from $\mathrm{Cay}(G, S)$ to $\mathrm{Cay}(G, S^\alpha)$. This means that essentially, a Cayley graph has the CI property if all of its isomorphisms to other Cayley graphs on the same group have algebraic justifications: group automorphisms that induce not necessarily that particular isomorphism, but an isomorphism to the same graph. The CI problem is the problem of determining which graphs have the CI property. The DCI (Directed Cayley Isomorphism) property and the DCI problem are defined analogously on digraphs.

Although work on the (D)CI problem dates back at least to 1967 [1], the standard terminology was coined and fundamental results about the problem were proved by Babai in [2]. A group G is a CI-group if every Cayley graph on G has the CI property, and is a DCI-group if every Cayley digraph on G has the DCI property. Since a graph is a special type of digraph, this means that every DCI-group is a CI-group, and if a group is not a CI-group then it is not a DCI-group, but there are well-known examples of groups that are CI-groups but not DCI-groups. For example, Muzychuk [8, 9] characterised cyclic groups according to which are DCI and which are CI: the cyclic group of order n is a DCI-group if and only if $n \in \{k, 2k, 4k\}$ where k is odd and square-free. It is a CI-group if and only if it is a DCI-group, or $n \in \{8, 9, 18\}$.

Once cyclic groups were completely understood with respect to the CI and DCI problems, elementary abelian groups became a natural class of groups to consider. This class of groups has become even more fundamentally important in understanding the (D)CI problem over time, since the combined work of a number of researchers has shown that any (D)CI group is a direct product of up to three factors, each of which is either small, abelian, or the semidirect product of an abelian group with a small cyclic group. (See for example [3, 4, 6], although Math Reviewers have noted some errors in the statements of the relevant results.)

In a 2003 paper, Muzychuk [10] proved that an elementary abelian group of sufficiently high rank is not a DCI-group. He did not consider the undirected problem in that paper, and the rank he achieved for an elementary abelian p-group was $2p - 1 + \binom{2p-1}{p}$. Spiga [13] improved this rank to $4p - 2$. Both of these papers may have introduced some confusion into the problem as they talk about the CI problem and property but use directed graphs throughout, so in fact prove that an elementary abelian p-group of sufficiently high rank is not a DCI-group although the statement of their results say that this is not a CI-group. Somlai [12] addressed this issue, and improved the previous results by showing that an elementary abelian p-group of rank at least $2p + 3$ is not a CI-group when $p \geq 5$. He did also prove a similar result when $p = 3$ but in this case was only able to show that the group is not a DCI-group, and noted that the problem of the existence of a non-CI elementary abelian 3-group remained open. For the $p = 3$ case, Spiga [14] had also previously shown that $\mathbb{Z}_3^8$ is not a DCI-group, by producing a digraph that does not have the DCI property.

On the other side of things, the best known result [5] shows that $\mathbb{Z}_p^5$ is a DCI-group. It is known [11] that $\mathbb{Z}_2^6$ is not a CI-group, but there remains a gap in our knowledge for every prime $p > 2$.

In a recent preprint with Dave Witte Morris [7], we show that $\mathbb{Z}_3^{10}$ is not a CI-group, and more generally demonstrate a method for using non-DCI digraphs to construct non-CI graphs whose order is a fairly small multiple of the order of the original digraph, and thereby find groups that are not CI-groups.

In this paper we show that a slightly modified version of the underlying undirected graph of the non-CI digraph of order 3^8 described by Spiga in [14] does not have the CI property, so $\mathbb{Z}_3^8$ is not a CI-group.

2 Two isomorphic Cayley graphs

Let $\{w_1, w_2, w_3, v_1, v_2, v_3, v_4, v_5\}$ be a generating set for $G \cong \mathbb{Z}_3^8$. We define the following sets:

$$\begin{aligned}
S_{0,0,0} &= \{v_1 - v_5, v_2 + v_3 - v_4 + v_5, v_3 - v_4 + v_5, v_4 + v_5, v_5\}\\
S_{1,0,0} &= \{w_1 + av_1 + bv_2 + cv_5 : a, b, c \in \mathbb{Z}_3\}\\
S_{0,1,0} &= \{w_2 + av_1 + bv_3 + cv_4 + dv_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{0,0,1} &= \{w_3 + av_2 + bv_3 + cv_4 + dv_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{1,1,0} &= \{w_1 + w_2 + av_1 + bv_2 + cv_3 + bv_4 + dv_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{1,0,1} &= \{w_1 + w_3 + av_1 + bv_2 + av_3 + cv_4 + dv_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{0,1,1} &= \{w_2 + w_3 + av_1 + bv_2 + cv_3 + dv_4 - (a + b)v_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{1,1,1} &= \{w_1 + w_2 + w_3 + av_1 + bv_2 + cv_3 + dv_4 + (-a - b + c + d)v_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{2,1,1} &= \{2w_1 + w_2 + w_3 + av_1 + bv_2 + cv_3 + dv_4 - (a + b + c + d)v_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{1,2,1} &= \{w_1 + 2w_2 + w_3 + av_1 + bv_2 + cv_3 + dv_4 + (a + b - c + d)v_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S_{1,1,2} &= \{w_1 + w_2 + 2w_3 + av_1 + bv_2 + cv_3 + dv_4 + (a + b + c - d)v_5 : a, b, c, d \in \mathbb{Z}_3\}\\
S &= S_{2,1,1} \cup S_{1,2,1} \cup S_{1,1,2} \bigcup_{0 \le i,j,k \le 1} S_{i,j,k}.
\end{aligned}$$

For $0 \le i, j \le 1$ let $T_{i,j,k} = S_{i,j,k}$ except let $T_{1,1,1} = S_{1,1,1} + v_5$. Also let

$$T_{2,1,1} = S_{2,1,1} - v_5, T_{1,2,1} = S_{1,2,1} - v_5, T_{1,1,2} = S_{1,1,2} - v_5.$$

Similar to S, let

$$T = T_{2,1,1} \cup T_{1,2,1} \cup T_{1,1,2} \bigcup_{0 \le i,j,k \le 1} T_{i,j,k}.$$

The graphs we will be studying throughout this paper are $\Gamma_1 = \mathrm{Cay}(G, S \cup -S)$ and $\Gamma_2 = \mathrm{Cay}(G, T \cup -T)$. We will often abuse notation and terminology by conflating a group element with the corresponding vertex in one or both of these Cayley graphs. We use additive notation throughout, and use a bold $\mathbf{0}$ to denote the identity element of $\mathbb{Z}_3^8$.

For convenience of notation, we also define a partition of the elements of G into subsets of cardinality 3^5 by

$$B_{i,j,k} = \{iw_1 + jw_2 + kw_3 + av_1 + bv_2 + cv_3 + dv_4 + fv_5 : a, b, c, d, f \in \mathbb{Z}_3\}.$$

Although the proof in [14] uses Schur rings, it does explicitly provide a connection set (the S on page 3398); if we use our S to define

$$\overrightarrow{\Gamma_1'} = \mathrm{Cay}(G, (S \setminus S_{0,0,0}) \cup \{v_1, v_3, v_4, v_5\})$$

then the connection set of $\overrightarrow{\Gamma_1'}$ is the one given in Spiga's paper. He also explicitly (on page 3397) defines a function f that is exactly the polynomial we will add to $\mathbf{v}$ in our next proof when we define the map ψ; if we apply ψ to Spiga's connection set, we get the connection set for

$$\overrightarrow{\Gamma_2'} = \mathrm{Cay}(G, (T \setminus T_{0,0,0}) \cup \{v_1, v_3, v_4, v_5\}).$$

Extracting these two connection sets from Spiga's paper and understanding these are the connection sets for Cayley digraphs that are isomorphic via the map ψ but not via a group automorphism, is a matter of translating the Schur ring language he uses into Cayley digraph language.

As we have made clear by our definitions of $\overrightarrow{\Gamma_1'}$ and $\overrightarrow{\Gamma_2'}$, the underlying graphs of these digraphs differ from our Γ_1 and Γ_2 only in the elements of the connection set that lie in $B_{0,0,0}$. If we try to apply our arguments (in Section 3 below) to the underlying graphs of Spiga's digraphs, too many of the values produced in the table of Lemma 3.3 coincide. Consequently, the arguments we use based on counting mutual neighbours do not suffice to prove that no group automorphism can act as a graph isomorphism between these graphs. Discovering the graphs Γ_1 and Γ_2 was a matter of making careful and intelligent adjustments to the elements of $S_{0,0,0}$ so as to produce more distinct values in Lemma 3.3 and thereby significantly reduce the number of group automorphisms that needed to be considered as possibly inducing a graph isomorphism, ultimately eliminating all of them. Computational evidence (directed using some counting arguments) suggests that the underlying graphs of Spiga's digraphs are probably not isomorphic via a group automorphism either. However, I could find no structure in them understandable without a computer that gave any significant intuition as to why this might be so. Since Spiga has privately communicated to me that his example was found by a random search, I believe there is more value in producing a new (but related) example with clearer structural rationale for the lack of a group automorphism that could act as a graph isomorphism, than in either largely appealing to computation to determine that Spiga's underlying graphs also work, or coming up with a much longer and more technical proof to explain his graphs.

Proposition 2.1. *There is a map from $S \cup -S$ to $T \cup -T$ that acts as a graph isomorphism from Γ_1 to Γ_2.*

Proof. According to [14], the map $\psi\colon G \to G$ defined by

$$\psi(\mathbf{v}) = \mathbf{v} + x_1 x_2^2 v_1 + x_1 x_3^2 v_2 + x_2^2 x_3 v_3 + x_2 x_3^2 v_4 + x_1 x_2 x_3 v_5$$

for each

$$\mathbf{v} = \sum_{i=1}^{3} x_i w_i + \sum_{j=1}^{5} y_j v_j \in G$$

is a digraph isomorphism from $\overrightarrow{\Gamma_1'}$ to $\overrightarrow{\Gamma_2'}$.

Our graphs Γ_1 and Γ_2 are very close to being the underlying undirected graphs of these digraphs $\overrightarrow{\Gamma_1'}$ and $\overrightarrow{\Gamma_2'}$, which must be isomorphic via ψ since the digraphs are. Indeed, aside from the edges and arcs that lie inside each $B_{i,j,k}$, they are the same. Since ψ fixes every $B_{i,j,k}$, it must act as an isomophism from Γ_1 to Γ_2 with respect to every edge that is not contained within some $B_{i,j,k}$. It remains to be shown that the edges that come from $\pm S_{0,0,0}$ are preserved by ψ.

For any fixed (i, j, k), ψ adds $\sum_{m=1}^{5} c_m v_m$ to each vertex of $B_{i,j,k}$, for some constants c_1 through c_5 that depend only on i, j, k. Thus the action of ψ on $B_{i,j,k}$ is a translation by some element of $\langle v_1, \ldots, v_5 \rangle$. This means that for any choice of $S \cap B_{0,0,0}$, as long as $T \cap B_{0,0,0} = S \cap B_{0,0,0}$, ψ must preserve the edges that lie within $B_{i,j,k}$ (the edges that come from $\pm S_{0,0,0}$). Thus, ψ is indeed an isomorphism from Γ_1 to Γ_2. □

3 They are not isomorphic via a group automorphism

We begin with a number of assertions about the structure of mutual neighbours of vertices in these graphs. These serve to limit how an arbitrary isomorphism between the graphs can act, even more so in the case where the isomorphism must also be a group automorphism.

The bound provided in our first lemma will shortly allow us to show that any isomorphism between the graphs must have an action on the partition $\{B_{i,j,k}\}$: that is, for any isomorphism φ, $B_{i,j,k}^{\varphi} = B_{i',j',k'}$ for some i', j', k' that depends on i, j, k.

Lemma 3.1. *Suppose $(i, j, k) \neq (0, 0, 0)$. Then for any element $g \in B_{i,j,k}$, the number of mutual neighbours of $\mathbf{0}$ and g in either Γ_1 or Γ_2 is at most 587.*

Proof. This can be verified by computer. To verify by hand, the following points may be helpful:

- if $\{x, y, z\} = \{0, 1, 2\}$ or $(x, y, z) = (0, 0, 0)$ or $(x, y, z) = \pm(i, j, k)$ then the number of mutual neighbours of $\mathbf{0}$ and g in this set is bounded by the minimum of the number of neighbours of each, for a total of 101 over all these sets;
- otherwise, any of the other 18 possible sets $B_{x,y,z}$ has at most 27 mutual neighbours of g and $\mathbf{0}$ (this is tedious but straightforward to check using the definitions of the sets).

This gives the bound of $101 + 18 \cdot 27 = 587$. □

In Lemma 3.3 (which is somewhat tedious and technical) we will specify how many mutual neighbours various vertices of $B_{0,0,0}$ have with the identity vertex $\mathbf{0}$ in Γ_1 and in Γ_2. Since any group automorphism of G fixes $\mathbf{0}$, to be a graph isomorphism from Γ_1 to Γ_2 it must map a vertex that has k mutual neighbours with $\mathbf{0}$ in Γ_1 to a vertex that has k mutual neighbours with $\mathbf{0}$ in Γ_2, so this lemma will be critical in limiting the possible actions of our group automorphism. Before we get there, we first prove an easy lemma showing that as long as $g \in B_{0,0,0}$, the number of mutual neighbours of g and $\mathbf{0}$ is the same in both graphs, so we don't have to calculate these values separately.

Lemma 3.2. *Suppose $g \in B_{0,0,0}$. Then the number of mutual neighbours of $\mathbf{0}$ and g in Γ_1 is the same as the number of mutual neighbours of $\mathbf{0}$ and g in Γ_2.*

Proof. For every i, j, k, we have $T_{i,j,k} = S_{i,j,k} + m_{i,j,k} v_5$ where $m_{i,j,k} \in \{0, 1, 2\}$. Now, h is a mutual neighbour of $\mathbf{0}$ and g in Γ_1 iff $h \in S_{i,j,k} \cap (S_{i,j,k} + g)$. This is true if and only if $h + m_{i,j,k} v_5 \in T_{i,j,k} \cap (T_{i,j,k} + g)$, which is true if and only if $h + m_{i,j,k} v_5$ is a mutual neighbour of $\mathbf{0}$ and g in Γ_2. □

Lemma 3.3. *The number of mutual neighbours that each vertex v in the table below has with $\mathbf{0}$ in each of Γ_1 and Γ_2, is as given in the corresponding column.*

v	$v_1 - v_5$	$v_2 + v_3 - v_4 + v_5$	$v_3 - v_4 + v_5$	$v_4 + v_5$	v_5	$v_2 + v_5$	v_4	$v_5 - v_4$
#	865	163	487	811	703	702	650	812

v	v_1	$-v_1 - v_5$	$v_3 + v_4 + v_5$	$-v_3 - v_5$	$v_2 - v_3 - v_4 + v_5$	$-v_2 + v_4 - v_5$
#	380	704	486	810	648	486

Proof. By Lemma 3.2, the number of mutual neighbours of $\mathbf{0}$ with any vertex of $B_{0,0,0}$ is the same in Γ_1 as in Γ_2, so we need only count one of these. We will count the mutual neighbours in Γ_1.

- $v_1 - v_5$: Mutual neighbours with $\mathbf{0}$ are $v_5 - v_1$; $\pm S_{1,0,0}$; $\pm S_{0,1,0}$, $\pm S_{1,1,0}$, $\pm S_{0,1,1}$, $\pm S_{1,1,1}$, $\pm S_{2,1,1}$. The total number of these is $1 + 54 + 81 \cdot 10 = 865$.
- $v_2 + v_3 - v_4 + v_5$: Mutual neighbours with $\mathbf{0}$ are $-v_2 - v_3 + v_4 - v_5$; $\pm S_{0,0,1}$. The total number of these is $1 + 81 \cdot 6 = 163$.
- $v_3 - v_4 + v_5$: Mutual neighbours with $\mathbf{0}$ are $-v_3 + v_4 - v_5$; $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{1,2,1}$. The total number of these is $1 + 81 \cdot 6 = 487$.
- $v_4 + v_5$: Mutual neighbours with $\mathbf{0}$ are $-v_4 - v_5$; $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{1,0,1}$, $\pm S_{1,1,1}$, $\pm S_{1,2,1}$. The total number of these is $1 + 81 \cdot 10 = 811$.
- v_5: Mutual neighbours with $\mathbf{0}$ are $-v_5$; $\pm S_{1,0,0}$; $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{1,1,0}$, $\pm S_{1,0,1}$. The total number of these is $1 + 54 + 81 \cdot 8 = 703$.
- $v_2 + v_5$: Mutual neighbours with $\mathbf{0}$ are $\pm S_{1,0,0}$; $\pm S_{0,0,1}$, $\pm S_{1,0,1}$, $\pm S_{1,2,1}$, $\pm S_{1,1,2}$. The total number of these is $54 + 81 \cdot 8 = 702$.
- v_4: Mutual neighbours with $\mathbf{0}$ are $v_4 + v_5$; $-v_5$; $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{1,0,1}$, $\pm S_{0,1,1}$. The total number of these is $2 + 81 \cdot 8 = 650$.
- $v_5 - v_4$: Mutual neighbours with $\mathbf{0}$ are $-v_5$; $-v_4 - v_5$; $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{1,0,1}$, $\pm S_{2,1,1}$, $\pm S_{1,1,2}$. The total number of these is $2 + 81 \cdot 10 = 812$.
- v_1: Mutual neighbours with $\mathbf{0}$ are v_5; $v_1 - v_5$; $\pm S_{1,0,0}$; $\pm S_{0,1,0}$, $\pm S_{1,1,0}$. The total number of these is $2 + 54 + 81 \cdot 4 = 380$.
- $-v_1 - v_5$: Mutual neighbours with $\mathbf{0}$ are v_5; $v_5 - v_1$; $\pm S_{1,0,0}$; $\pm S_{0,1,0}$, $\pm S_{1,1,0}$, $\pm S_{1,2,1}$, $\pm S_{1,1,2}$. The total number of these is $2 + 54 + 81 \cdot 8 = 704$.
- $v_3 + v_4 + v_5$: Mutual neighbours with $\mathbf{0}$ are $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{2,1,1}$. The total number of these is $81 \cdot 6 = 486$.
- $-v_3 - v_5$: Mutual neighbours with $\mathbf{0}$ are $\pm S_{0,1,0}$, $\pm S_{0,0,1}$, $\pm S_{1,1,0}$, $\pm S_{1,1,1}$, $\pm S_{1,1,2}$. The total number of these is $81 \cdot 10 = 810$.
- $v_2 - v_3 - v_4 + v_5$: Mutual neighbours with $\mathbf{0}$ are $\pm S_{0,0,1}$, $\pm S_{2,1,1}$, $\pm S_{1,2,1}$, $\pm S_{1,1,2}$. The total number of these is $81 \cdot 8 = 648$.
- $-v_2 + v_4 - v_5$: Mutual neighbours with $\mathbf{0}$ are $\pm S_{0,0,1}$, $\pm S_{1,0,1}$, $\pm S_{1,1,1}$. The total number of these is $81 \cdot 6 = 486$.

□

With this result in hand, we can show that a group automorphism acting as a graph isomorphism must either fix some of the elements of $\pm S_{0,0,0}$ pointwise, and have very small potential orbits on the other elements, or must have these properties after being combined with another group automorphism that acts as a graph automorphism of Γ_1.

Lemma 3.4. *If there is a group automorphism α of G that maps $S \cup -S$ to $T \cup -T$, then there is one that fixes v_5 and $-v_5$. Moreover, any such automorphism fixes each of the sets $\{v_1 - v_5, v_5 - v_1\}$, $\{v_2 + v_3 - v_4 + v_5, -v_2 - v_3 + v_4 - v_5\}$, $\{v_3 - v_4 + v_5, -v_3 + v_4 - v_5\}$, and $\{v_4 + v_5, -v_4 - v_5\}$.*

Proof. Any group automorphism fixes $\mathbf{0}$. A group automorphism α that maps $S \cup -S$ to $T \cup -T$ must map any vertex that has a certain number of mutual neighbours with $\mathbf{0}$ in Γ_1, to a vertex that has that number of mutual neighbours with $\mathbf{0}$ in Γ_2.

By Lemma 3.3, the vertices $v_1 - v_5$, $v_2 + v_5$, $-v_3 - v_5$, $v_4 + v_5$, and v_5 each has more than 587 mutual neighbours with $\mathbf{0}$, so by Lemma 3.1 each of these vertices must map to a vertex in $B_{0,0,0}$, and must be the image of a vertex in $B_{0,0,0}$. Note that $B_{0,0,0}$ is actually a subgroup of G, and is generated by these five elements. This implies that α must map this generating set for $B_{0,0,0}$ to a generating set for $B_{0,0,0}$, so $B_{0,0,0}^{\alpha} = B_{0,0,0}$.

For convenience in this paragraph, let $S_0 = S_{0,0,0} \cup -S_{0,0,0}$ and $T_0 = T_{0,0,0} \cup -T_{0,0,0}$. Since

$$(S \cup -S) \cap B_{0,0,0} = S_0 = T_0 = (T \cup -T) \cap B_{0,0,0}$$

and $B_{0,0,0}^{\alpha} = B_{0,0,0}$, we must have $S_0^{\alpha} = T_0 = S_0$. In particular, since the numbers of mutual neighbours that each vertex in each inverse-closed pair in S_0 has with $\mathbf{0}$ is distinct from the number of mutual neighbours that each vertex of any other inverse-closed pair in S_0 has with $\mathbf{0}$ (see Lemma 3.3), each inverse-closed pair in S_0 must be mapped to the same inverse-closed pair in S_0. This completes the proof unless $v_5^{\alpha} = -v_5$ (in which case $(-v_5)^{\alpha} = v_5$), which we now assume.

Let σ be the automorphism of G that inverts every element of G; note that σ fixes $S \cup -S$, and therefore $\sigma\alpha$ maps $S \cup -S$ to $T \cup -T$. Now $v_5^{\sigma\alpha} = v_5$, and $\sigma\alpha$ also fixes each of the other inverse-closed pairs separately since α did, completing the proof. $\square$

In fact, we can now show that a group automorphism acting as a graph isomorphism must fix every element of $\pm S_{0,0,0}$ pointwise (possibly after being combined in the preceding lemma with another group automorphism that acts as a graph automorphism).

Lemma 3.5. *If there is a group automorphism α of G that maps $S \cup -S$ to $T \cup -T$ and fixes v_5 and $-v_5$, then it must also fix every other vertex of $S_{0,0,0} \cup -S_{0,0,0}$.*

Proof. We first show that it fixes $v_4 + v_5$ and its inverse.

Any such α induces a graph automorphism from Γ_1 to Γ_2. Since Γ_1 is a Cayley graph, the number of mutual neighbours of v_5 with $v_4 + v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with v_4. Likewise, the number of mutual neighbours of v_5 with $-v_4 - v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with $v_5 - v_4$. Since we see from Lemma 3.3 that these numbers are not equal, α must fix both $v_4 + v_5$ and $-v_4 - v_5$.

Next we show that $v_1 - v_5$ and its inverse are fixed.

Since Γ_1 is a Cayley graph, the number of mutual neighbours of $-v_5$ with $v_1 - v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with v_1. Likewise, the number of mutual neighbours of $-v_5$ with $v_5 - v_1$ is the same as the number of mutual neighbours of $\mathbf{0}$ with $-v_1 - v_5$. Since we see from Lemma 3.3 that these numbers are not equal, α must fix both $v_1 - v_5$ and $v_5 - v_1$.

Now we show that $v_3 - v_4 + v_5$ and its inverse are fixed. At this point, notice that since α fixes v_5 and $v_4 + v_5$, it also fixes v_4.

Since Γ_1 is a Cayley graph, the number of mutual neighbours of v_4 with $v_3 - v_4 + v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with $v_3 + v_4 + v_5$. Likewise, the number of mutual neighbours of v_4 with $-v_3 + v_4 - v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with $-v_3 - v_5$. Since we see from Lemma 3.3 that these numbers are not equal, α must fix both $v_3 - v_4 + v_5$ and $-v_3 + v_4 - v_5$.

Finally, we must show that $v_2 + v_3 - v_4 + v_5$ and its inverse are fixed. At this point, notice that since α fixes v_4, v_5, and $v_3 - v_4 + v_5$, it also fixes $-v_3$.

Since Γ_1 is a Cayley graph, the number of mutual neighbours of $-v_3$ with $v_2+v_3-v_4+v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with $v_2 - v_3 - v_4 + v_5$. Likewise, the number of mutual neighbours of $-v_3$ with $-v_2-v_3+v_4-v_5$ is the same as the number of mutual neighbours of $\mathbf{0}$ with $-v_2 + v_4 - v_5$. Since we see from Lemma 3.3 that these numbers are not equal, α must fix both $v_2 + v_3 - v_4 + v_5$ and $-v_2 - v_3 + v_4 - v_5$. □

At this point we have enough information to show the invariant action on the partition $\{B_{i,j,k}\}$, as mentioned earlier.

Lemma 3.6. *Any group automorphism α of G that fixes every vertex of $B_{0,0,0}$ has an invariant action on the collection $\{B_{i,j,k} : 0 \leq i, j, k \leq 2\}$.*

Proof. Since α is an automorphism of G, once we know its action on a generating set for G, this completely determines its action. Since α fixes every vertex of $B_{0,0,0}$, it fixes each v_i for $1 \leq i \leq 5$. This means that if $g \in B_{i,j,k}$ with $g = iw_1 + jw_2 + kw_3 + h$ then $g^\alpha = iw_1^\alpha + jw_2^\alpha + kw_3^\alpha + h$ since $h \in B_{0,0,0}$. So $B_{i,j,k}^\alpha$ has the form $B_{i',j',k'}$ for some $0 \leq i', j', k' \leq 2$. □

In fact, the invariant action on the partition can have only two possible forms.

Lemma 3.7. *If there is a group automorphism α of G that maps $S \cup -S$ to $T \cup -T$ and fixes every vertex of $B_{0,0,0}$, then it must either leave every $B_{i,j,k}$ invariant, or map every $B_{i,j,k}$ to $B_{-i,-j,-k}$.*

Proof. By Lemma 3.6, α must have an invariant action on the collection $\{B_{i,j,k} : 0 \leq i, j, k \leq 2\}$.

The sets $B_{1,0,0}$ and $B_{-1,0,0}$ are the only sets that have exactly 27 neighbours of $\mathbf{0}$ in both Γ_1 and Γ_2, so must be left invariant by α.

The sets $B_{0,1,0}$ and $B_{0,-1,0}$ are the only sets for which all neighbours of $\mathbf{0}$ in both Γ_1 and Γ_2 are also neighbours of $iv_1 + jv_3 + kv_4 + \ell v_5$ for every $0 \leq i, j, k, \ell \leq 2$, so these sets must be left invariant by α.

Similarly, the sets $B_{0,0,1}$ and $B_{0,0,-1}$ are the only sets for which all neighbours of $\mathbf{0}$ in both Γ_1 and Γ_2 are also neighbours of $iv_2 + jv_3 + kv_4 + \ell v_5$ for every $0 \leq i, j, k, \ell \leq 2$, so these sets must be left invariant by α.

Likewise, the sets $B_{1,1,1}$ and $B_{-1,-1,-1}$ are the only sets for which (in both Γ_1 and Γ_2) all neighbours of $\mathbf{0}$ are also neighbours of $iv_1+jv_2+kv_3+\ell v_4$ for every $0 \leq i, j, k, \ell \leq 2$. Notice this is true even though $S_{1,1,1} \neq T_{1,1,1}$. So these sets must be left invariant by α.

Taken together, these force $w_1^\alpha \in B_{\pm 1,0,0}$; $w_2^\alpha \in B_{0,\pm 1,0}$; and $w_3^\alpha \in B_{0,0,\pm 1}$. However, the previous paragraph also tells us that $(w_1+w_2+w_3)^\alpha \in B_{1,1,1} \cup B_{-1,-1,-1}$. This forces the signs of each of the $\pm$ in our first three conclusions to be the same, yielding the desired conclusion. □

We can even show that after possibly combining with a group automorphism that acts as a graph automorphism, the invariant action fixes every set in the partition.

Lemma 3.8. *If there is a group automorphism α of G that maps $S \cup -S$ to $T \cup -T$ and fixes every vertex of $B_{0,0,0}$, then there is one that leaves every $B_{i,j,k}$ invariant.*

Proof. By Lemma 3.7, the only other possibility is that α maps every $B_{i,j,k}$ to $B_{-i,-j,-k}$.

Let σ_W be the automorphism of G determined by $w_i^{\sigma_W} = -w_i$ for every $1 \leq i \leq 3$, and $v_i^{\sigma_W} = v_i$ for every $1 \leq i \leq 5$. Note that σ_W fixes S, and therefore $\sigma_W\alpha$ maps S to T. Also σ_W fixes every vertex of $B_{0,0,0}$ and maps every $B_{i,j,k}$ to $B_{-i,-j,-k}$. Therefore $\sigma_W\alpha$ has all of the properties we claimed. □

In our final lemma, we show that a group automorphism that has all of the properties we have been deducing, cannot exist.

Lemma 3.9. *A group automorphism α of G that maps $S \cup -S$ to $T \cup -T$, fixes every vertex of $B_{0,0,0}$, and leaves every $B_{i,j,k}$ invariant must map $(S \setminus S_{0,0,0}) \cup S'_{0,0,0}$ to $(T \setminus T_{0,0,0}) \cup S'_{0,0,0}$ for any $S'_{0,0,0} \subseteq B_{0,0,0}$. In fact, there is no such group automorphism.*

Proof. Notice that for every $(i,j,k) \neq (0,0,0)$ we have either $B_{i,j,k} \cap S_{i,j,k} = \emptyset$ or $B_{i,j,k} \cap -S_{i,j,k} = \emptyset$ (or both), and $T_{i,j,k} = \emptyset$ if and only if $S_{i,j,k} = \emptyset$. Since $B_{i,j,k}^\alpha = B_{i,j,k}$, this means that $S_{i,j,k}^\alpha = T_{i,j,k}$. Hence, since α fixes $B_{0,0,0}$ pointwise and $S_{0,0,0} = T_{0,0,0}$, we have $S^\alpha = T$. In fact, since α fixes $B_{0,0,0}$ pointwise, for any $S'_{0,0,0} \subseteq B_{0,0,0}$ we have

$$((S \setminus T_{0,0,0}) \cup S'_{0,0,0})^\alpha = (T \setminus T_{0,0,0}) \cup S'_{0,0,0},$$

as claimed.

Since the connection sets of $\overrightarrow{\Gamma_1'}$ and $\overrightarrow{\Gamma_2'}$ have this form, such an α would act as a digraph isomorphism between them, but since [14] proved these digraphs are not isomorphic via any group automorphism, this is impossible. Hence no such α exists. □

We pull all of our results in this section together in our conclusion.

Corollary 3.10. *There is no automorphism of G that maps $S \cup -S$ to $T \cup -T$.*

Proof. By Lemma 3.4, if there were such an automorphism, then there must be one that fixes v_5 and $-v_5$. Furthermore, by Lemma 3.5, any such automorphism fixes every vertex of $S_{0,0,0} \cup -S_{0,0,0}$. Since it is a group automorphism and fixes every element of $S_{0,0,0}$, and this generates $B_{0,0,0}$, it must fix every vertex of $B_{0,0,0}$.

By Lemma 3.8, this would imply the existence of an automorphism that maps $S \cup -S$ to $T \cup -T$, fixes every vertex of $B_{0,0,0}$, and leaves every $B_{i,j,k}$ invariant. Finally, by Lemma 3.9, no such automorphism exists. □

Putting this result together with Proposition 2.1, and using the well-known fact that every subgroup of a CI-group must be a CI-group, yields the main result of this paper.

Theorem 3.11. *The group $\mathbb{Z}_3^8$ is not a CI-group. Neither is any group containing $\mathbb{Z}_3^8$ as a subgroup. In particular, $\mathbb{Z}_3^n$ is not a CI-group for $n \geq 8$.*

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Complexity function of jammed configurations of Rydberg atoms*

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Abstract

In this article, we determine the complexity function (configurational entropy) of jammed configurations of Rydberg atoms on a one-dimensional lattice. Our method consists of providing asymptotics for the number of jammed configurations determined by direct combinatorial reasoning. In this way we reduce the computation of complexity to solving a constrained optimization problem for the Shannon's entropy function. We show that the complexity can be expressed explicitly in terms of the root of a certain polynomial of degree b, where b is the so-called blockade range of a Rydberg atom. Our results are put in a relation with the model of irreversible deposition of k-mers on a one-dimensional lattice.

Keywords: Dynamic lattice systems, equilibrium lattice systems, complexity function, configurational entropy, jammed configuration, maximal packing, Rydberg atoms.

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1 Introduction

Rydberg atom is a name given to an atom which has been excited into a high energy level so that one of its electrons is able to travel much farther from the nucleus than usual (up to 10^6 times more, see [22]). In physics community, Rydberg atoms have been intensely studied and have become a testing ground for various quantum mechanical problems in quantum information processing, quantum computation and quantum simulation [58]. See [29] for a comprehensive description of the physics of Rydberg atoms and their remarkable properties. Due to their large size, Rydberg atoms can exhibit very large electric dipole moments which results in strong interactions between two close Rydberg atoms. This causes a blockage effect that prohibits the excitation of an atom located close to an atom that is already excited to a Rydberg state [3, 12, 34, 37, 54, 63]. The simplest setting for studying Rydberg atoms and their blockage effect is on a finite one-dimensional lattice. In this setting, each atom occupies one site and each two excited atoms are at least $b \geq 1$ sites apart. The positive integer b is referred to as the *blockade range* of the model. We will be interested in maximal (or *jammed*) configurations where no further atoms can be excited. Note that in such a configuration each two excited atoms are at most $2b$ sites apart. In physics literature, jammed states in similar deposition models have the interpretation of metastable states at low enough temperature and/or high enough density, and are referred to as valleys, pure states, quasi-states, and inherent structures [4, 5, 17, 33, 38, 50, 62].

The main question related to maximal configurations concerns the expected density of the atoms excited to a Rydberg state. There are two natural ways to interpret this question. One way to look at this problem is to consider the set of all the possible maximal configurations and to sample one such configuration at random (which implies that all the maximal configurations are equiprobable). This is referred to as the static (or equilibrium) model. The static model is usually described by the so-called complexity function (also known as configurational entropy), and the expected density of particles in a jammed configuration converges to the argument of the maximum of the complexity function. This is exactly the approach we take in this paper and our main result is the derivation of the mentioned complexity function. Static model can be compared with the random sequential adsorption (RSA) model (also refered to as the dynamic model) where initially all atoms are in the ground state, and are excited sequentially, at random, until a jammed configuration is reached. The expected density of excited atoms with this underlying probability space is called *jamming limit*. Assumption that the two models result in the same distribution of maximal configurations has come to be known as Edwards's flatness hypothesis (see [2] for a recent review). However, there seems to be no *a priori* reason for the two models to have similar properties. It is interesting to note that there is a long history to the question of how similar the two models are (see e.g. the discussion in [8, page 681], or, in a more subtle continuum context, how a similar confusion of different probability models led to some extended discussion over a false "proof" [53]).

The dynamic version of the problem was already studied in literature. In [28, 42, 48] it was found that the jamming limit is

$$\rho_\infty^{b\text{-Ryd}} = \int_0^1 \exp\left[-2\sum_{j=1}^{b}\frac{1-y^j}{j}\right] dy.$$

The jamming limit was also computed for an equivalent model of deposition of linear polymers (k-mers) in [44, §7.1]

$$\rho_\infty^{k\text{-mer}} = k\int_0^\infty \exp\left[-u - 2\sum_{j=1}^{k-1}\frac{1-e^{-ju}}{j}\right]du = k\int_0^1 \exp\left[-2\sum_{j=1}^{k-1}\frac{1-y^j}{j}\right]dy.$$

The equivalence of models is reflected in the fact that $\rho_\infty^{k\text{-mer}} = k\cdot\rho_\infty^{b\text{-Ryd}}$ for $b = k-1$.

In the static model, it all comes down to counting the maximal configurations. It is known that in similar models, the number of different maximal configurations with prescribed density $0 \le \rho \le 1$ tends to grow exponentially with the length L of configuration, see [9, 10, 13, 14, 15, 16, 18, 23, 27, 35, 40, 45, 46, 49, 52, 55, 56, 59]. Denoting this number by $J_L(\rho)$, it is common to describe it using the so-called complexity function (also called configurational entropy) $f(\rho)$ for which it holds that $J_L(\rho) \sim e^{Lf(\rho)}$. It turns out (see e.g. Figure 9) that the density $\rho_\star^{b\text{-Ryd}}$ maximizing the complexity function is slightly different than the expected density (jamming limit) of the dynamic model. This falsifies the above mentioned Edward's flatness hypothesis. Recall that $\rho_\star^{b\text{-Ryd}}$ is the limit (as L tends to infinity) of the most probable densities in the equilibrium models that assign equal probabilities to all jammed configurations.

Our main goal is to compute the complexity $f(\rho)$ of jammed configurations of Rydberg atoms using direct combinatorial reasoning. The problem reduces to solving a constrained optimization problem for the Shannon's entropy function. We show that the complexity function can be expressed explicitly in terms of the root of a certain polynomial of degree b. This work has been carried out simultaneously with [43]. The authors there introduce a novel method for determining the same complexity function. Their method is inspired by the theory of renewal processes.

The described model of Rydberg atoms on a one-dimensional lattice is equivalent to a number of other models already present in the literature. The case $b = 1$ is the famous model introduced by Flory [26] describing the mechanism of vinyl polymerization. This is in turn essentially equivalent to the Page-Rényi car parking problem [31, 51] (which is a discrete version of the famous model introduced by Rényi in [57]) describing the jammed configurations of cars of length 2. The equivalence is obtained by replacing each excited atom with a car taking up both the atom's and its right neighbor's site. Clearly, this only works for configurations not having an excited atom at the rightmost site. This means that the total number of jammed configurations is actually different in these two models, but only up to a constant factor, which does not affect the shape of the complexity function of these models. In chemistry, this model appears in the context of the irreversible deposition of dimers [26, 36], and in graph theory, the jammed configurations correspond to maximal matchings in a path graph, see [21].

Similarly, the general case $b > 1$ corresponds to irreversible deposition of k-mers ($k = b+1$) in a linear polymer of length L. The equivalence (again, up to a constant factor) is obtained by replacing each excited atom with a polymer taking up $b+1$ consecutive sites, starting from the atom's position, see Figure 1. In this, and all the following figures, bullets ($\bullet$) represent Rydberg atoms (in the Rydberg model) or occupied sites (in the k-mer deposition model), while empty bullets ($\circ$) represent neutral atoms (in the Rydberg model) or vacant sites (in the k-mer deposition model). Notice that the gaps between adjacent k-mers in jammed configurations of this deposition model are of size at most $k-1$. This equivalence allows us to easily transfer our results on Rydberg atoms to the setting of k-

mer deposition model. The problem of irreversible deposition of k-mers was extensively studied in the literature, see [1, 6, 24, 32, 42, 44, 61].

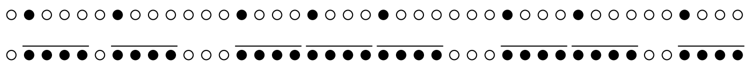

Figure 1: A jammed configuration of Rydberg atom model with blockade range b and the corresponding jammed configuration of the k-mer deposition model when $b = 3$, $k = 4$.

In graph theory, the k-mer deposition model is equivalent to P_k-packings of a path graph P_L, and jammed configurations in the former correspond to maximal packings in the latter. The maximal P_k-packings of P_L were previously studied in [20].

Another equivalent formulation of the Rydberg atom model appeared recently in [19, §3.2.1] where the authors of the present paper considered the settlement model consisting of k-story buildings on a one-dimensional tract of land. The tract of land is oriented east-west and each story of each building has to receive the sunlight from both east and west.

The rest of the paper is organized as follows. In Section 2 we calculate the asymptotics for the number of jammed configurations in the model of Rydberg atoms, which is expressed in terms of the maximum of the Shannon's entropy function over a certain finite set determined by the constraints of the model. In Section 3 we use these results in order to obtain the formula for the associated complexity function. We derive the expression for the complexity $f(\rho)$ which, for a chosen density ρ, depends explicitly on a positive root of a certain polynomial whose degree coincides with the blockade range of the model. Further on, in Section 4, we put our findings in relation with the model for the deposition of k-mers on the linear polymer and draw conclusions from the obtained results. There, we also provide some results on the qualitative properties of the maximizers of mentioned complexity functions, for various blockade ranges b, and put them in comparison with their counterparts in the theory of RSA. Finally, in Section 5 we recapitulate our findings and indicate several possible directions of future research.

Notation

We write $M_L \sim N_L$ if the two positive sequences $(M_L)_L$ and $(N_L)_L$ have the same growth, as $L \to \infty$, up to a sub-exponential factor, i.e. if

$$\lim_{L\to\infty} \frac{\ln M_L - \ln N_L}{L} = 0.$$

2 Jammed configurations of Rydberg atoms

As already stated in the introduction, the main goal of this paper is to compute the complexity function $f(\rho)$ of jammed configurations of Rydberg atoms. Crucial step towards obtaining a complexity function of such models in general is to inspect the set of all jammed configurations of a model. Each configuration is a binary 0/1 sequence which we sometimes interpret as a sequence of empty/occupied sites or, in Rydberg model, as neutral/excited atoms. The total number of all configurations of length L in the model is denoted by J_L. The total number of configurations of length L consisting of N ones (occupied sites, excited atoms) is denoted by $J_{N,L}$. The *density (saturation, coverage)* of any such configuration of length L with N ones is defined as $N/L \in [0,1]$.

In order to determine the complexity function, it is not enough to work only with J_L. We need to be more precise. We need to know the behavior of the number of different jammed configurations of length L, where precisely N atoms are excited to the Rydberg state. The main result of this section (see Lemma 2.4) provides asymptotics of the quantity $J_{N,L}$ for Rydberg atom model.

Let us first consider several concrete examples of jammed configurations of our model to get a better feeling of their possible shapes. Figure 2 displays three different jammed configurations in the chain of $L = 16$ atoms, where the blockade range b is equal to two, i.e. each two excited atoms are at least two sites apart. Since Rydberg atoms in a jammed

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Figure 2: Three jammed configurations in the chain of $L = 16$ atoms with blockade range $b = 2$. The number of Rydberg atoms in these configurations is $N = 6, 5, 4$ (from top to bottom).

configuration are separated by clusters of empty sites whose length is at least b (so that the constraint imposed by the blockage effect is satisfied), and at most $2b$ (since we can excite another atom in the middle of an empty range of size $2b + 1$, hence such a configuration would not be jammed), it is easy to see that it holds

$$\left\lceil \frac{L}{2b+1} \right\rceil \leq N \leq \left\lceil \frac{L}{b+1} \right\rceil, \tag{2.1}$$

where N is the number of excited atoms, L is the length of the configuration, and b is the blockade range. In the particular case of $L = 16$ and $b = 2$, this implies that $4 \leq N \leq 6$. Hence, Figure 2 shows one jammed configuration for each possible value of N. Notice that relation (2.1) implies that

$$\frac{1}{2b+1} - \frac{1}{L} < \frac{N}{L} \leq \frac{1}{b+1}, \tag{2.2}$$

and this in turn implies that in the limit, as $L \to \infty$, the density $\rho = N/L$, of Rydberg atoms in jammed configurations, lies within the bounds

$$\frac{1}{2b+1} \leq \rho \leq \frac{1}{b+1}. \tag{2.3}$$

As a first result in the direction of better understanding the double sequence $J_{N,L}$ for Rydberg atom model, we provide the bivariate generating function for this sequence in the general case of blockade range $b \geq 1$.

Lemma 2.1. *The bivariate generating function of the sequence $J_{N,L}$ associated with jammed configurations of Rydberg atoms, when the blockade range is equal to b, is given by*

$$F_b(x,y) = \sum_L \sum_N J_{N,L} x^N y^L = \frac{(1-y)^2 + xy - xy^{b+1} - xy^{b+2} + xy^{2b+2}}{(1-y)(1-y-xy^{b+1}+xy^{2b+2})}.$$

Proof. As already mentioned, configurations of Rydberg atoms can be represented as $0/1$ sequences. Due to the fact that we can determine whether the blockage effect has been taken into account, and whether the configuration represented with such a sequence is jammed, just by inspecting finite size patches of a given sequence, we can apply the so-called transfer matrix method (see [60, §4.7] or [25, §V], and also [47, §2–4]). This is a well known method for counting words of a regular language. Since Rydberg atoms in a jammed configuration are separated with at least b, and at most $2b$ neutral atoms, every jammed configuration will be composed of blocks that start with a Rydberg atom and then have a cluster of neutral atoms of length between b and $2b$. Such blocks are displayed in Figure 3.

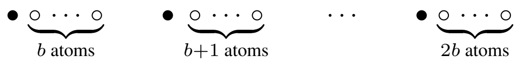

Figure 3: Building blocks of jammed configurations of Rydberg atoms with blockade range b.

These building blocks are encoded with the polynomial

$$p_b(x,y) = xy^{b+1} + xy^{b+2} + \cdots + xy^{2b+1}.$$

Now we only need to take care of the beginning and the end of jammed configurations. Notice that in front of the first block we can have some neutral atoms. More precisely, the number of neutral atoms that can appear at the left end of the jammed configuration is between 0 and b. These starting blocks are encoded with the polynomial

$$s_b(x,y) = 1 + y + y^2 + \cdots + y^b.$$

Similarly, after the last block from the set of blocks shown in Figure 3 (if there are any, i.e. if we want to have more than just one atom in the Rydberg state), we need to have a block that again starts with a Rydberg atom, and then has a cluster of neutral atoms of length between 0 and b. These ending blocks are encoded with the polynomial

$$e_b(x,y) = xy + xy^2 + \cdots + xy^{b+1}.$$

Notice that each of the blocks shown in Figure 3 can be glued to any other block listed in this figure. This implies that we do not even need to work with powers of the transfer matrix, but we can directly take powers of the polynomial $p_b(x,y)$ in order to obtain the desired bivariate generating function. A simple calculation gives

$$\begin{aligned} F_b(x,y) &= 1 + \sum_{n=0}^{\infty} s_b(x,y) \cdot p_b(x,y)^n \cdot e_b(x,y) \\ &= 1 + \frac{s_b(x,y) \cdot e_b(x,y)}{1 - p_b(x,y)} \\ &= \frac{(1-y)^2 + xy - xy^{b+1} - xy^{b+2} + xy^{2b+2}}{(1-y)(1-y-xy^{b+1}+xy^{2b+2})}. \end{aligned}$$

$\square$

Remark 2.2. By using the same technique, we can easily compute the bivariate generating function enumerating the number of jammed configurations of prescribed length, and with some fixed number of occupied sites, in the k-mer deposition model. The building blocks here are composed of a cluster of k consecutive sites occupied by a single k-mer, followed by a cluster of empty sites of length between 0 and $k-1$ (see Figure 4). These building

$$\underbrace{\bullet\cdots\bullet}_{k\text{ sites}} \qquad \underbrace{\bullet\cdots\bullet}_{k\text{ sites}}\circ \qquad \underbrace{\bullet\cdots\bullet}_{k\text{ sites}}\circ\circ \qquad \cdots \qquad \underbrace{\bullet\cdots\bullet}_{k\text{ sites}}\underbrace{\circ\cdots\circ}_{k-1\text{ sites}}$$

Figure 4: Building blocks of jammed configurations of k-mer deposition model.

blocks are encoded with a polynomial

$$p_k(x,y) = x^k y^k + x^k y^{k+1} + \cdots + x^k y^{2k-1},$$

where x is again a formal variable associated with the number of occupied sites, and y is a formal variable associated with the length of a configuration. Similarly as in the case of the Rydberg atom model, at the left end of a jammed configuration, we can have a cluster of vacant sites of length between 0 and $k-1$. These starting blocks are encoded with the polynomial

$$s_k(x,y) = 1 + y + y^2 + \cdots + y^{k-1}.$$

It is clear that we can end a jammed configuration with any of the building blocks shown in Figure 4, so we can set $e_k(x,y) = 1$. Using again the fact that each of the blocks from Figure 4 can be glued to any other block listed in that figure, we can work directly with powers of the polynomial $p_k(x,y)$ to obtain

$$F_k(x,y) = \sum_{n=0}^{\infty} a_k(x,y)\cdot p_k(x,y)^n = \frac{a_k(x,y)}{1-p_k(x,y)} = \frac{1-y^k}{1-y-x^k y^k + x^k y^{2k}}. \tag{2.4}$$

Notice that we are not adding 1 to the bivariate generating function in (2.4). The reason is that starting with a cluster of 0 vacant sites and setting $n=0$ already counts the empty configuration.

The sequence $J_{N,L}$ has already been studied in the literature, but in the context of maximal P_k-packings of a path graph P_L (see [20]). The bivariate generating function enumerating the total number of maximal k-packings in P_L, with exactly N copies of P_k, is given in [20, Corollary 2.4], and the only difference between that bivariate generating function and the one we obtained in (2.4), is that x is not raised to power k. The reason is that the author in [20] is interested in the number of copies of P_k (i.e. the number of deposited k-mers) in jammed configurations, and we are interested in the total number of sites occupied by those deposited k-mers. The bivariate generating function from (2.4) is also obtained in [43, formula (5.3)], where authors use a novel approach inspired by the theory of renewal processes. Using the same technique, they also obtain the bivariate generating function which coincides with the one we obtained in Lemma 2.1, which enumerates the total number of jammed configurations of length L of Rydberg atoms with blockade range b, with precisely N excited atoms (see [43, formula (6.5)]).

It is easy to see from the bivariate generating function from Lemma 2.1 that, for $b=2$, $J_{16} = 96$ (i.e. there are 96 jammed configurations in the chain of $L=16$ atoms, when the blockade range is $b = 2$). Out of those 96 jammed configurations, 45 of them have 4 Rydberg atoms ($J_{4,16} = 45$), 50 of them have 5 Rydberg atoms ($J_{5,16} = 50$), and only one has 6 Rydberg atoms ($J_{6,16} = 1$). This particular one is exactly the first jammed configuration shown in Figure 2.

We could now proceed like the authors in [43] and use the bivariate generating function developed in Lemma 2.1 to obtain the complexity function of jammed configurations of Rydberg atoms by means of the Legendre transform. However, we will use a direct combinatorial argument. To this end, we introduce a slightly different way of counting jammed configurations in the Rydberg model with blockade range b, than the one introduced in Lemma 2.1. Denote with B the block of $b+1$ adjacent atoms where only the first one is excited to the Rydberg state (see Figure 5). Using again the fact that each two Rydberg

$$B = \bullet \underbrace{\circ\circ\cdots\circ}_{b \text{ atoms}}$$

Figure 5: Block consisting of $b+1$ adjacent atoms where only the first one is excited to the Rydberg state.

atoms have at least b and at most $2b$ neutral atoms separating them, it is clear that every jammed configuration consists of blocks B separated by clusters of neutral atoms of length $0 \le a \le b$ (see Figure 6). Denote by M_a the number of gaps with a neutral atoms. The

$$\underbrace{\circ\cdots\circ}_{a_1 \text{ atoms}} B \underbrace{\circ\cdots\circ}_{a_2 \text{ atoms}} B \underbrace{\circ\cdots\circ}_{a_3 \text{ atoms}} B \cdots B \underbrace{\circ\cdots\circ}_{a_N \text{ atoms}} B$$

Figure 6: The shape of jammed configurations in Rydberg model with blockade range b and exactly N Rydberg atoms, ending with a block B (displayed in Figure 5). Gaps between blocks B, and in front of the first block B, consist of neutral atoms and are of length $0 \le a_i \le b$.

total number of jammed configurations of the shape shown in Figure 6, with L atoms in total, out of which precisely N atoms are excited to the Rydberg state, is given as

$$\binom{N}{M_0, M_1, \ldots, M_b} = \frac{N!}{\prod_{0\le a\le b} M_a!}, \tag{2.5}$$

with M_a satisfying

$$\sum_{a=0}^{b} M_a = N, \tag{2.6}$$

$$\sum_{a=0}^{b} aM_a = L - (b+1)N. \tag{2.7}$$

The constraint (2.6) expresses that the total number of gaps is N. Notice that we have N blocks B (since we want to have precisely N Rydberg atoms), and that gaps of size $0 \le a \le b$ can be added in front of the first block B, and between each two blocks B.

The constraint (2.7) implies that the total number of neutral atoms is $L - N$. Clearly we need $L - N$ neutral atoms in addition to N Rydberg atoms to have a configuration of length L. Equation (2.5) accounts for the jammed configurations ending precisely on B. There are also jammed configurations where the last block B is truncated, and there are only $0 \le c < b$ neutral atoms after the last atom excited to the Rydberg state. The contribution of such jammed configurations to the value of $J_{N,L}$ is comparable to (2.5), but since complexity function ignores sub-exponential factors, it suffices to determine the asymptotics of the sum

$$J_{N,L} \sim \sum_{(M_0,M_1,\ldots,M_b)\in R_{N,L}} \binom{N}{M_0, M_1, \ldots, M_b}, \tag{2.8}$$

where

$$R_{N,L} = \{(M_0, M_1, \ldots, M_b) \in \mathbb{N}_0^{b+1} : M_0 + M_1 + \cdots + M_b = N \text{ and } \\ M_1 + 2M_2 + \cdots + bM_b = L - (b+1)N\}. \tag{2.9}$$

We write H for the Shannon's entropy function given as

$$H(p_0, p_1, \ldots, p_b) = -\sum_{i=0}^{b} p_i \ln p_i, \tag{2.10}$$

where $p_i \ge 0$, for $0 \le i \le b$, and $p_0 + p_1 + \cdots + p_b = 1$.

Remark 2.3. In case $p_i = 0$ for some i, we set $0 \cdot \ln 0 = 0$.

The following lemma is the key result of this section, and it constitutes a crucial step in computing the complexity function of our model as it provides the asymptotics of $J_{N,L}$ in terms of the maximum of the entropy function.

Lemma 2.4.

$$J_{N,L} \sim \exp\left(L \cdot \max_{(M_0,M_1,\ldots,M_b)\in R_{N,L}} \frac{N}{L} \cdot H\left(\frac{M_0}{N}, \frac{M_1}{N}, \ldots, \frac{M_b}{N}\right)\right), \text{ as } L \to \infty.$$

where the set $R_{N,L}$ *is defined in* (2.9)*, and the function* H *is defined in* (2.10).

Proof. Note that

$$\max_{(M_0,M_1,\ldots,M_b)\in R_{N,L}} \binom{N}{M_0, M_1, \ldots, M_b} \le \sum_{(M_0,M_1,\ldots,M_b)\in R_{N,L}} \binom{N}{M_0, M_1, \ldots, M_b} \\ \le |R_{N,L}| \max_{(M_0,M_1,\ldots,M_b)\in R_{N,L}} \binom{N}{M_0, M_1, \ldots, M_b}.$$

As the number $|R_{N,L}|$ of terms in the sum is at most $(N+1)^{b+1} \le (L+1)^{b+1}$, which is polynomial in L, the sum, asymptotically, grows as its largest term. It is, therefore, enough to determine the asymptotics of

$$J_{N,L} \sim \max_{(M_0,M_1,\ldots,M_b)\in R_{N,L}} \binom{N}{M_0, M_1, \ldots, M_b}, \text{ as } L \text{ (and } N) \to \infty.$$

By following the proof of Lemma 2.2 in [11] we can conclude that

$$\binom{N+b}{b}^{-1} \frac{N^N}{{M_0}^{M_0} {M_1}^{M_1} \cdots {M_b}^{M_b}} \leq \binom{N}{M_0, M_1, \ldots, M_b} \leq \frac{N^N}{{M_0}^{M_0} {M_1}^{M_1} \cdots {M_b}^{M_b}}.$$

Note that in case any M_a is zero, the expression 0^0 is to be interpreted as 1. Since $\binom{N+b}{b}$ is of polynomial growth, we get

$$\begin{aligned} \binom{N}{M_0, M_1, \ldots, M_b} &\sim \frac{N^N}{{M_0}^{M_0} {M_1}^{M_1} \cdots {M_b}^{M_b}} \\ &= \left(\frac{N}{M_0}\right)^{M_0} \left(\frac{N}{M_1}\right)^{M_1} \cdots \left(\frac{N}{M_b}\right)^{M_b}, \end{aligned} \tag{2.11}$$

as $N \to \infty$. Note that

$$\left(\frac{N}{M_0}\right)^{M_0} \left(\frac{N}{M_1}\right)^{M_1} \cdots \left(\frac{N}{M_b}\right)^{M_b} = \exp\left(N \cdot H\left(\frac{M_0}{N}, \frac{M_1}{N}, \ldots, \frac{M_b}{N}\right)\right).$$

Hence

$$J_{N,L} \sim \max_{(M_0, M_1, \ldots, M_b) \in R_{N,L}} \exp\left(N \cdot H\left(\frac{M_0}{N}, \frac{M_1}{N}, \ldots, \frac{M_b}{N}\right)\right), \text{ as } L \to \infty,$$

and consequentially

$$J_{N,L} \sim \exp\left(L \cdot \max_{(M_0, M_1, \ldots, M_b) \in R_{N,L}} \frac{N}{L} \cdot H\left(\frac{M_0}{N}, \frac{M_1}{N}, \ldots, \frac{M_b}{N}\right)\right), \text{ as } L \to \infty,$$

which is exactly what we wanted to prove. □

Remark 2.5. One could obtain the asymptotics in (2.11) from Stirling's approximation $N! \sim (N/e)^N$, as $N \to \infty$, where sub-exponential factors are ignored.

3 Complexity function of jammed configurations of Rydberg atoms

In this section we compute the *complexity function*, sometimes referred to as *configurational entropy*, of jammed configurations of Rydberg atoms. We first recall the definition of complexity function of a certain model.

Definition 3.1. For a fixed density $\rho \in [0, 1]$, let $J_{\lfloor \rho L \rfloor, L}$ denote the number of configurations of length L with density $\lfloor \rho L \rfloor / L \approx \rho$. The complexity function $f \colon [0, 1] \to \mathbb{R}$ is then defined as

$$f(\rho) = \lim_{L \to \infty} \frac{\ln J_{\lfloor \rho L \rfloor, L}}{L}, \tag{3.1}$$

for each $\rho \in [0, 1]$ for which this limit exists.

Remark 3.2. If the limit above does not exist for a certain ρ, one can still define (upper) complexity at that point by replacing $\lim$ in the definition with $\limsup$. And if there are no configurations with a certain density ρ, we still write $f(\rho) = 0$.

Remark 3.3. This definition implies that the number of configurations with the density $\lfloor \rho L \rfloor / L \approx \rho$ grows as $e^{Lf(\rho)}$ for large L.

The guiding idea behind introducing the complexity function is to describe what portion of the total number of configurations take up configurations with a particular density. The problem is that, as L grows to infinity, the actual proportions tend to the delta distribution concentrated on the 'most probable' density $\rho_\star$.

As an example, the distribution of densities (the sum of digits divided by the length) of binary sequences of length L is a symmetric binomial distribution re-scaled to the interval $[0, 1]$. The limiting distribution is then the delta distribution $\delta_{0.5}$ which is, essentially, the consequence of the law of large numbers.

This convergence to a delta distribution results from the fact that the number of configurations with a certain density grows exponentially with a rate that depends on the density. For large L, the number of configurations with density having the largest rate overtakes, in proportion, configurations having any other density. The complexity function then quantifies the distribution of all configurations with respect to their densities in a more refined way.

Another consequence of the fact that the number of configurations having density with the largest rate dominates, in proportion, any other density is that the total number of all configurations grows at the same exponential rate as the number of configurations having this 'most probable density'. To be precise, if $\rho_\star$ denotes the density at which the complexity function f attains its maximum and if J_L is the total number of all configurations of length L, then $J_L \sim e^{Lf(\rho_\star)}$ for large L.

Remark 3.4. In Lemma 2.1 we derived the generating function for the sequence $J_{N,L}$ within the Rydberg atom model. Plugging $x = 1$ into this generating function gives the generating function for J_L, the total number of configurations of length L in Rydberg atom model

$$\begin{aligned} F_b(1, y) &= \frac{(1-y)^2 + y - y^{b+1} - y^{b+2} + y^{2b+2}}{(1-y)(1-y-y^{b+1}+y^{2b+2})} \\ &= \frac{1 + y(1 + y + \cdots + y^b)(1 + y + \cdots + y^{b-1})}{1 - y^{b+1}(1 + y + \cdots + y^b)}. \end{aligned}$$

From here, we can infer the asymptotics of J_L for large L by inspecting the roots of the polynomial $1 - y^{b+1}(1 + y + \cdots + y^b)$ in the denominator. More precisely, if y_b is the root with the smallest modulus, then the logarithm of $w_b = |y_b|^{-1}$ gives the exponential growth rate of the sequence J_L

$$J_L \sim w_b^L = e^{L \ln w_b}.$$

The discussion in the previous paragraph now implies the relation $f(\rho_\star^{b\text{-Ryd}}) = \ln w_b$.

The following theorem is the main result of this paper and provides an elegant expression for the complexity function of jammed configurations of Rydberg atoms $f(\rho)$ in terms of a root of a certain polynomial.

Theorem 3.5. *The complexity function of jammed configurations of Rydberg atoms with blockade range $b \in \mathbb{N}$ is given as*

$$f(\rho) = \begin{cases} \rho\left[-\ln\frac{1-z}{1-z^{b+1}} - \left(\frac{1}{\rho} - (b+1)\right)\ln z\right], & \text{if } \frac{1}{2b+1} < \rho \le \frac{1}{b+1}, \\ 0, & \text{otherwise,} \end{cases}$$

where $z \geq 0$ is a real root of the polynomial

$$p(z) = \sum_{i=0}^{b} \left(i + b + 1 - \frac{1}{\rho} \right) z^i \tag{3.2}$$

for which the expression $f(\rho)$ is the largest.

Remark 3.6. When $\frac{1}{2b+1} < \rho < \frac{1}{b+1}$ the leading coefficient of the polynomial $p(z)$ given in (3.2) is positive, while the constant term is negative. This guaranties the existence of at least one positive real root $z > 0$. If $\rho = \frac{1}{b+1}$, then $z = 0$ is the root of $p(z)$ and the formula gives $f(\frac{1}{b+1}) = 0$.

Remark 3.7. Since (3.2) is a polynomial of degree b, it is possible to find its roots explicitly for $b \leq 4$ and numerically for $b > 4$. The explicit expression for the complexity in case $b = 1$ is

$$f^{\text{1-Ryd}}(\rho) = \rho \ln \rho - (1 - 2\rho) \ln(1 - 2\rho) - (3\rho - 1) \ln(3\rho - 1),$$

and for $b = 2$

$$\begin{aligned} f^{\text{2-Ryd}}(\rho) = (3\rho - 1) \ln \frac{\sqrt{-44\rho^2 + 24\rho - 3} - 4\rho + 1}{10\rho - 2} - \\ \rho \ln \frac{-350\rho^3 + (25\rho^2 - 10\rho + 1)\sqrt{-44\rho^2 + 24\rho - 3} + 215\rho^2 - 44\rho + 3}{\rho^2 \sqrt{-44\rho^2 + 24\rho - 3} - 134\rho^3 + 57\rho^2 - 6\rho}. \end{aligned}$$

In the case $b = 1$, the function $f^{\text{1-Ryd}}(\rho)$ recovers the result from [44, formula (7.20)] and [41, §VII]. The graphs of the complexity function of jammed configurations of Rydberg atoms with blockade range $1 \leq b \leq 10$ are given in Figure 7. In that figure we also see that, for each b, the maximum of the complexity function matches $\ln w_b$, the growth rate of all jammed configurations. This was already discussed in Remark 3.4.

Proof of Theorem 3.5. Recall that in (2.2) we showed that

$$\frac{1}{2b+1} - \frac{1}{L} < \frac{N}{L} \leq \frac{1}{b+1},$$

and therefore, there are no jammed configurations with densities $\rho > \frac{1}{b+1}$ nor with densities $\rho < \frac{1}{2b+1}$, for sufficiently large L. Thus, $f(\rho) = 0$ when $\rho > \frac{1}{b+1}$ or $\rho < \frac{1}{2b+1}$. In case $\rho = \frac{1}{2b+1}$, it is not hard to see that the number of configurations $J_{\lfloor \frac{L}{2b+1} \rfloor, L}$ is

$$J_{\lfloor \frac{L}{2b+1} \rfloor, L} = \begin{cases} 1, & \text{if } (2b+1) \mid L, \\ 0, & \text{otherwise.} \end{cases}$$

This implies $f(\frac{1}{2b+1}) = 0$ by the definition of complexity.

In the remainder, we fix $\frac{1}{2b+1} < \rho \leq \frac{1}{b+1}$. By Lemma 2.4, and by using the definition of the complexity function (3.1), we have

$$f(\rho) = \lim_{L \to \infty} \max_{(M_0, M_1, \ldots, M_b) \in R_{N,L}} \frac{N}{L} \cdot H\left(\frac{M_0}{N}, \frac{M_1}{N}, \ldots, \frac{M_b}{N} \right), \tag{3.3}$$

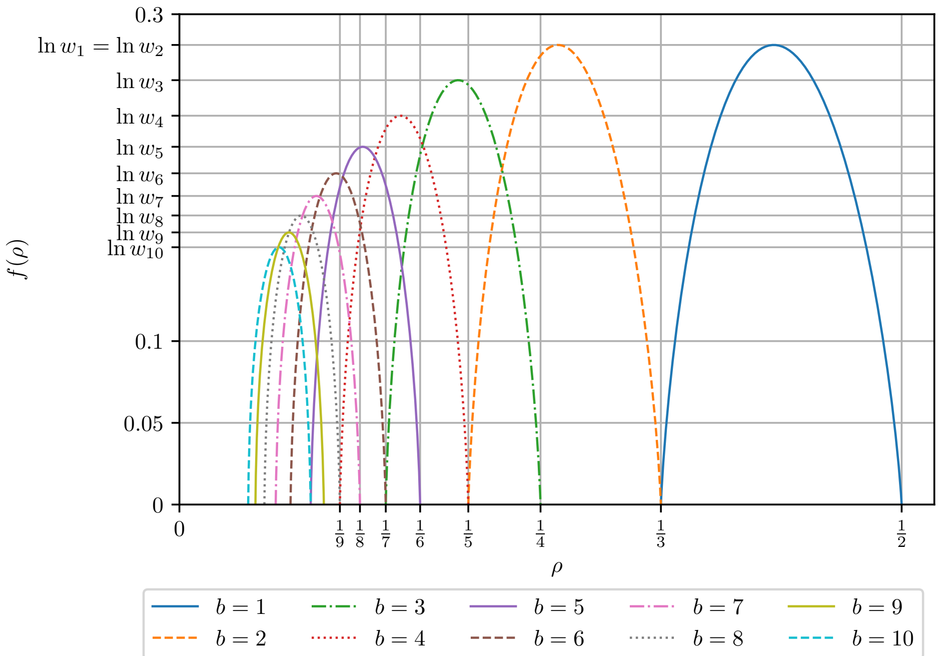

Figure 7: The complexity function of jammed configurations of Rydberg atoms with blockade range $1 \leq b \leq 10$.

where $N = \lfloor \rho L \rfloor$, provided that this limit exists. By rewriting $(M_0, M_1, \dots, M_b) \in R_{N,L}$ as

$$\begin{gathered}
\frac{M_0}{N} \geq 0, \frac{M_1}{N} \geq 0, \dots, \frac{M_b}{N} \geq 0 \\
\frac{M_0}{N} + \frac{M_1}{N} + \cdots + \frac{M_b}{N} = 1 \\
\frac{M_1}{N} + 2\frac{M_2}{N} + \cdots + b\frac{M_b}{N} = \frac{L}{N} - (b+1)
\end{gathered}$$

and denoting $p_i = \frac{M_i}{N} \in \frac{1}{\lfloor \rho L \rfloor}\mathbb{Z}$, the complexity (3.3) can be written as

$$f(\rho) = \lim_{L\to\infty} \max_{(p_0,p_1,\dots,p_b)\in \frac{1}{\lfloor \rho L \rfloor} R_{\lfloor \rho L \rfloor, L}} \hat{\rho} H\left(p_0, p_1, \dots, p_b\right), \tag{3.4}$$

where $\hat{\rho} = \hat{\rho}(L) = \frac{N}{L} = \frac{\lfloor \rho L \rfloor}{L}$. We claim that this limit exists and is equal to the maximum of the constrained optimization problem

$$\max_{\substack{p_0,p_1,\dots,p_b \geq 0 \\ p_0+p_1+\cdots+p_b=1 \\ p_1+2p_2+\cdots+bp_b=\frac{1}{\rho}-(b+1)}} \rho H\left(p_0, p_1, \dots, p_b\right), \tag{3.5}$$

where $p_i \in \mathbb{R}$ are no longer required to be fractions.

We argue as follows. Denote by $(p_0^*, p_1^*, \ldots, p_b^*)$ the point at which the maximum in (3.5) is attained. For each $L \in \mathbb{N}$, let $(p_0(L), p_1(L), \ldots, p_b(L))$ be the point at which maximum in (3.4) is attained. Clearly,

$$\hat{\rho} H\left(p_0(L), p_1(L), \ldots, p_b(L)\right) \leq \hat{\rho} H(p_0^*, p_1^*, \ldots, p_b^*) \leq \rho H(p_0^*, p_1^*, \ldots, p_b^*).$$

The first inequality follows by substituting $\hat{\rho}$ for ρ in (3.5) and the fact that one is now optimizing over a larger set. The second inequality follows from $\hat{\rho} \leq \rho$. Note that the right hand side no longer depends on L, and thus

$$\limsup_{L \to \infty} \hat{\rho} H\left(p_0(L), p_1(L), \ldots, p_b(L)\right) \leq \rho H(p_0^*, p_1^*, \ldots, p_b^*).$$

Next, for each $L \in \mathbb{N}$, we consider the point $(t_0(L), t_1(L), \ldots, t_b(L)) \in \frac{1}{\lfloor \rho L \rfloor} R_{\lfloor \rho L \rfloor, L}$, which is closest to the to the optimizer $(p_0^*, p_1^*, \ldots, p_b^*)$. Note that, due to the density argument, $(t_0(L), t_1(L), \ldots, t_b(L)) \to (p_0^*, p_1^*, \ldots, p_b^*)$ as $L \to \infty$. This, along with the continuity of H and the fact that $\hat{\rho} \to \rho$ implies the lower bound

$$\begin{aligned} \rho H(p_0^*, p_1^*, \ldots, p_b^*) = \lim_{L \to \infty} \hat{\rho} H(t_0(L), t_1(L), \ldots, t_b(L)) \leq \\ \leq \liminf_{L \to \infty} \hat{\rho} H\left(p_0(L), p_1(L), \ldots, p_b(L)\right). \end{aligned}$$

Putting everything together completes the argument that the limit

$$f(\rho) = \lim_{L \to \infty} \hat{\rho} H\left(p_0(L), p_1(L), \ldots, p_b(L)\right)$$

exists and that the complexity function is

$$f(\rho) = \rho H(p_0^*, p_1^*, \ldots, p_b^*) = \max_{\substack{p_0, p_1, \ldots, p_b \geq 0 \\ p_0 + p_1 + \cdots + p_b = 1 \\ p_1 + 2p_2 + \cdots + bp_b = \frac{1}{\rho} - (b+1)}} \rho \cdot H\left(p_0, p_1, \ldots, p_b\right).$$

In order to obtain the expression for complexity $f(\rho)$, it only remains to solve the constrained optimization problem (3.5). We define the Lagrangian function

$$\begin{aligned} \mathcal{L}(p_0, \ldots, p_b; \lambda, \mu) = \rho \cdot H(p_0, p_1, \ldots, p_b) - \lambda(p_0 + p_1 + \cdots + p_b - 1) \\ - \mu(p_1 + 2p_2 \cdots + bp_b - \frac{1}{\rho} + (b+1)), \end{aligned}$$

and find the stationary point by solving the system

$$\begin{aligned} -\rho(\ln p_i + 1) - \lambda - \mu i = 0, \qquad & \text{for } i = 0, 1, \ldots, b; \\ p_0 + p_1 + \cdots + p_b = 1; \\ p_1 + 2p_2 \cdots + bp_b = \frac{1}{\rho} - (b+1). \end{aligned} \tag{3.6}$$

By multiplying i-th of the first $(b+1)$ equations by p_i and adding them together we get

$$-\rho \sum_{i=0}^{b} (p_i \ln p_i + p_i) - \lambda \sum_{i=0}^{b} p_i - \mu \sum_{i=0}^{b} i p_i = 0,$$

and from here we obtain the expression for complexity in terms of the Lagrange multipliers λ and μ which solve the system (3.6)

$$f(\rho) = \rho H(p_0, p_1, \ldots, p_b) = \rho + \lambda + \mu\left(\frac{1}{\rho} - (b+1)\right). \tag{3.7}$$

Subtracting successive equations in (3.6) we get

$$-\rho(\ln p_i - \ln p_{i-1}) - \mu = 0,$$

or equivalently

$$\frac{p_i}{p_{i-1}} = e^{-\mu/\rho}.$$

Therefore $p_i = p_0 e^{-\mu i/\rho}$, for $i = 1, \ldots, b$. From the very first equation in (3.6) we get

$$p_0 = e^{-\lambda/\rho - 1},$$

and the whole system (3.6) now reduces to just two equations

$$e^{-\lambda/\rho-1}\sum_{i=0}^{b} e^{-\mu i/\rho} = 1; \tag{3.8}$$

$$e^{-\lambda/\rho-1}\sum_{i=0}^{b} i e^{-\mu i/\rho} = \frac{1}{\rho} - (b+1). \tag{3.9}$$

Setting $z = e^{-\mu/\rho}$, and eliminating $e^{-\lambda/\rho-1}$ from equations (3.8) and (3.9), gives a single polynomial equation of degree b

$$bz^b + (b-1)z^{b-1} + \cdots + 2z^2 + z = \left[\frac{1}{\rho} - (b+1)\right](z^b + z^{b-1} + \cdots + z + 1), \tag{3.10}$$

which can be written as $p(z) = 0$ where $p(z)$ is given in (3.2).

Now, in order to obtain the complexity, all we need is, for a fixed $\frac{1}{2b+1} < \rho < \frac{1}{b+1}$, to find a real root $z > 0$ of the polynomial $p(z)$ for which the expression (3.7) is the largest. The case $\rho = \frac{1}{b+1}$, which gives $z = 0$, has to be treated separately. From relation $z = e^{-\mu/\rho}$ and equation (3.8) we have

$$\begin{aligned} \mu &= -\rho \ln z; \\ \lambda &= -\rho\left(1 + \ln\frac{1-z}{1-z^{b+1}}\right). \end{aligned} \tag{3.11}$$

Plugging (3.11) into (3.7), gives the complexity expressed in terms of the root of $p(z)$

$$f(\rho) = \rho\left[-\ln\frac{1-z}{1-z^{b+1}} - \left(\frac{1}{\rho} - (b+1)\right)\ln z\right].$$

Lastly, in case $\rho = \frac{1}{b+1}$, already from the last two equations in (3.6) we can conclude $p_1 = p_2 = \cdots = p_b = 0$ and $p_0 = 1$. This immediately gives $f(\rho) = 0$ as $H(1, 0, 0, \ldots, 0) = 0$, completing the proof. $\square$

Remark 3.8. Using the standard summation formulas, we can rewrite (3.10) as

$$\frac{bz^{b+2}-(b+1)z^{b+1}+z}{(1-z)^2}=\left[\frac{1}{\rho}-(b+1)\right]\frac{1-z^{b+1}}{1-z}, \tag{3.12}$$

or equivalently

$$\left[(2b+1)-\frac{1}{\rho}\right]z^{b+2}-\left[(2b+2)-\frac{1}{\rho}\right]z^{b+1}-\left[b-\frac{1}{\rho}\right]z+\left[(b+1)-\frac{1}{\rho}\right]=0.$$

As discussed in the introduction, the complexity function is associated to *equilibrium* (or *static*) models of a certain phenomena and $\rho_\star$, the point at which the complexity function attains its maximum, is interpreted as the expected and most probable density observed in such a model. This value $\rho_\star$ is sometimes called the *equilibrium density* of the model and Theorem 3.9 below shows how to calculate it. A different (and perhaps more natural) way to look at Rydberg atom model is *dynamically*, within the framework of random sequential adsorption (RSA). Initially neutral atoms are sequentially and at random excited (obeying the blockade range constraint) until the jammed configuration is reached. The expected density of the reached jammed configuration (the *jamming limit*) in this dynamical version of the model, denoted by $\rho_\infty^{b\text{-Ryd}}$, was computed in [42, §IV]

$$\rho_\infty^{b\text{-Ryd}}=\int_0^1\exp\left[-2\sum_{j=1}^{b}\frac{1-y^j}{j}\right]dy.$$

It is interesting to compare $\rho_\star^{b\text{-Ryd}}$ and $\rho_\infty^{b\text{-Ryd}}$ for different blockade ranges b. Even though

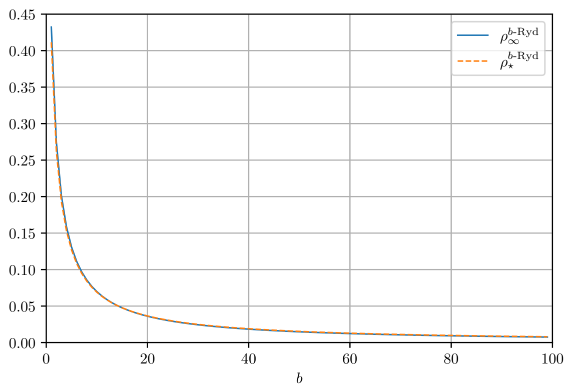

Figure 8: Comparison of $\rho_\star^{b\text{-Ryd}}$ and $\rho_\infty^{b\text{-Ryd}}$ for $1 \leq b \leq 99$.

they are not the same, they seem to match quite nicely, see Figure 8. Additionally, as one would expect, they both tend to zero for large b. One can see their differences more clearly in Figure 9. This violation of Edwards flatness hypothesis is even more pronounced when one inspects the asymptotics of the two sequences more closely. In Figure 10 we see the graph of quantities $b \cdot \rho_\star^{b\text{-Ryd}}$ and $b \cdot \rho_\infty^{b\text{-Ryd}}$.

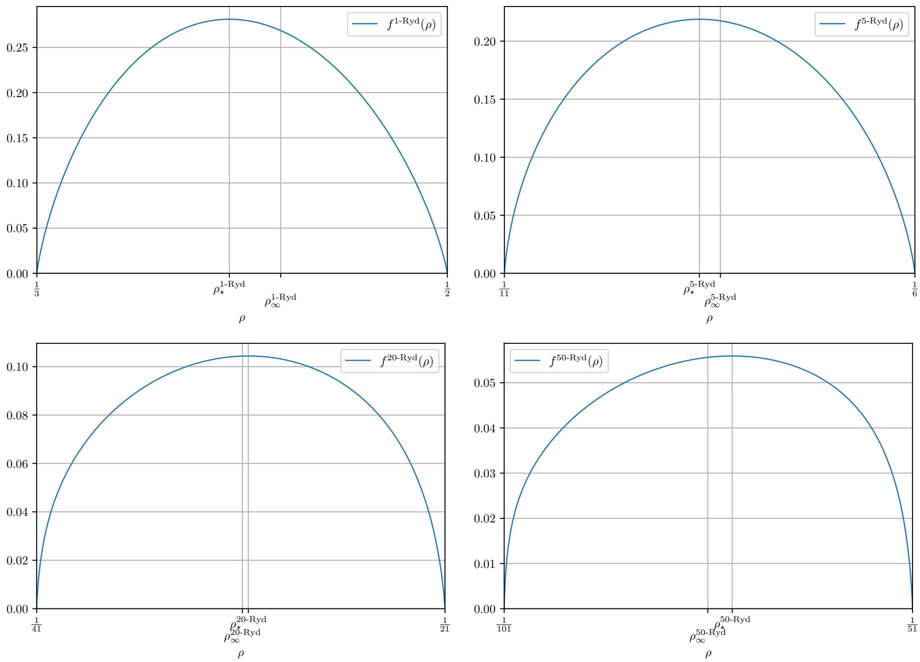

Figure 9: Complexity function of Rydberg atom model with blockade range b, for $b \in \{1, 5, 20, 50\}$. Also plotted in each graph are the equilibrium density $\rho_\star^{b\text{-Ryd}}$ and the jamming density $\rho_\infty^{b\text{-Ryd}}$.

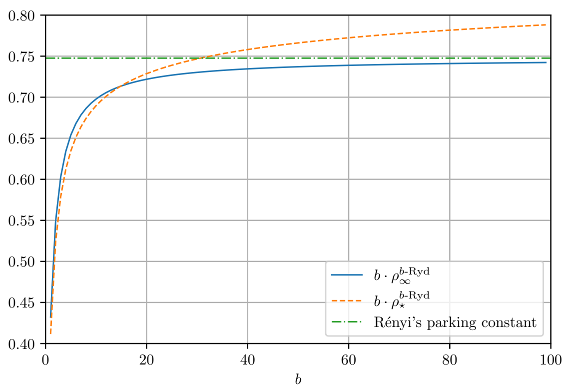

Figure 10: Comparison of $b \cdot \rho_\star^{b\text{-Ryd}}$ and $b \cdot \rho_\infty^{b\text{-Ryd}}$ for $1 \le b \le 99$.

It can be shown that these two sequences approach different constants as b grows large

$$\begin{aligned} \lim_{b\to\infty} b \cdot \rho_\infty^{b\text{-Ryd}} &= \int_0^\infty \exp\left[-2\int_0^y \frac{1-e^{-x}}{x}dx\right] dy = 0.7475979202\ldots \\ \lim_{b\to\infty} b \cdot \rho_\star^{b\text{-Ryd}} &= 1. \end{aligned} \tag{3.13}$$

The constant appearing in the first limit is known as Rényi's parking constant [57]. Both of these two limits are easier to understand in the context of irreversible deposition of k-mers. We deal with the k-mer deposition model in the following section where we revisit those limits.

The calculation below, showing how to obtain the first limit in (3.13), and which we provide for completeness, appears in [32]. First note

$$\sum_{j=1}^{b} \frac{1-y^j}{j} = \sum_{j=1}^{b} \int_y^1 t^{j-1}\, dt = \int_y^1 \sum_{j=1}^{b} t^{j-1}\, dt = \int_y^1 \frac{1-t^b}{1-t}\, dt$$
$$= \begin{bmatrix} x = b(1-t) \\ dx = -b\, dt \end{bmatrix} = \int_0^{b(1-y)} \frac{1-(1-\frac{x}{b})^b}{x}\, dx,$$

and therefore

$$\begin{aligned} b \cdot \rho_\infty^{b\text{-Ryd}} &= b \int_0^1 \exp\left[-2 \sum_{j=1}^{b} \frac{1-y^j}{j}\right] dy \\ &= b \int_0^1 \exp\left[-2 \int_0^{b(1-y)} \frac{1-(1-\frac{x}{b})^b}{x}\, dx\right] dy \\ &= \begin{bmatrix} \tilde{y} = b(1-y) \\ d\tilde{y} = -b\, dy \end{bmatrix} = \int_0^b \exp\left[-2 \int_0^{\tilde{y}} \frac{1-(1-\frac{x}{b})^b}{x}\, dx\right] d\tilde{y}. \end{aligned}$$

The dominated convergence theorem now implies

$$\lim_{b\to\infty} b \cdot \rho_\infty^{b\text{-Ryd}} = \int_0^\infty \exp\left[-2 \int_0^y \frac{1-e^{-x}}{x} dx\right] dy = 0.7475979202\ldots$$

Before we calculate the second limit in (3.13), we give a characterization of the value $\rho_\star^{b\text{-Ryd}}$ in terms of a root of a certain polynomial. Compare this with the same results obtained by Došlić [20, discussion after Theorem 2.10] and Krapivsky–Luck [43, (3.4), (3.14) and (6.6)].

Theorem 3.9. *The value $\rho_\star^{b\text{-Ryd}}$, at which the complexity of the Rydberg atom model with blockade range b, given in* Theorem 3.5*, attains its maximum, can be calculated as*

$$\rho_\star^{b\text{-Ryd}} = \frac{(1-z)(1-z^{b+1})}{1+b-bz-2z^{b+1}-2bz^{b+1}+z^{b+2}+2bz^{b+2}}, \tag{3.14}$$

where z is the unique root of the polynomial

$$z^{2b+1} + \cdots + z^{b+2} + z^{b+1} - 1,$$

on the interval $0 < z < 1$.

Proof. We seek to find the density $\frac{1}{2b+1} < \rho_\star^{b\text{-Ryd}} < \frac{1}{b+1}$ at which the complexity $f = f^{b\text{-Ryd}}$ in Theorem 3.5 attains its maximum. Again, we employ the Lagrangian function method by setting

$$\begin{aligned}\mathcal{L}(\rho, z; \lambda) &= \rho\left[-\ln\frac{1-z}{1-z^{b+1}} - \left(\frac{1}{\rho} - (b+1)\right)\ln z\right] - \lambda\sum_{i=0}^{b}\left(i+b+1-\frac{1}{\rho}\right)z^i \\ &= \rho\ln\frac{1-z^{b+1}}{1-z} - (1-\rho(b+1))\ln z - \lambda\sum_{i=0}^{b}\left(i+b+1-\frac{1}{\rho}\right)z^i.\end{aligned}$$

The stationary points of this function solve the following system

$$\begin{gathered}\ln\frac{1-z^{b+1}}{1-z} + (b+1)\ln z - \frac{\lambda}{\rho^2}\cdot\frac{1-z^{b+1}}{1-z} = 0 \\ -\frac{\rho(b+1)z^b}{1-z^{b+1}} + \frac{\rho}{1-z} - \frac{(1-\rho(b+1))}{z} - \lambda\sum_{i=1}^{b} i\left(i+b+1-\frac{1}{\rho}\right)z^{i-1} = 0 \\ \sum_{i=0}^{b}\left(i+b+1-\frac{1}{\rho}\right)z^i = 0.\end{gathered}$$

Using standard summation formulas, as in (3.12), it is possible to express ρ from the third equation as

$$\rho = \frac{(1-z)(1-z^{b+1})}{1+b-bz-2z^{b+1}-2bz^{b+1}+z^{b+2}+2bz^{b+2}}.$$

Plugging this into the second equation gives

$$0 = \lambda\sum_{i=1}^{b} i\left(i+b+1-\frac{1}{\rho}\right)z^{i-1}.$$

From here, we conclude $\lambda = 0$. Finally, from the first equation we get

$$\lambda = \rho^2\frac{1-z}{1-z^{b+1}}\ln\frac{z^{b+1}(1-z^{b+1})}{1-z}$$

and, combining this with $\lambda = 0$, gives

$$\ln\frac{z^{b+1}(1-z^{b+1})}{1-z} = 0,$$

or

$$z^{b+1}(1-z^{b+1}) = 1-z.$$

We know from Theorem 3.5 that $z \neq 1$, so we can rewrite this equation as

$$z^{2b+1} + \cdots + z^{b+2} + z^{b+1} - 1 = 0.$$

Clearly, there is a unique $0 < z < 1$ solving this equation, and the corresponding

$$\rho_\star^{b\text{-Ryd}} = \frac{(1-z)(1-z^{b+1})}{1+b-bz-2z^{b+1}-2bz^{b+1}+z^{b+2}+2bz^{b+2}}$$

is the density at which the complexity in the Rydberg atom model with blockade range b is the largest. □

The previous theorem can be used to give a proof of the second limit in (3.13).

Corollary 3.10.

$$\lim_{b\to\infty} b \cdot \rho_\star^{b\text{-}Ryd} = 1.$$

Proof. Since $0 < z = z(b) < 1$ solves the equation

$$\frac{z^{b+1}(1-z^{b+1})}{1-z} = z^{2b+1} + \cdots + z^{b+2} + z^{b+1} = 1 \tag{3.15}$$

it follows

$$bz^{2b+1} < 1 < bz^{b+1}$$

and therefore

$$\lim_{b\to\infty} z^{2b+1} = 0.$$

Multiplying by z and taking square root we also get

$$\lim_{b\to\infty} z^{b+1} = 0.$$

Finally, letting $b \to \infty$ in the identity $z^{b+1}(1-z^{b+1}) = 1-z$, gives

$$\lim_{b\to\infty} z = 1.$$

Note that

$$b \cdot \rho_\star^{b\text{-Ryd}} = \frac{b(1-z)(1-z^{b+1})}{1 + b(1-z)[1-2z^{b+1}] - 2z^{b+1} + z^{b+2}}$$

so in order to get $\lim_{b\to\infty} b \cdot \rho_\star^{b\text{-Ryd}} = 1$, it suffices to show $\lim_{b\to\infty} b(1-z) = \infty$. To see this, note that from (3.15) it follows

$$(b+1)\ln z = \ln(1-z) - \ln(1-z^{b+1})$$

and hence

$$\lim_{b\to\infty} (b+1)(1-z) = \lim_{b\to\infty} \frac{1-z}{\ln z} \cdot \left[\ln(1-z) - \ln(1-z^{b+1})\right] = -1 \cdot [-\infty - 0] = +\infty$$

which completes the argument. □

4 Complexity function of jammed configurations for irreversible deposition of k-mers

It is easy to see that the Rydberg atom model with blockade range b is, up to scaling all densities by a factor $b+1$, equivalent to the irreversible deposition of k-mers model where $k = b+1$. As an immediate consequence of Theorem 3.5 we get the complexity of jammed configurations for irreversible deposition of k-mers.

Corollary 4.1. *For $k \in \mathbb{N}$, $k > 1$, the complexity function of jammed configurations for irreversible deposition of k-mers is*

$$f(\rho) = \begin{cases} \frac{\rho}{k}\left[-\ln\frac{1-z}{1-z^k} - \left(\frac{k}{\rho} - k\right)\ln z\right], & \text{if } \frac{k}{2k-1} < \rho \le 1, \\ 0, & \text{otherwise,} \end{cases}$$

where $z \geq 0$ is a real root of the polynomial

$$\sum_{i=0}^{k-1} \left(i + k - \frac{k}{\rho}\right) z^i$$

for which the expression $f(\rho)$ is the largest.

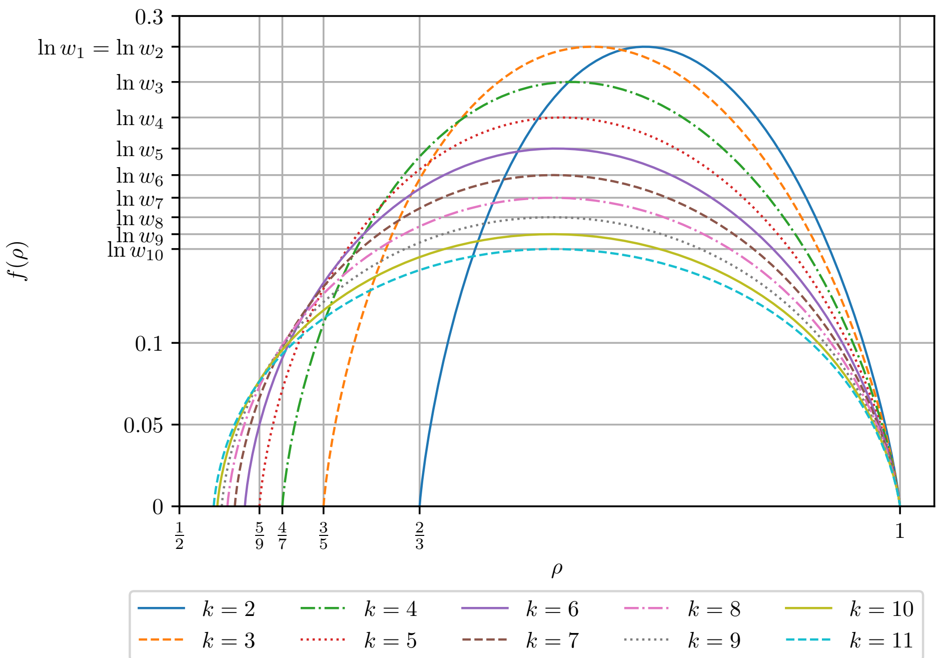

Figure 11: The complexity function of jammed configurations for irreversible deposition of k-mers, for $2 \leq k \leq 11$.

Figure 11 shows the complexity function for all $2 \leq k \leq 11$. Note that the support of the complexity function is now contained in the interval $[1/2, 1]$. In Figure 12 we compare the equilibrium density $\rho_\star^{k\text{-mer}}$ and the jamming density $\rho_\infty^{k\text{-mer}}$, for $2 \leq k \leq 100$. In this model it is even more obvious that the Edwards hypothesis is violated. The limits of these two sequences as k grows large are

$$\begin{aligned} \lim_{k\to\infty} \rho_\infty^{k\text{-mer}} &= \int_0^\infty \exp\left[-2\int_0^y \frac{1-e^{-x}}{x} dx\right] dy = 0.7475979202\ldots \\ \lim_{k\to\infty} \rho_\star^{k\text{-mer}} &= 1. \end{aligned} \tag{4.1}$$

Note that these limits are equivalent to those in (3.13). The convergence of jamming limits of k-mer deposition models (as k grows to infinity) to the Rényi's parking constant is discussed in [44, §7.1] (see also [28, 32]).

Clearly, the second limit from (4.1) follows from Corollary 3.10 as $\rho_\star^{k\text{-mer}} = k \cdot \rho_\star^{b\text{-Ryd}}$ for $b = k - 1$. Below, we provide a direct alternative proof of this fact.

Theorem 4.2.

$$\lim_{k\to\infty} \rho_\star^{k\text{-}mer} = 1.$$

Proof. The quantity we are interested in, $\rho_\star^{k\text{-mer}}$, is equivalent to the quantity called the *efficiency* $\varepsilon(k)$ in the context of packing P_k into P_n. It was shown in [20] that the efficiency is determined by the smallest singularity w_k of the generating function $F_k(1, y)$, i.e., by the smallest zero of its denominator. Hence we start by setting $x = 1$ into the rightmost expression in (2.4),

$$F_k(1, y) = \frac{1 - y^k}{1 - y - y^k - y^{2k}} = \frac{\frac{1-y^k}{1-y}}{1 - y^k \frac{1-y^k}{1-y}}.$$

We rewrite its denominator as $1 - q_k(y)$, where $q_k(y) = q^k \frac{1-y^k}{1-y}$, and denote the smallest solution of equation $q_k(y) = 1$ by w_k. This equation has only one positive solution, since $q_k(0) = 0$, $q_k(1) = k > 1$ for large k and $q_k'(y) > 0$ for all $y > 0$. Moreover, the same reasoning provides a better lower bound for w_k, since $q_k(\frac{1}{2}) = 2^{(1-k)}(1 - 2^{-k}) < 1$. Hence $1/2 < w_k < 1$.

Consider now the expression

$$\varepsilon(k) = \rho_\star^{k\text{-mer}} = \frac{k}{w_k q_k'(x)}$$

derived in [20]. First we rewrite $q_k'(w_k)$ as

$$q_k'(x) = x^k \frac{1 - x^k}{1 - x} \left[\frac{2k}{x} - \frac{k}{x(1 - x^k)} + \frac{1}{1 - x}\right].$$

After plugging in $x = w_k$, the term outside the brackets becomes equal to one, and by multiplying through by w_k we arrive at

$$w_k q_k'(w_k) = \left(2 - \frac{1}{1 - w_k^k}\right) k + \frac{w_k}{1 - w_k}.$$

We are seeking upper bounds to the right-hand side. The first term is bounded from above by k, since the expression in parentheses cannot exceed one. It remains to bound the second term. As mentioned before, w_k is the only positive solution of the equation $1 - q_k(x) = 0$. We claim that, for a given (large) positive a, $w_k < 1 - \frac{a}{k}$ for large enough k. So let us suppose otherwise, that for a given $a > 0$, $w_k > 1 - \frac{a}{k}$ is valid for all k. It means that the function $1 - q_k(x)$ has a positive value for $x = 1 - \frac{a}{k}$. By evaluating both sides, we obtain that

$$\left(1 - \frac{a}{k}\right)^k - \left(1 - \frac{a}{k}\right)^{2k} < \frac{a}{k}$$

is valid for all k. This is a contradiction, since the left-hand side has a positive limit, $e^{-a} - e^{-2a} > 0$, while the right-hand side tends to zero as k tends to infinity. Hence, $w_k < 1 - \frac{a}{k}$ for large enough k. Now the second term can be bounded from above by $\frac{a}{k}$, and the whole expression for $w_k q_k'(w_k)$ is bounded from above by $\frac{a+1}{a} k$. Since a can be taken arbitrarily large, it means that the reciprocal value of $w_k q_k'(w_k)$, which is equal to our $\rho_\star^{k\text{-mer}}$, comes arbitrarily close to one, and our claim follows. □

The convergence is quite slow, most likely logarithmic. We note another unusual thing in Figure 12. The equilibrium density $\rho_\star^{k\text{-mer}}$ attains the minimum value for $k = 9$. The interpretation being that the polymers of length 9 pack the least efficiently of all polymers assuming the equilibrium model. This phenomenon was previously observed in [20].

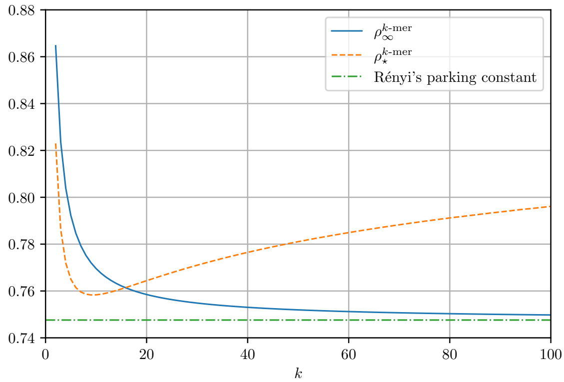

Figure 12: Comparison of $\rho_\star^{k\text{-mer}}$ and $\rho_\infty^{k\text{-mer}}$ for $2 \leq k \leq 100$.

5 Conclusions

In this paper we have computed the complexity function (or configurational entropy) of jammed configurations of Rydberg atoms with a given blockade range on a one-dimensional lattice. We employed a purely combinatorial method which allowed us to compute the complexity function by solving a constrained optimization problem. Along the way we have explored and elucidated numerous connections between the considered problem and other models, such as, e.g., the random sequential adsorption and packings of blocks of a given length into one-dimensional lattices. In most cases, we have not followed those links very far. We believe that many interesting results could be obtained by deeper investigations of those connections. As an example, we mention here that explicit expressions for the number of maximal packings of given size from reference [20] could be directly translated into expressions for the number of jammed configurations of Rydberg atoms. By the same reasoning one can show that the total number of all jammed configurations of N Rydberg atoms with blockade range b on all one-dimensional lattices is given by $(b+1)^{N+1}$.

The methods employed here could be easily adapted for other one-dimensional structures with low connectivity such as, e.g., cactus chains. Another class of promising structures could be various simple graphs decorated by addition of certain number of vertices of degree one to each of their vertices.

Similar problems were considered under various guises also for finite portions of rectangular lattices, mostly for narrow strips of varying length. Among the best known problems of this type are the so-called unfriendly seating arrangements. See [7, 30] for their history and some recent developments. To the same class belong the problems concerned with privacy, such as the ones considered in [39]. All cited references were concerned with one-dimensional lattices and/or narrow strips in the square grid, mostly with ladders. It would be interesting to consider those problems in finite portions of the regular hexagonal lattice.

Another interesting thing to do would be to study the behavior (and the difference) of ρ_∞ and $\rho_\star$ for different lattices/substrates. In other words, to investigate the difference between the jamming limit of dynamical models and the most probable densities in the equilibrium models. A drastic example is presented by the expected density of independent sets in stars: there are exactly two maximal independent sets in $S_n = K_{1,n-1}$, one of them with size 1 and the other with size $n-1$. If both of them are equally probable, the expected size is $n/2$. Under dynamical model, however, the smaller one is much less probable than the bigger one, and the expected size is $\frac{1}{n} + \frac{n-1}{n}(n-1) = n-2+\frac{2}{n}$. It would be interesting to know more about such differences and to know for which classes of graphs they are extremal.

Our final remark is that the jammed configurations of Rydberg atoms with a given blockade range b are known as maximal b-independent sets in the language of graph theory. It might be worth investigating to what extent can similar problems be formulated also in terms of b-dominance in graphs.

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Distinguishing colorings, proper colorings, and covering properties without AC*

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Abstract

We work with simple graphs in ZF (i.e., the Zermelo–Fraenkel set theory without the Axiom of Choice (AC)) and assume that the sets of colors can be either well-orderable or non-well-orderable, to prove that the following statements are equivalent to Kőnig's Lemma:

(a) Any infinite locally finite connected graph G such that the minimum degree of G is greater than k, has a chromatic number for any fixed integer k greater than or equal to 2.

(b) Any infinite locally finite connected graph has a chromatic index.

(c) Any infinite locally finite connected graph has a distinguishing number.

(d) Any infinite locally finite connected graph has a distinguishing index.

The above results strengthen some recent results of Stawiski since he assumed that the sets of colors can be well-ordered. We formulate new conditions for the existence of irreducible proper coloring, minimal edge cover, maximal matching, and minimal dominating set in connected bipartite graphs and locally finite connected graphs, which are either equivalent to AC or Kőnig's Lemma. Moreover, we show that if the Axiom of Choice for families of 2-element sets holds, then the Shelah-Soifer graph has a minimal dominating set.

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1 Introduction

In 1991, Galvin–Komjáth proved that the statements "Any graph has a chromatic number" and "Any graph has an irreducible proper coloring" are equivalent to AC in ZF using Hartogs's theorem (cf. [7]). In 1977, Babai [1] introduced distinguishing vertex colorings under the name asymmetric colorings, and distinguishing edge colorings were introduced by Kalinowski–Pilśniak [14] in 2015. Recently, Stawiski [20] proved that the statements (b)–(d) mentioned in the abstract above and the statement "Any infinite locally finite connected graph has a chromatic number" are equivalent to Kőnig's Lemma (a weak form of AC) by assuming that the sets of colors can be well-ordered (cf. [20, Lemma 3.3 and Section 2]).

1.1 Proper and distinguishing colorings

An infinite cardinal in ZF can either be an ordinal or a set that is not well-orderable. Herrlich–Tachtsis [10, Proposition 23] proved that no Russell graph has a chromatic number in ZF. We refer the reader to [10] for the details concerning Russell graph and Russell sequence. In Theorem 4.2, the first and the second authors study new combinatorial proofs (mainly inspired by the arguments of [10, Proposition 23]) to show that the statements (a)–(d) mentioned in the abstract above are equivalent to Kőnig's Lemma (without assuming that the sets of colors can be well-ordered).[1]

1.2 New equivalents of Kőnig's lemma and AC

The role of AC and Kőnig's Lemma in the existence of graph-theoretic properties like irreducible proper coloring, chromatic numbers, maximal independent sets, spanning trees, and distinguishing colorings were studied by several authors in the past (cf. [2, 3, 5, 6, 7, 11, 19, 20]). We list a few known results apart from the above-mentioned results due to Galvin–Komjáth [7] and Stawiski [20]. In particular, Friedman [6, Theorem 6.3.2, Theorem 2.4] proved that AC is equivalent to the statement "Any graph has a maximal independent set". Höft–Howard [11] proved that the statement "Any connected graph contains a partial subgraph which is a tree" is equivalent to AC. Fix any even integer $m \geq 4$ and any integer $n \geq 2$. Delhommé–Morillon [5] studied the role of AC in the existence of spanning subgraphs and observed that AC is equivalent to "Any connected bipartite graph has a spanning subgraph without a complete bipartite subgraph $K_{n,n}$" as well as "Any connected graph admits a spanning m-bush" (cf. [5, Corollary 1, Remark 1]). They also proved that the statement "Any locally finite connected graph has a spanning tree" is equivalent to Kőnig's lemma in [5, Theorem 2]. Banerjee [2, 3] observed that the statements "Any infi-

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[1] We note that statement (a) mentioned in the abstract is a new equivalent of Kőnig's Lemma. Stawiski's graph from [20, Theorem 3.6] shows that Kőnig's Lemma is equivalent to "Every infinite locally finite connected graph G such that $\delta(G)$ (the minimum degree of G) is 2 has a chromatic number".

nite locally finite connected graph has a maximal independent set" and "Any infinite locally finite connected graph has a spanning m-bush" are equivalent to Kőnig's lemma. However, the existence of maximal matching, minimal edge cover, and minimal dominating set in ZF were not previously investigated. The following table summarizes the new results (cf. Theorem 5.1, Theorem 6.4).[2]

New equivalents of Kőnig's lemma	New equivalents of AC
$\mathcal{P}_{\text{lf,c}}$(irreducible proper coloring)	
$\mathcal{P}_{\text{lf,c}}$(minimal dominating set)	$\mathcal{P}_{\text{c}}$(minimal dominating set)
$\mathcal{P}_{\text{lf,c}}$(maximal matching)	$\mathcal{P}_{\text{c,b}}$(maximal matching)
$\mathcal{P}_{\text{lf,c}}$(minimal edge cover)	$\mathcal{P}_{\text{c,b}}$(minimal edge cover)

In the table, $\mathcal{P}_{\text{lf,c}}$(property X) denotes "Any infinite locally finite connected graph has property X", $\mathcal{P}_{\text{c,b}}$(property X) denotes "Any connected bipartite graph has property X" and $\mathcal{P}_{\text{c}}$(property X) denotes "Any connected graph has property X".

2 Basics

Definition 2.1. Suppose X and Y are two sets. We write:

1. $X \preceq Y$, if there is an injection $f\colon X \to Y$.
2. X and Y are equipotent if $X \preceq Y$ and $Y \preceq X$, i.e., if there is a bijection $f\colon X \to Y$.
3. $X \prec Y$, if $X \preceq Y$ and X is not equipotent with Y.

Definition 2.2. Without AC, a set m is called a *cardinal* if it is the cardinality $|x|$ of some set x, where $|x| = \{y : y \sim x$ and y is of least rank$\}$ where $y \sim x$ means the existence of a bijection $f\colon y \to x$ (see [15, Definition 2.2, page 83] and [13, Section 11.2]).

Definition 2.3. A graph $G = (V_G, E_G)$ consists of a set V_G of vertices and a set $E_G \subseteq [V_G]^2$ of edges.[3] Two vertices $x, y \in V_G$ are *adjacent vertices* if $\{x, y\} \in E_G$, and two edges $e, f \in E_G$ are *adjacent edges* if they share a common vertex. The *degree* of a vertex $v \in V_G$, denoted by $\deg(v)$, is the number of edges emerging from v. We denote by $\delta(G)$ the minimum degree of G. Given a non-negative integer n, a *path of length* n in G is a one-to-one finite sequence $\{x_i\}_{0\leq i\leq n}$ of vertices such that for each $i < n$, $\{x_i, x_{i+1}\} \in E_G$; such a path joins x_0 to x_n.

(1) G is *locally finite* if every vertex of G has a finite degree.

(2) G is *connected* if any two vertices are joined by a path of finite length.

(3) A *dominating set* of G is a set D of vertices of G, such that any vertex of G is either in D, or has a neighbor in D.

(4) An *independent set* of G is a set of vertices of G, no two of which are adjacent vertices. A *dependent set* of G is a set of vertices of G that is not an independent set.

[2] We note that Theorem 5.1 is a combined effort of the first and the second authors. Moreover, all remarks in Section 6 including Theorem 6.4 are due to all the authors.

[3] i.e., E_G is a subset of the set of all two-element subsets of V_G.

(5) A *vertex cover* of G is a set of vertices of G that includes at least one endpoint of every edge of the graph G.

(6) A *matching* M in G is a set of pairwise non-adjacent edges.

(7) An *edge cover* of G is a set C of edges such that each vertex in G is incident with at least one edge in C.

(8) A *minimal dominating set (minimal vertex cover, minimal edge cover)* is a dominating set (a vertex cover, an edge cover) that is not a superset of any other dominating set (vertex cover, edge cover). A *maximal independent set (maximal matching)* is an independent set (a matching) that is not a subset of any other independent set (matching).

(9) A *proper vertex coloring* of G with a color set C is a mapping $f\colon V_G \to C$ such that for every $\{x, y\} \in E_G$, $f(x) \neq f(y)$. A *proper edge coloring* of G with a color set C is a mapping $f\colon E_G \to C$ such that for any two adjacent edges e_1 and e_2, $f(e_1) \neq f(e_2)$.

(10) Let $|C| = \kappa$. We say G is *κ-proper vertex colorable* or *C-proper vertex colorable* if there is a proper vertex coloring $f\colon V_G \to C$ and G is *κ-proper edge colorable* or *C-proper edge colorable* if there is a proper edge coloring $f\colon E_G \to C$. The least cardinal κ for which G is κ-proper vertex colorable (if it exists) is the *chromatic number* of G and the least cardinal κ for which G is κ-proper edge colorable (if it exists) is the *chromatic index* of G.

(11) A proper vertex coloring $f\colon V_G \to C$ is a *C-irreducible proper coloring* if $f^{-1}(c_1) \cup f^{-1}(c_2)$ is a dependent set whenever $c_1, c_2 \in C$ and $c_1 \neq c_2$ (cf. [7]).

(12) An automorphism of G is a bijection $\phi\colon V_G \to V_G$ such that $\{u, v\} \in E_G$ if and only if $\{\phi(u), \phi(v)\} \in E_G$. Let f be an assignment of colors to either vertices or edges of G. We say that an automorphism ϕ of G *preserves* f if each vertex of G is mapped to a vertex of the same color or each edge of G is mapped to an edge of the same color. We say that f is a *distinguishing coloring* if the only automorphism that preserves f is the identity. Let $|C| = \kappa$. We say G is *κ-distinguishing vertex colorable* or *C-distinguishing vertex colorable* if there is a distinguishing vertex coloring $f\colon V_G \to C$ and G is *κ-distinguishing edge colorable* or *C-distinguishing edge colorable* if there is a distinguishing edge coloring $f\colon E_G \to C$. The least cardinal κ for which G is κ-distinguishing vertex colorable (if it exists) is the *distinguishing number* of G and the least cardinal κ for which G is κ-distinguishing edge colorable (if it exists) is the *distinguishing index* of G.

(13) The automorphism group of G, denoted by $\mathrm{Aut}(G)$, is the group consisting of automorphisms of G with composition as the operation. Let τ be a group acting on a set S and let $a \in S$. The orbit of a, denoted by $\mathrm{Orb}_\tau(a)$, is the set $\{\phi(a) : \phi \in \tau\}$.

(14) G is *complete* if each pair of vertices is connected by an edge. We denote by K_n, the complete graph on n vertices for any natural number $n \geq 1$.

(15) *Kőnig's Lemma* states that every infinite locally finite connected graph has a ray.

Let ω be the set of natural numbers, $\mathbb{Z}$ be the set of integers, $\mathbb{Q}$ be the set of rational numbers, $\mathbb{R}$ be the set of real numbers, and $\mathbb{Q}+a = \{a+r : r \in \mathbb{Q}\}$ for any $a \in \mathbb{R}$. Shelah–Soifer [17] constructed a graph whose chromatic number is 2 in ZFC and uncountable in some model of ZF (e.g. in Solovay's model from [18, Theorem 1]).

Definition 2.4 (cf. [17])**.** The *Shelah–Soifer Graph* $G = (\mathbb{R}, \rho)$ is defined by $x\rho y \Leftrightarrow (x-y) \in (\mathbb{Q}+\sqrt{2}) \cup (\mathbb{Q}+(-\sqrt{2}))$.

Definition 2.5. A set X is *Dedekind-finite* if it satisfies the following equivalent conditions (cf. [10, Definition 1]):

- $\omega \not\preceq X$,[4]
- $A \prec X$ for every proper subset A of X.

Definition 2.6. For every family $\mathcal{B} = \{B_i : i \in I\}$ of non-empty sets, $\mathcal{B}$ is said to have a *partial choice function* if $\mathcal{B}$ has an infinite subfamily $\mathcal{C}$ with a choice function.

Definition 2.7 (A list of choice forms)**.**

(1) AC_2: Every family of 2-element sets has a choice function.

(2) $\mathsf{AC}_{\mathsf{fin}}$: Every family of non-empty finite sets has a choice function.

(3) $\mathsf{AC}^{\omega}_{\mathsf{fin}}$: Every countably infinite family of non-empty finite sets has a choice function. We recall that $\mathsf{AC}^{\omega}_{\mathsf{fin}}$ is equivalent to Kőnig's Lemma as well as the statement "The union of a countable family of finite sets is countable".

(4) $\mathsf{AC}^{\omega}_{k\times\mathsf{fin}}$ for $k \in \omega\backslash\{0,1\}$: Every countably infinite family $\mathcal{A} = \{A_i : i \in \omega\}$ of non-empty finite sets, where k divides $|A_i|$, has a choice function.

(5) $\mathsf{PAC}^{\omega}_{k\times\mathsf{fin}}$ for $k \in \omega\backslash\{0,1\}$: Every countably infinite family $\mathcal{A} = \{A_i : i \in \omega\}$ of non-empty finite sets, where k divides $|A_i|$ has a partial choice function.

Definition 2.8. From the point of view of model theory, the *language of graphs* $\mathcal{L}$ consists of a single binary relational symbol E depicting edges, i.e., $\mathcal{L} = \{E\}$ and a graph is an $\mathcal{L}$-structure $G = \langle V, E\rangle$ consisting of a non-empty set V of vertices and the edge relation E on V. Let $G = \langle V, E\rangle$ be an $\mathcal{L}$-structure, $\phi(x_1, ..., x_n)$ be a first-order $\mathcal{L}$-formula, and let $a_1, ..., a_n \in V$ for some $n \in \omega\backslash\{0\}$. We write $G \models \phi(a_1, ..., a_n)$, if the property expressed by ϕ is true in G for $a_1, ..., a_n$. Let $G_1 = \langle V_{G_1}, E_{G_1}\rangle$ and $G_2 = \langle V_{G_2}, E_{G_2}\rangle$ be two $\mathcal{L}$-structures. We recall that if $j\colon V_{G_1} \to V_{G_2}$ is an isomorphism, $\varphi(x_1, ..., x_r)$ is a first-order $\mathcal{L}$-formula on r variables for some $r \in \omega\backslash\{0\}$, and $a_i \in V_{G_1}$ for each $1 \le i \le r$, then by induction on the complexity of formulae, one can see that $G_1 \models \varphi(a_1, ..., a_r)$ if and only if $G_2 \models \varphi(j(a_1), ..., j(a_r))$ (cf. [16, Theorem 1.1.10]).

3 Known and basic results

3.1 Known results

Fact 3.1 (ZF)**.** *The following hold:*

[4] i.e., there is no injection $f\colon \omega \to X$.

(1) (Galvin–Komjáth; cf. [7, Lemma 3 and the proof of Lemma 2]). *Any graph based on a well-ordered set of vertices has an irreducible proper coloring and a chromatic number.*

(2) (Delhommé–Morillon; cf. [5, Lemma 1]). *Given a set X and a set A which is the range of no mapping with domain X, consider a mapping $f\colon A \to \mathcal{P}(X)\backslash\{\emptyset\}$ (with values non-empty subsets of X). Then there are distinct a and b in A such that $f(a) \cap f(b) \neq \emptyset$.*

(3) (Herrlich–Rhineghost; cf. [9, Theorem]). *For any measurable subset X of $\mathbb{R}$ with a positive measure there exist $x \in X$ and $y \in X$ with $y - x \in \mathbb{Q} + \sqrt{2}$.*

(4) (Stawiski; cf. [20, proof of Theorem 3.8]). *Any graph based on a well-ordered set of vertices has a chromatic index, a distinguishing number, and a distinguishing index.*

3.2 Basic results

Proposition 3.2 (ZF)**.** *The Shelah-Soifer Graph $G = (\mathbb{R}, \rho)$ has the following properties:*

(1) *If AC_2 holds, then G has a minimal dominating set.*

(2) *Any independent set of G is either non-measurable or of measure zero.*

Proof. First, we note that each component of G is infinite, since $x, y \in \mathbb{R}$ are connected if and only if $x - y = q + \sqrt{2}z$ for some $q \in \mathbb{Q}$ and $z \in \mathbb{Z}$, and G has no odd cycles.

(1). Under AC_2, G has a 2-proper vertex coloring $f\colon V_G \to 2$ (see [9]). This is because, since G has no odd cycles, each component of G has precisely two 2-proper vertex colorings. Using AC_2 one can select a 2-proper vertex coloring for each component, in order to obtain a 2-proper vertex coloring of G. We claim that $f^{-1}(i)$ (which is an independent set of G) is a maximal independent set (and hence a minimal dominating set) of G for any $i \in \{0, 1\}$. Fix $i \in \{0, 1\}$ and assume that $f^{-1}(i)$ is not a maximal independent set. Then $f^{-1}(i) \cup \{v\}$ is an independent set for some $v \in \mathbb{R}\backslash f^{-1}(i) = f^{-1}(1 - i)$ and so $\{v, x\} \notin \rho$ for any $x \in f^{-1}(i)$. Since $f^{-1}(1 - i)$ is an independent set, $\{v, x\} \notin \rho$ for any $x \in f^{-1}(1 - i)$. This contradicts the fact that G has no isolated vertices.

(2). Let M be an independent set of G. Pick any $x, y \in M$ such that $x \neq y$. Then,

$$\neg(y\rho x) \implies (y-x) \notin (\mathbb{Q}+\sqrt{2})\cup(\mathbb{Q}+(-\sqrt{2})) = \{r+\sqrt{2} : r \in \mathbb{Q}\}\cup\{r-\sqrt{2} : r \in \mathbb{Q}\}.$$

Thus, there are no $x, y \in M$ where $x \neq y$ such that $y - x \in \mathbb{Q} + \sqrt{2}$. By Fact 3.1(3), M is not a measurable set of $\mathbb{R}$ with a positive measure. □

Proposition 3.3 (ZF)**.** *The following hold:*

(1) *Any graph based on a well-ordered set of vertices has a minimal vertex cover.*

(2) *Any graph based on a well-ordered set of vertices has a minimal dominating set.*

(3) *Any graph based on a well-ordered set of vertices has a maximal matching.*

(4) *Any graph based on a well-ordered set of vertices with no isolated vertex, has a minimal edge cover.*

Proof. (1). Let $G = (V_G, E_G)$ be a graph based on a well-ordered set of vertices and let $<$ be a well-ordering of V_G. We use transfinite recursion, without invoking any form of choice, to construct a minimal vertex cover. Let $M_0 = V_G$. Clearly, M_0 is a vertex cover. Assume that M_0 is not a minimal vertex cover. Now, assume that for some ordinal number α we have constructed a sequence $(M_\beta)_{\beta<\alpha}$ of vertex covers such that M_β is not a minimal vertex cover for any $\beta < \alpha$. If $\alpha = \gamma + 1$ is a successor ordinal for some ordinal γ, then let $M_\alpha = M_{\gamma+1} = M_\gamma \backslash \{v_\gamma\}$ where v_γ is the $<$-minimal element of the well-ordered set $\{v \in M_\gamma : M_\gamma \backslash \{v\}$ is a vertex cover$\}$. If α is a limit ordinal, we use $M_\alpha = \bigcap_{\beta\in\alpha} M_\beta$. For any ordinal α, if M_α is a minimal vertex cover, then we are done. Since the class of all ordinal numbers is a proper class, it follows that the recursion must terminate at some ordinal stage, say λ. Then, M_λ is the minimal vertex cover.

(2). This follows from (1) and the fact that if I is a minimal vertex cover of G, then $V_G \backslash I$ is a maximal independent set (and hence a minimal dominating set) of G.

(3). If V_G is well-orderable, then $E_G \subseteq [V_G]^2$ is well-orderable as well. Thus, similar to the arguments of (1) we can obtain a maximal matching by using transfinite recursion in ZF and modifying the greedy algorithm to construct a maximal matching.

(4). Let $G = (V_G, E_G)$ be a graph on a well-ordered set of vertices without isolated vertices. Let $\prec'$ be a well-ordering of E_G. By (3), we can obtain a maximal matching M in G. Let W be the set of vertices not covered by M. For each vertex $w \in W$, the set $E_w = \{e \in E_G : e$ is incident with $w\}$ is well-orderable being a subset of the well-orderable set $(E_G, \prec')$. Let f_w be the $(\prec' \restriction E_w)$-minimal element of E_w. Let $F = \{f_w : w \in W\}$ and let $M_1 = \{e \in M :$ at least one endpoint of e is not covered by $F\}$. Then $F \cup M_1$ is a minimal edge cover of G. □

Remark 3.4. We remark that the direct proofs of items (1)–(3) of Proposition 3.3 do not adapt immediately to give a proof of item (4); the issue is in the limit steps, where a vertex of infinite degree might not be covered anymore by the intersection of edge covers.

4 Proper and distinguishing colorings

Definition 4.1. Let $\mathcal{A} = \{A_n : n \in \omega\}$ be a disjoint countably infinite family of non-empty finite sets and $T = \{t_n : n \in \omega\}$ be a countably infinite sequence disjoint from $A = \bigcup_{n\in\omega} A_n$. Let $G_1(\mathcal{A}, T) = (V_{G_1(\mathcal{A},T)}, E_{G_1(\mathcal{A},T)})$ be the infinite locally finite connected graph such that

$$V_{G_1(\mathcal{A},T)} := (\bigcup_{n\in\omega} A_n) \cup T,$$

$$E_{G_1(\mathcal{A},T)} := \big\{\{t_n, t_{n+1}\} : n \in \omega\big\} \cup \big\{\{t_n, x\} : n \in \omega, x \in A_n\big\} \cup \big\{\{x, y\} : n \in \omega, x, y \in A_n, x \neq y\big\}.$$

We denote by $\mathcal{C}$ the statement "For any disjoint countably infinite family of non-empty finite sets $\mathcal{A}$, and any countably infinite sequence $T = \{t_n : n \in \omega\}$ disjoint from $A = \bigcup_{n\in\omega} A_n$, the graph $G_1(\mathcal{A}, T)$ has a chromatic number" and we denote by $\mathcal{C}_k$ the statement "Any infinite locally finite connected graph G such that $\delta(G) \geq k$ has a chromatic number".

Theorem 4.2 (ZF). *Fix a natural number $k \geq 3$. The following statements are equivalent:*

(1) *Kőnig's Lemma.*

(2) $\mathcal{C}$.

(3) $\mathcal{C}_k$.

(4) *Any infinite locally finite connected graph has a chromatic number.*

(5) *Any infinite locally finite connected graph has a chromatic index.*

(6) *Any infinite locally finite connected graph has a distinguishing number.*

(7) *Any infinite locally finite connected graph has a distinguishing index.*

Proof. (1)⇒(2)–(7) Let $G = (V_G, E_G)$ be an infinite locally finite connected graph. Pick some $r \in V_G$. Let $V_0(r) = \{r\}$. For each integer $n \geq 1$, define $V_n(r) = \{v \in V_G : d_G(r, v) = n\}$ where "$d_G(r, v) = n$" means there are n edges in the shortest path joining r and v. Each $V_n(r)$ is finite by the local finiteness of G, and $V_G = \bigcup_{n\in\omega} V_n(r)$ since G is connected. By $\mathsf{AC}^{\omega}_{\mathsf{fin}}$, V_G is countably infinite (and hence, well-orderable). The rest follows from Fact 3.1(1), (4) and the fact that $G_1(\mathcal{A}, T)$ is an infinite locally finite connected graph for any given disjoint countably infinite family $\mathcal{A}$ of non-empty finite sets and any countably infinite sequence $T = \{t_n : n \in \omega\}$ disjoint from $A = \bigcup_{n\in\omega} A_n$.

(2)⇒(1) Since $\mathsf{AC}^{\omega}_{\mathsf{fin}}$ is equivalent to its partial version $\mathsf{PAC}^{\omega}_{\mathsf{fin}}$ (Every countably infinite family of non-empty finite sets has an infinite subfamily with a choice function) (cf. [12], [4, the proof of Theorem 4.1(i)] or footnote 5), it suffices to show that $\mathcal{C}$ implies $\mathsf{PAC}^{\omega}_{\mathsf{fin}}$. In order to achieve this, we modify the arguments of Herrlich–Tachtsis [10, Proposition 23] suitably. Let $\mathcal{A} = \{A_n : n \in \omega\}$ be a countably infinite set of non-empty finite sets without a partial choice function. Without loss of generality, we assume that $\mathcal{A}$ is disjoint. Pick a countably infinite sequence $T = \{t_n : n \in \omega\}$ disjoint from $A = \bigcup_{i\in\omega} A_i$ and consider the graph $G_1(\mathcal{A}, T) = (V_{G_1(\mathcal{A},T)}, E_{G_1(\mathcal{A},T)})$ as in Figure 1.

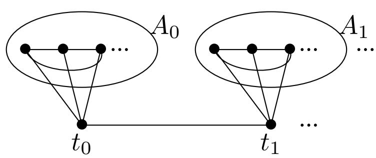

Figure 1: Graph $G_1(\mathcal{A}, T)$, an infinite locally finite connected graph.

Let $f : V_{G_1(\mathcal{A},T)} \to C$ be a C-proper vertex coloring of $G_1(\mathcal{A}, T)$, i.e., a map such that if $\{x, y\} \in E_{G_1(\mathcal{A},T)}$ then $f(x) \neq f(y)$. Then for each $c \in C$, the set $M_c = \{v \in f^{-1}(c) : v \in A_i \text{ for some } i \in \omega\}$ must be finite, otherwise M_c will generate a partial choice function for $\mathcal{A}$.

Claim 4.3. $f[\bigcup_{n\in\omega} A_n]$ *is infinite.*

Proof. Otherwise, $\bigcup_{n\in\omega} A_n = \bigcup_{c\in f[\bigcup_{n\in\omega} A_n]} M_c$ is finite since the finite union of finite sets is finite in ZF and we obtain a contradiction. □

Claim 4.4. $f[\bigcup_{n\in\omega} A_n]$ *is Dedekind-finite.*

Proof. First, we note that $\bigcup_{n\in\omega} A_n$ is Dedekind-finite since $\mathcal{A}$ has no partial choice function. For the sake of contradiction, assume that $C = \{c_i : i \in \omega\}$ is a countably infinite subset of $f[\bigcup_{n\in\omega} A_n]$. Fix a well-ordering $<$ of $\mathcal{A}$ (since $\mathcal{A}$ is countable, and hence well-orderable). Define d_i to be the *unique* element of $M_{c_i} \cap A_n$ where n is the $<$-least element of $\{m \in \omega : M_{c_i} \cap A_m \neq \emptyset\}$. Such an n exists since $c_i \in f[\bigcup_{n<\omega} A_n]$ and $M_{c_i} \cap A_n$ has a single element since f is a proper vertex coloring. Then $\{d_i : i \in \omega\}$ is a countably infinite subset of $\bigcup_{n\in\omega} A_n$ which contradicts the fact that $\bigcup_{n\in\omega} A_n$ is Dedekind-finite. $\square$

The following claim states that $\mathcal{C}$ fails.

Claim 4.5. *There is a C_1-proper vertex coloring $f\colon V_{G_1(\mathcal{A},T)} \to C_1$ of $G_1(\mathcal{A}, T)$ such that $C_1 \prec C$. Thus, $G_1(\mathcal{A}, T)$ has no chromatic number.*

Proof. Fix some $c_0 \in f[\bigcup_{n\in\omega} A_n]$. Then $\mathrm{Index}(M_{c_0}) = \{n \in \omega : M_{c_0} \cap A_n \neq \emptyset\}$ is finite. By Claim 4.3, there exists some $b_0 \in (f[\bigcup_{n\in\omega} A_n] \backslash \bigcup_{m\in\mathrm{Index}(M_{c_0})} f[A_m])$ since the finite union of finite sets is finite. Define a proper vertex coloring $g\colon \bigcup_{n\in\omega} A_n \to (f[\bigcup_{n\in\omega} A_n] \backslash c_0)$ as follows:

$$g(x) = \begin{cases} f(x) & \text{if } f(x) \neq c_0, \\ b_0 & \text{otherwise.} \end{cases}$$

Similarly, define a proper vertex coloring $h\colon \bigcup_{n\in\omega} A_n \to (f[\bigcup_{n\in\omega} A_n] \backslash \{c_0, c_1, c_2\})$ for some $c_0, c_1, c_2 \in f[\bigcup_{n\in\omega} A_n]$. Let $h(t_{2n}) = c_0$ and $h(t_{2n+1}) = c_1$ for all $n \in \omega$. Thus, $h\colon V_{G_1} \to (f[\bigcup_{n\in\omega} A_n] \backslash \{c_2\})$ is a $f[\bigcup_{n\in\omega} A_n] \backslash \{c_2\}$-proper vertex coloring of G_1. We define $C_1 = f[\bigcup_{n\in\omega} A_n] \backslash \{c_2\}$. By Claim 4.4, $C_1 \prec f[\bigcup_{n\in\omega} A_n] \preceq C$. $\square$

Similarly, we can see (4)⇒(1).

(3)⇒(1) Let $\mathcal{A} = \{A_n : n \in \omega\}$ be a disjoint countably infinite set of non-empty finite sets without a partial choice function, such that k divides $|A_n|$ for each $n \in \omega$ and $k \in \omega \backslash \{0, 1\}$. Assume T and $G_1(\mathcal{A}, T)$ as in the proof of (2)⇒(1). Then $\delta(G_1(\mathcal{A}, T)) \geq k$. By the arguments of (2)⇒(1), $\mathcal{C}$ implies $\mathsf{PAC}^{\omega}_{k\times\mathsf{fin}}$. Following the arguments of [4, Theorem 4.1], we can see that $\mathsf{PAC}^{\omega}_{k\times\mathsf{fin}}$ implies $\mathsf{AC}^{\omega}_{\mathsf{fin}}$.[5]

(5)⇒(1) Let $\mathcal{A} = \{A_n : n \in \omega\}$ be a disjoint countably infinite set of non-empty finite sets without a partial choice function and $T = \{t_n : n \in \omega\}$ be a sequence disjoint from $A = \bigcup_{n\in\omega} A_n$. Let H_1 be the graph obtained from the graph $G_1(\mathcal{A}, T)$ of (2)⇒(1) after deleting the edge set $\{\{x, y\} : n \in \omega, x, y \in A_n, x \neq y\}$. Clearly, H_1 is an infinite locally finite connected graph.

Claim 4.6. *H_1 has no chromatic index.*

[5] For the reader's convenience, we write down the proof. First, we can see that $\mathsf{PAC}^{\omega}_{k\times\mathsf{fin}}$ implies $\mathsf{AC}^{\omega}_{k\times\mathsf{fin}}$. Fix a family $\mathcal{A} = \{A_i : i \in \omega\}$ of disjoint nonempty finite sets such that k divides $|A_i|$ for each $i \in \omega$. Then the family

$$\mathcal{B} = \{B_i : i \in \omega\} \text{ where } B_i = \textstyle\prod_{j\leq i} A_j$$

is a disjoint family such that k divides $|B_i|$ and any partial choice function on $\mathcal{B}$ yields a choice function for $\mathcal{A}$.

Finally, fix a family $\mathcal{C} = \{C_i : i \in \omega\}$ of disjoint nonempty finite sets. Then $\mathcal{D} = \{D_i : i \in \omega\}$ where $D_i = C_i \times k$ is a pairwise disjoint family of finite sets where k divides $|D_i|$ for each $i \in \omega$. Thus $\mathsf{AC}^{\omega}_{k\times\mathsf{fin}}$ implies that $\mathcal{D}$ has a choice function f which determines a choice function for $\mathcal{C}$.

Proof. Assume that the graph H_1 has a chromatic index. Let $f\colon E_{H_1} \to C$ be a proper edge coloring with $|C| = \kappa$, where κ is the chromatic index of H_1. Let $B = \{\{t_n, x\} : n \in \omega, x \in A_n\}$. Similar to Claims 4.3, 4.4, and 4.5, $f[B]$ is an infinite, Dedekind-finite set and there is a proper edge coloring $h\colon B \to f[B] \setminus \{c_0, c_1, c_2\}$ for some $c_0, c_1, c_2 \in f[B]$. Finally, define $h(\{t_{2n}, t_{2n+1}\}) = c_0$ and $h(\{t_{2n+1}, t_{2n+2}\}) = c_1$ for all $n \in \omega$. Thus, we obtain a $f[B] \setminus \{c_2\}$-proper edge coloring $h\colon E_{H_1} \to f[B] \setminus \{c_2\}$, with $f[B] \setminus \{c_2\} \prec f[B] \preceq C$ as $f[B]$ is Dedekind-finite, contradicting the fact that κ is the chromatic index of H_1. □

(6)⇒(1) Assume $\mathcal{A}$ and T as in the proof of (5)⇒(1). Let H_1^1 be the graph obtained from H_1 of (5)⇒(1) by adding two new vertices t' and t'' and the edges $\{t'', t'\}$ and $\{t', t_0\}$ (see Figure 2).

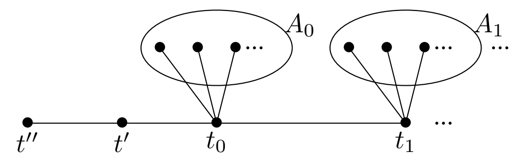

Figure 2: Graph H_1^1, an infinite locally finite connected graph.

It suffices to show that H_1^1 has no distinguishing number. We recall that whenever $j\colon V_{H_1^1} \to V_{H_1^1}$ is an automorphism, $\varphi(x_1, ..., x_r)$ is a first-order $\mathcal{L}$-formula on r variables (where $\mathcal{L}$ is the language of graphs) for some $r \in \omega\backslash\{0\}$ and $a_i \in V_{H_1^1}$ for each $1 \leq i \leq r$, then $H_1^1 \models \varphi(a_1, ..., a_r)$ if and only if $H_1^1 \models \varphi(j(a_1), ..., j(a_r))$ (cf. Definition 2.8).

Claim 4.7. *t', t'', and t_m are fixed by any automorphism for each non-negative integer m.*

Proof. Fix non-negative integers n, m, r. The first-order $\mathcal{L}$-formula

$$\mathsf{Deg}_n(x) := \exists x_0 \ldots \exists x_{n-1}\Big(\bigwedge_{i \neq j}^{n-1} x_i \neq x_j \wedge \bigwedge_{i<n} x \neq x_i \wedge \bigwedge_{i<n} Exx_i \wedge \forall y(Exy \to \bigvee_{i<n} y = x_i)\Big)$$

expresses the property that a vertex x has degree n, where Eab denotes the existence of an edge between vertices a and b. We define the following first-order $\mathcal{L}$-formula:

$$\varphi(x) := \mathsf{Deg}_1(x) \wedge \exists y(Exy \wedge \mathsf{Deg}_2(y)).$$

It is easy to see the following:

(i) t'' is the unique vertex such that $H_1^1 \models \varphi(t'')$. This means t'' is the unique vertex such that $\deg(t'') = 1$ and t'' has a neighbor of degree 2.

(ii) t' is the unique vertex such that $H_1^1 \models \mathsf{Deg}_2(t')$. So t' is the unique vertex with $\deg(t') = 2$.

Fix any automorphism τ. Since every automorphism preserves the properties mentioned in (i)–(ii), t' and t'' are fixed by τ. The vertices t_m are fixed by τ by induction as follows: Since t_i is the unique vertex of path length $i+1$ from t'' such that the degree of t_i is greater than 1, where $i \in \{0, 1\}$, we have that t_0 and t_1 are fixed by τ. Assume that $\tau(t_l) = t_l$ for all $l < m - 1$. We show that $\tau(t_m) = t_m$. Now, $\tau(t_m)$ is a neighbour of $\tau(t_{m-1}) = t_{m-1}$ which is of degree at least 2, so $\tau(t_m)$ must be either t_{m-2} or t_m, but $t_{m-2} = \tau(t_{m-2})$ is already taken. So, $\tau(t_m) = t_m$. □

Claim 4.8. *Fix $m \in \omega$ and $x \in A_m$. Then* $\mathrm{Orb}_{\mathrm{Aut}(H_1^1)}(x) = \{g(x) : g \in \mathrm{Aut}(H_1^1)\} = A_m$.

Proof. This follows from the fact that each $y \in \bigcup_{n\in\omega} A_n$ has path length 1 from t_m if and only if $y \in A_m$. □

Claim 4.9. *H_1^1 has no distinguishing number.*

Proof. Assume that the graph H_1^1 has a distinguishing number. Let $f\colon V_{H_1^1} \to C$ be a distinguishing vertex coloring with $|C| = \kappa$, where κ is the distinguishing number of H_1^1. Similar to Claims 4.3 and 4.4, $f[\bigcup_{n\in\omega} A_n]$ is infinite and Dedekind-finite. Consider a coloring $h\colon \bigcup_{n\in\omega} A_n \to f[\bigcup_{n\in\omega} A_n]\backslash\{c_0, c_1, c_2\}$ for some $c_0, c_1, c_2 \in f[\bigcup_{n\in\omega} A_n]$, just as in Claim 4.5. Let $h(t) = c_0$ for all $t \in \{t'', t'\} \cup T$. Then, $h\colon V_{H_1^1} \to (f[\bigcup_{n\in\omega} A_n]\backslash\{c_1, c_2\})$ is a $f[\bigcup_{n\in\omega} A_n] \setminus \{c_1, c_2\}$-distinguishing vertex coloring of H_1^1. Finally, $f[\bigcup_{n\in\omega} A_n] \setminus \{c_1, c_2\} \prec f[\bigcup_{n\in\omega} A_n] \preceq C$ contradicts the fact that κ is the distinguishing number of H_1^1. □

(7)⇒(1) Assume $\mathcal{A}$, T, and H_1^1 as in the proof of (6)⇒(1). By Claim 4.7, every automorphism fixes the edges $\{t'', t'\}$, $\{t', t_0\}$ and $\{t_n, t_{n+1}\}$ for each $n \in \omega$. Moreover, if H_1^1 has a distinguishing edge coloring f, then for each $n \in \omega$ and $x, y \in A_n$ such that $x \neq y$, $f(\{t_n, x\}) \neq f(\{t_n, y\})$.

Claim 4.10. *H_1^1 has no distinguishing index.*

Proof. This follows modifying the arguments of Claims 4.6 and 4.9. □

□

5 Irreducible proper coloring and covering properties

Theorem 5.1 (ZF)**.** *The following statements are equivalent:*

(1) *Kőnig's Lemma.*

(2) *Every infinite locally finite connected graph has an irreducible proper coloring.*

(3) *Every infinite locally finite connected graph has a minimal dominating set.*

(4) *Every infinite locally finite connected graph has a minimal edge cover.*

(5) *Every infinite locally finite connected graph has a maximal matching.*

Proof. Implications (1)⇒(2)–(5) follow from Proposition 3.3, and the fact that $\mathsf{AC}_{\mathsf{fin}}^{\omega}$ implies every infinite locally finite connected graph is countably infinite.

(2)⇒(1) In view of the proof of Theorem 4.2((2)⇒(1)), it suffices to show that the given statement implies $\mathsf{PAC}_{\mathsf{fin}}^{\omega}$. Let $\mathcal{A} = \{A_n : n \in \omega\backslash\{0\}\}$ be a disjoint countably infinite set of non-empty finite sets without a partial choice function. Pick $t \notin \bigcup_{i\in\omega\backslash\{0\}} A_i$. Let

$A_0 = \{t\}$. Consider the following infinite locally finite connected graph $G_2 = (V_{G_2}, E_{G_2})$ (see Figure 3):

$$V_{G_2} := \bigcup_{n\in\omega} A_n,$$

$$E_{G_2} := \Big\{\{t,x\} : x \in A_1\Big\} \cup \Big\{\{x,y\} : n \in \omega\backslash\{0\}, x, y \in A_n, x \neq y\Big\} \cup \Big\{\{x,y\} : n \in \omega\backslash\{0\}, x \in A_n, y \in A_{n+1}\Big\}.$$

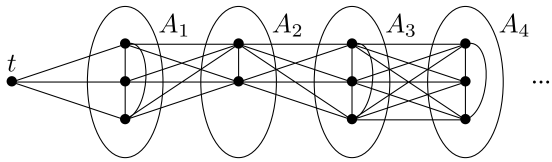

Figure 3: The graph G_2 when $|A_1| = |A_3| = |A_4| = 3$, and $|A_2| = 2$.

Claim 5.2. *G_2 has no irreducible proper coloring.*

Proof. Let $f\colon V_{G_2} \to C$ be a C-irreducible proper coloring of G_2, i.e., a map such that $f(x) \neq f(y)$ if $\{x,y\} \in E_{G_2}$ and $(\forall c_1, c_2 \in C) f^{-1}(c_1) \cup f^{-1}(c_2)$ is dependent. Similar to the proof of Theorem 4.2((2)⇒(1)), $f^{-1}(c)$ is finite for all $c \in C$, and $f[\bigcup_{n\in\omega\backslash\{0\}} A_n]$ is infinite. Fix $c_0 \in f[\bigcup_{n\in\omega\backslash\{0\}} A_n]$. Then $\mathrm{Index}(f^{-1}(c_0)) = \{n \in \omega\backslash\{0\} : f^{-1}(c_0) \cap A_n \neq \emptyset\}$ is finite. So there exists some

$$c_1 \in f[\textstyle\bigcup_{n\in\omega\backslash\{0\}} A_n]\backslash \bigcup_{m\in\mathrm{Index}(f^{-1}(c_0))}(f[A_m] \cup f[A_{m-1}] \cup f[A_{m+1}])$$

as $\bigcup_{m\in\mathrm{Index}(f^{-1}(c_0))}(f[A_m] \cup f[A_{m-1}] \cup f[A_{m+1}])$ is finite. Clearly, $f^{-1}(c_0) \cup f^{-1}(c_1)$ is independent, and we obtain a contradiction. □

(3)⇒(1) Assume $\mathcal{A}$ as in the proof of (2)⇒(1). Let G_2^1 be the infinite locally finite connected graph obtained from G_2 of (2)⇒(1) after deleting t and $\{\{t,x\} : x \in A_1\}$. Consider a minimal dominating set D of G_2^1. The following conditions must be satisfied:

(i) Since D is a dominating set, for each $n \in \omega \setminus \{0,1\}$, there is an $a \in D$ such that $a \in A_{n-1} \cup A_n \cup A_{n+1}$ (otherwise, no vertices from A_n belongs to D or have a neighbor in D).

(ii) By the minimality of D, we have $|A_n \cap D| \leq 1$ for each $n \in \omega \setminus \{0\}$.

Clearly, (i) and (ii) determine a partial choice function over $\mathcal{A}$, contradicting the assumption that $\mathcal{A}$ has no partial choice function.

(4)⇒(1) Let $\mathcal{A} = \{A_n : n \in \omega\}$ be a disjoint countably infinite set of non-empty finite sets and let $A = \bigcup_{n\in\omega} A_n$. Consider a countably infinite family $(B_i, <_i)_{i\in\omega}$ of well-ordered sets such that the following hold (cf. the proof of [5, Theorem 1, Remark 6]):

(i) $|B_i| = |A_i| + k$ for some fixed $1 \leq k \in \omega$ and thus, there is no mapping with domain A_i and range B_i.

(ii) for each $i \in \omega$, B_i is disjoint from A and the other B_j's.

Let $B = \bigcup_{i\in\omega} B_i$. Pick a countably infinite sequence $T = \{t_i : i \in \omega\}$ disjoint from A and B and consider the following infinite locally finite connected graph $G_3 = (V_{G_3}, E_{G_3})$ (see Figure 4):

$$\begin{aligned} V_{G_3} &:= A \cup B \cup T, \\ E_{G_3} &:= \Big\{\{t_i, t_{i+1}\} : i \in \omega\Big\} \cup \Big\{\{t_i, x\} : i \in \omega, x \in A_i\Big\} \\ &\qquad \cup \Big\{\{x, y\} : i \in \omega, x \in A_i, y \in B_i\Big\}. \end{aligned}$$

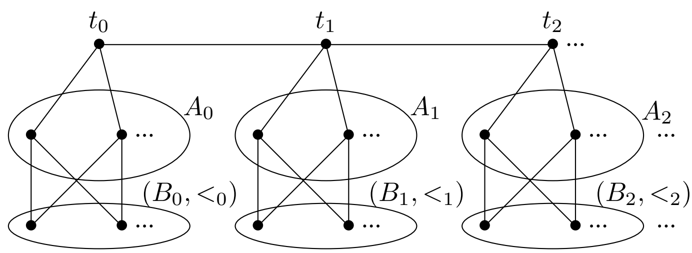

Figure 4: Graph G_3.

By assumption, G_3 has a minimal edge cover, say G_3'. For each $i \in \omega$, let $f_i \colon B_i \to \mathcal{P}(A_i)\backslash\{\emptyset\}$ map each vertex of B_i to its neighborhood in G_3'.

Claim 5.3. *Fix $i \in \omega$. For any two distinct ϵ_1 and ϵ_2 in B_i, $|f_i(\epsilon_1) \cap f_i(\epsilon_2)| \leq 1$.*

Proof. This follows from the fact that G_3' does not contain a complete bipartite subgraph $K_{2,2}$. In particular, each component of G_3' has at most one vertex of degree greater than 1. If any edge $e \in G_3'$ has both of its endpoints incident on edges of $G_3'\backslash\{e\}$, then $G_3'\backslash\{e\}$ is also an edge cover of G_3, contradicting the minimality of G_3'. □

By Fact 3.1(2) and (i), there are tuples $(\epsilon_1', \epsilon_2') \in B_i \times B_i$ such that $f_i(\epsilon_1') \cap f_i(\epsilon_2') \neq \emptyset$. Consider the first such tuple $(\epsilon_1'', \epsilon_2'')$ with respect to the lexicographical ordering of $B_i \times B_i$. Then $\{f_i(\epsilon_1'') \cap f_i(\epsilon_2'') : i \in \omega\}$ is a choice function of $\mathcal{A}$ by Claim 5.3.

(5)⇒(1) Assume $\mathcal{A}$, and A as in the proof of (4)⇒(1). Let $R = \{r_n : n \in \omega\}$ and $T = \{t_n : n \in \omega\}$ be two disjoint countably infinite sequences disjoint from A. We define the following locally finite connected graph $G_4 = (V_{G_4}, E_{G_4})$ (see Figure 5):

$$\begin{aligned} V_{G_4} &:= (\bigcup_{n\in\omega} A_n) \cup R \cup T, \\ E_{G_4} &:= \Big\{\{t_n, t_{n+1}\} : n \in \omega\Big\} \cup \Big\{\{t_n, x\} : n \in \omega, x \in A_n\Big\} \\ &\qquad \cup \Big\{\{r_n, x\} : n \in \omega, x \in A_n\Big\}. \end{aligned}$$

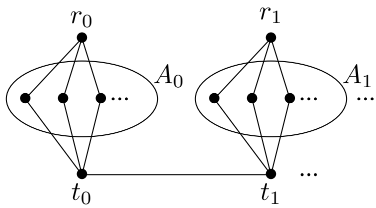

Figure 5: Graph G_4.

Let M be a maximal matching of G_4. For all $i \in \omega$, there is at most one $x \in A_i$ such that $\{r_i, x\} \in M$ since M is a matching and there is at least one $x \in A_i$ such that $\{r_i, x\} \in M$ since M is maximal. These unique $x \in A_i$ determine a choice function for $\mathcal{A}$.

This concludes the proof of the Theorem. $\square$

6 Remarks on new equivalents of AC

Remark 6.1. We remark that the statement "Any connected graph has a minimal dominating set" implies AC.[6] Consider a family $\mathcal{A} = \{A_i : i \in I\}$ of pairwise disjoint non-empty sets. For each $i \in I$, let $B_i^0 = A_i \times \{0\}$ and $B_i^1 = A_i \times \{1\}$. Pick $t \notin \bigcup_{i \in I} B_i^0 \cup \bigcup_{i \in I} B_i^1$ and consider the following connected graph $G_5 = (V_{G_5}, E_{G_5})$ in Figure 6:

$$V_{G_5} := \{t\} \cup \bigcup_{i \in I} B_i^0 \cup \bigcup_{i \in I} B_i^1,$$

$$E_{G_5} := \Big\{\{x, t\} : i \in I, x \in B_i^0\Big\} \cup \Big\{\{x, y\} : i \in I, x \in B_i^0, y \in B_i^1\Big\}$$
$$\cup \Big\{\{x, y\} : i \in I, x, y \in B_i^0, x \neq y\Big\} \cup \Big\{\{x, y\} : i \in I, x, y \in B_i^1, x \neq y\Big\}.$$

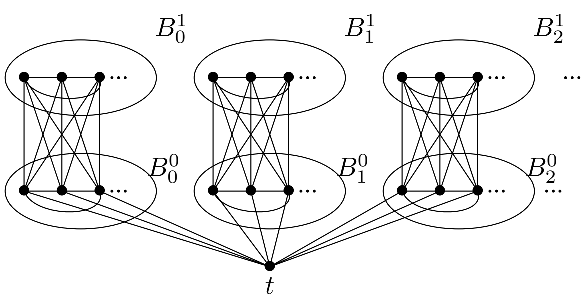

Figure 6: Graph G_5, a connected graph. If each A_i is finite, then G_5 is rayless.

[6]The authors are very thankful to one of the referees for pointing out to us an error that appeared in this remark in a former version of the paper and especially for guiding us to eliminate the error.

Let D be a minimal dominating set of G_5. Define $M_i = (B_i^0 \cup B_i^1) \cap D$ for every $i \in I$. We claim that for every $i \in I$, $|M_i| = 1$.

Case (i): If there exists an $i \in I$ such that $M_i = \emptyset$, then any member of B_i^1 is neither in D nor it has a neighbour in D. This contradicts the fact that D is a dominating set of G_5.

Case (ii): If there exists an $i \in I$ such that $|M_i| \geq 2$, then pick $x, y \in M_i$.

- Case (ii(a)): If $x, y \in B_i^0$, or $x, y \in B_i^1$, then $D \backslash \{x\}$ is a dominating set, which contradicts the minimality of D.

- Case (ii(b)): If $x \in B_i^0$, and $y \in B_i^1$, then $D \backslash \{y\}$ is a dominating set, which contradicts the minimality of D. Similarly, we can obtain a contradiction if $y \in B_i^0$, and $x \in B_i^1$.

Let $M_i = \{a_i\}$ for every $i \in I$. Define,

$$g(i) = \begin{cases} p_i^1(a_i) & \text{if } a_i \in B_i^1 \cap D, \\ p_i^0(a_i) & \text{if } a_i \in B_i^0 \cap D, \end{cases}$$

where for $m \in \{0,1\}$, $p_i^m : B_i^m \to A_i$ is the projection map to the first coordinate for each $i \in I$. Then, g is a choice function for $\mathcal{A}$.

Remark 6.2. The statement "Any connected bipartite graph has a minimal edge cover" implies AC. Assume $\mathcal{A} = \{A_i : i \in I\}$ as in the proof of Remark 6.1. Consider a family $\{(B_i, <_i) : i \in I\}$ of well-ordered sets with fixed well-orderings such that for each $i \in I$, B_i is disjoint from $A = \bigcup_{i \in I} A_i$ and the other B_j's, and there is no mapping with domain A_i and range B_i (see the proofs of [5, Theorem 1] and Theorem 5.1((4)⇒(1))). Let $B = \bigcup_{i \in I} B_i$. Then given some $t \notin B \cup (\bigcup_{i \in I} A_i)$, consider the following connected bipartite graph $G_6 = (V_{G_6}, E_{G_6})$ in Figure 7:

$$V_{G_6} := \{t\} \cup B \cup (\bigcup_{i \in I} A_i),$$

$$E_{G_6} := \Big\{\{x, t\} : i \in I, x \in A_i\Big\} \cup \Big\{\{x, y\} : i \in I, x \in A_i, y \in B_i\Big\}.$$

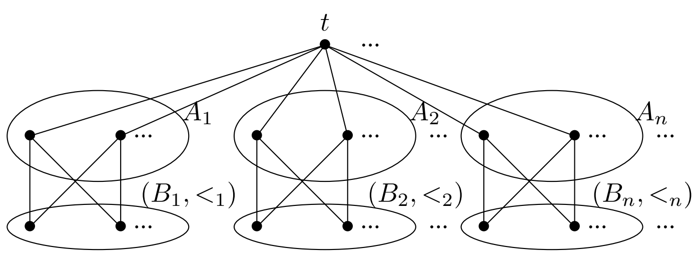

Figure 7: Graph G_6, a connected bipartite graph. If each A_i is finite, then G_6 is rayless.

The rest follows from the arguments of the implication (4)⇒(1) in Theorem 5.1.

Remark 6.3. The statement "Any connected bipartite graph has a maximal matching" implies AC. Assume $\mathcal{A}$ as in the proof of Remark 6.1. Pick a sequence $T = \{t_n : n \in I\}$ disjoint from $\bigcup_{i\in I} A_i$, a $t \notin \bigcup_{i\in I} A_i \cup T$ and consider the following connected bipartite graph $G_7 = (V_{G_7}, E_{G_7})$ in Figure 8:

$$V_{G_7} := \bigcup_{i\in I} A_i \cup T \cup \{t\}, \qquad E_{G_7} := \Big\{\{t_i, x\} : x \in A_i\Big\} \cup \Big\{\{t, t_i\} : i \in I\Big\}.$$

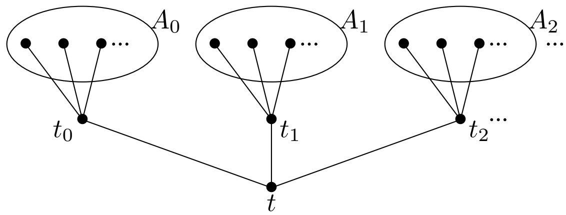

Figure 8: Graph G_7, a connected rayless bipartite graph.

Let M be a maximal matching of G_7. Clearly, $S = \{i \in I : \{t_i, t\} \in M\}$ has at most one element and for each $j \in I \backslash S$, there is exactly one $x \in A_j$ (say x_j) such that $\{x, t_j\} \in M$. Let $f(A_j) = x_j$ for each $j \in I \backslash S$. If $S \neq \emptyset$, pick any $r \in A_i$ if $i \in S$, since selecting an element from a set does not involve any form of choice. Let $f(A_i) = r$. Clearly, f is a choice function for $\mathcal{A}$.

Theorem 6.4 (ZF). *The following statements are equivalent:*

(1) AC

(2) *Any connected graph has a minimal dominating set.*

(3) *Any connected bipartite graph has a maximal matching.*

(4) *Any connected bipartite graph has a minimal edge cover.*

Proof. Implications (1)⇒(2)–(4) are straightforward (cf. Proposition 3.3). The other directions follow from Remarks 6.1, 6.2, and 6.3. □

Remark 6.5. The locally finite connected graphs forbid those graphs that contain vertices of infinite degrees but may contain rays. There is another class of connected graphs that forbid rays but may contain vertices of infinite degrees. For a study of some properties of the class of rayless connected graphs, the reader is referred to Halin [8].

(1). We can see that the statement "Every connected rayless graph has a minimal dominating set" implies $\mathsf{AC}_{\mathsf{fin}}$. Consider a non-empty family $\mathcal{A} = \{A_i : i \in I\}$ of pairwise disjoint finite sets and the graph G_5 from Remark 6.1. Clearly, G_5 is connected and rayless. The rest follows by the arguments of Remark 6.1.

(2). By applying Remark 6.3 and Proposition 3.3, we can see that the statement "Every connected rayless graph has a maximal matching" is equivalent to AC.

(3). The statement "Every connected rayless graph has a minimal edge cover" implies $\mathsf{AC}_{\mathsf{fin}}$. Let $\mathcal{A} = \{A_i : i \in I\}$ be as in (1) and G_6 be the graph from Remark 6.2. Then G_6 is connected and rayless. By the arguments of Remark 6.2, the rest follows.

7 Questions

Question 7.1. Do the following statements imply AC (without assuming that the sets of colors can be well-ordered)?

(1) Any graph has a chromatic index.

(2) Any graph has a distinguishing number.

(3) Any graph without a component isomorphic to K_1 or K_2 has a distinguishing index.

Stawiski [20, Theorem 3.8] proved that the statements (1)–(3) mentioned above are equivalent to AC by assuming that the sets of colors can be well-ordered.

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Selected topics on Wiener index*

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Abstract

The Wiener index is defined as the sum of distances between all unordered pairs of vertices in a graph. It is one of the most recognized and well-researched topological indices, which is on the other hand still a very active area of research. This work presents a natural continuation of the paper *Mathematical aspects of Wiener index* (Ars Math. Contemp., 2016) in which several interesting open questions on the topic were outlined. Here we collect answers gathered so far, give further insights on the topic of extremal values of Wiener index in different settings, and present further intriguing problems and conjectures.

Keywords: Graph distance, Wiener index, average distance, topological index, molecular descriptor, chemical graph theory.

Math. Subj. Class. (2020): 05C05, 05C12, 05C20, 05C92, 92E10

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1 Introduction

The *Wiener index*, $W(G)$, is a topological index of a connected graph, defined as the sum of the lengths of the shortest paths between all unordered pairs of vertices in the graph. In other words, for a connected graph

$$W(G) = \sum_{\{u,v\} \in V(G)} d(u,v),$$

where $d(u,v)$ denotes the distance between vertices u and v in G. This graph invariant has been investigated by numerous authors (see e.g. [24, 26, 27, 52, 56, 81]) under a variety of other names like transmission, total status, sum of all distances, path number and Wiener number of a graph. Due to its basic character and applicability, it has arisen in diverse contexts, including efficiency of information, sociometry, mass transport, cryptography, theory of communication, molecular structure, complex network topology and many more.

The index was originally introduced in 1947 by Harold Wiener for the purpose of determining the approximation formula of the boiling point of paraffin [80]. The definition of Wiener index in terms of distances between vertices of a graph was first given by Hosoya [40].

The *transmission* (also called the *distance*) of $u \in V(G)$ is $t_G(u) = \sum_{v \in V(G)} d_G(u,v)$. Thus the Wiener index can be expressed as

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} t_G(v).$$

Another view on the Wiener index was presented in [3] as follows. Suppose that $\{t_G(u) \,|\, u \in V(G\} = \{d_1, d_2, \ldots, d_k\}$. Assume in addition that G contains t_i vertices whose transmission is d_i, $1 \leq i \leq k$. Then the Wiener index of G can be expressed as

$$W(G) = \frac{1}{2} \sum_{i=1}^{k} t_i d_i.$$

We therefore say that the *Wiener dimension* $\dim_W(G)$ of G is k. That is, the Wiener dimension of a graph is the number of different transmissions of its vertices.

Fundamental properties regarding extremal values of Wiener index are already a part of the folklore. In [30] and later in many subsequent papers (e.g. [36, 37]) it was shown that for trees on n vertices, the maximum Wiener index is obtained for the path P_n, and the minimum for the star S_n. Thus, for every tree T on n vertices, it holds

$$(n-1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \binom{n+1}{3}.$$

Since the distance between any two distinct vertices is at least one, we have that among all graphs on n vertices K_n has the smallest Wiener index. In general, removing (resp. adding) of an edge from a connected graph results in increased (resp. decreased) Wiener index, which leads to the observation that Wiener index of a connected graph is less than or equal to the Wiener index of its spanning tree. Therefore, for any connected graph G on n vertices, it holds

$$\binom{n}{2} = W(K_n) \leq W(G) \leq W(P_n) = \binom{n+1}{3}.$$

Despite extensive literature on the Wiener index, many interesting and basic questions remain open. In our previous survey [56] we have exposed some of them that mainly pertain to extremal values of Wiener index in different settings. In this paper we continue with summarizing knowledge accumulated since then, and integrate some new conjectures, problems and ideas for possible future work.

2 Minimum Wiener index for chemical graphs

The *degree* $\deg_G(v)$ of a vertex $v \in V(G)$ in a graph G is $|N_G(v)|$, where $N_G(v)$ denotes the neighborhood of v in G. The *maximum degree* of a graph G, $\max_{v\in V(G)} \deg_G(v)$, is denoted by $\Delta(G)$, and the *minimum degree*, $\min_{v\in V(G)} \deg_G(v)$, is denoted by $\delta(G)$.

Since every atom has a certain valency, chemists are often interested in graphs with restricted degrees, which correspond to valencies. Particularly interesting is the class of *chemical graphs*, i.e. graphs for which the degrees of its vertices do not exceed 4. In [60] the authors addressed an "overlooked" problem of determining the minimum value of Wiener index and corresponding extremal graphs among chemical graphs with prescribed number of vertices. Note that the upper bound for this class of graphs is attained by paths.

Problem 2.1. Find all the chemical graphs G on n vertices with the minimum value of Wiener index.

Inserting of an edge in a graph decreases the Wiener index, thus one would expect that its minimum in the class of chemical graphs is attained by 4-regular graphs. Using a computer it was verified that for $n \in \{1, 2, \ldots, 5\}$ minimum is attained for K_n. Extremal graphs in cases $n = 6, 7$ are presented in Figure 1. Observe that the first two graphs in this figure are circulant graphs $C_6(1, 2)$ and $C_7(1, 2)$, respectively, and they are vertex-transitive. There are 1929 simple connected graphs on 8 vertices and the minimum Wiener index value is 40, which is attained by only 6 graphs depicted in Figure 2. Note that the first three graphs, which are the circulant graph $C_8(1, 2)$, the Cartesian product $K_4 \square P_2$ and the complete bipartite graph $K_{4,4} = C_8(1, 3)$, respectively, are vertex-transitive. The above cases support the following conjecture.

Conjecture 2.2. *Every chemical graph G on $n \geq 5$ vertices with the minimum value of Wiener index is 4-regular.*

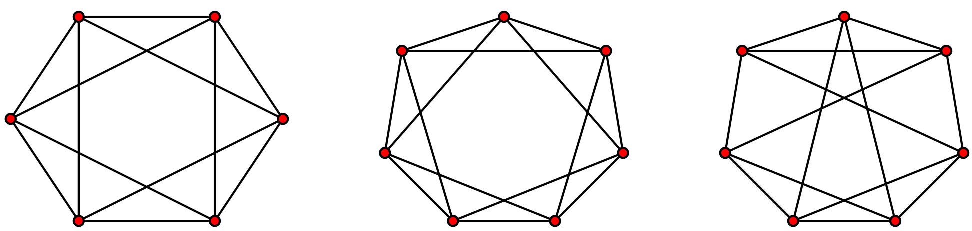

Figure 1: Extremal graphs for $n = 6$ and $n = 7$.

Although computer results indicate the above conjecture to be true, the problem seems to be far from tractable. In [60] it is shown that a chemical graph with the minimum value of Wiener index has at most 3 vertices of degree smaller than 4. In fact, a more general statement holds.

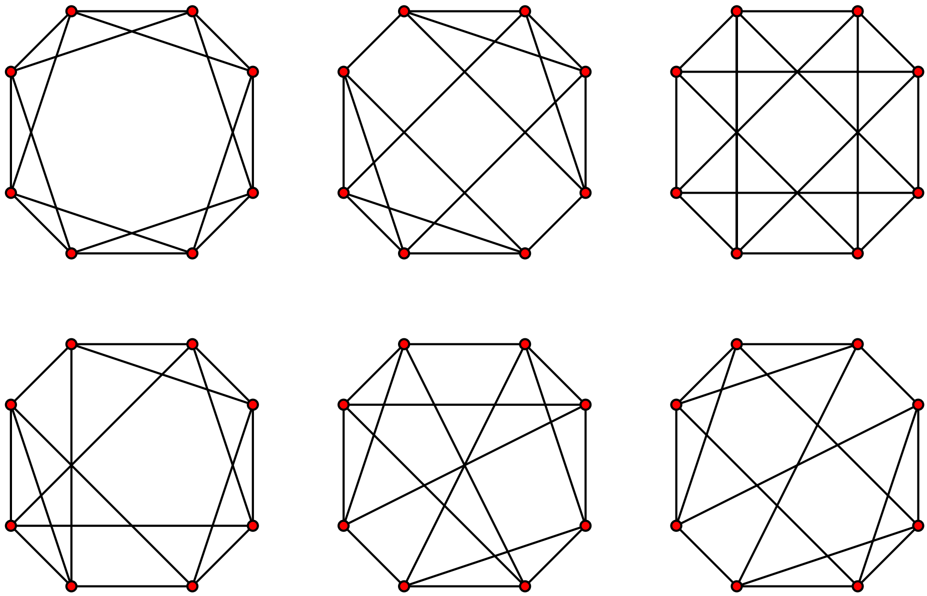

Figure 2: Extremal graphs for $n = 8$.

Observation 2.3. If G is a graph on n vertices with maximum degree Δ, $n \geq \Delta + 1$, and with the minimum possible value of Wiener index, then G contains at most $\Delta - 1$ vertices whose degree is strictly smaller than Δ, and these vertices induce a clique.

3 Prescribed degrees

As mentioned earlier, among n-vertex graphs with minimum degree at least 1, the maximum Wiener index is attained by P_n. But when restricting to minimum degree at least 2, the extremal graph is different. Observe that with the reasonable assumptions $\Delta \geq 2$ and $\delta \leq n - 1$, the following holds:

- $W(P_n) = \max\{W(G);\ G \text{ has maximum degree at most } \Delta \text{ and } n \text{ vertices}\}$,
- $W(K_n) = \min\{W(G);\ G \text{ has minimum degree at least } \delta \text{ and } n \text{ vertices}\}$.

Analogous reasons motivate the following two problems from [56].

Problem 3.1. What is the maximum Wiener index among n-vertex graphs with minimum degree at least δ?

Problem 3.2. What is the minimum Wiener index among n-vertex graphs with maximum degree at most Δ?

Both problems are still on the list of unsolved problems, but several results were obtained under additional requirements. Fischermann et al. [33], and independently Jelen and Trisch [44, 45] solved Problem 3.2 for trees. In addition, they determined the trees which maximize the Wiener index among all trees of given order whose vertices are either end-vertices or of maximum degree Δ.

Stevanović [73] solved Problem 3.1 for trees (where $\delta = 1$) under the assumption that the maximum degree is precisely Δ. Let $T_{n,\Delta}$ be the tree on n vertices obtained by taking a path on $n - \Delta + 1$ vertices and joining new $\Delta - 1$ vertices to one end-vertex of the path, see Figure 3.

Theorem 3.3. *For every n-vertex graph G with maximum degree $\Delta \geq 2$ it holds that $W(G) \leq W(T_{n,\Delta})$ with equality if and only if G is $T_{n,\Delta}$.*

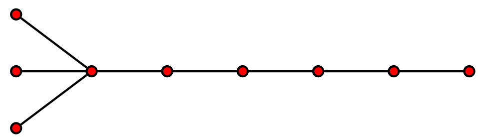

Figure 3: Graph $T_{9,4}$.

Dong and Zhou [29] determined the maximum Wiener index of unicyclic graphs with fixed maximum degree and they characterized the unique extremal graph.

Lin [62] characterized trees with the maximal Wiener index in the class of trees of order n with exactly k vertices of maximum degree, and proposed analogous problem for the minimum. The solution of this problem was recently presented by Božović et al. in [13]. The same authors considered a similar problem with a predetermined value of the maximum degree, i.e. they obtained the maximal value of Wiener index in the class of trees of order n with exactly k vertices of a given maximum degree and showed that the corresponding maximal trees are caterpillars with certain properties.

Recently Alochukwu and Dankelmann [4] obtained the following asymptotically sharp upper bound in terms of given minimum and maximum degree.

Theorem 3.4. *Let G be a graph of order n, minimum degree δ and maximum degree Δ. Then $W(G) \leq \binom{n-\Delta+\delta}{2}\frac{n+2\Delta}{\delta+1} + 2n(n-1)$, and this bound is sharp apart from an additive constant.*

Another interesting class of graphs with restrictions on degrees is the class of *regular graphs*, i.e. graphs for which $\Delta(G) = \delta(G)$. In general, introducing edges in a graph decreases the Wiener index, but in the class of r-regular graphs on n vertices the number of edges is fixed, therefore the following conjecture from [54] seems to be reasonable. The *diameter*, $\mathrm{diam}(G)$, of a graph G is the maximum distance between all pairs of vertices, i.e. $\mathrm{diam}(G) = \max\{d(u,v) |\ u, v \in V(G)\}$.

Conjecture 3.5. *Among all r-regular graphs on n vertices, the maximum Wiener index is attained by a graph with the maximum possible diameter.*

The above conjecture can be supported by the fact that in the case of trees, where the number of edges is fixed as well, the maximum Wiener index is attained by P_n which has the largest diameter. In fact, Chen et al. [18] recently proved that the conjecture is valid for $r = 3$. More precisely, they proved a conjecture from [54], that cubic graphs of the form L_n, presented in Figure 4, have maximum Wiener index among all cubic graphs of order n.

The minimum Wiener index in the class of trees is attained by S_n, which has the smallest diameter. A similar claim may hold for regular graphs [54].

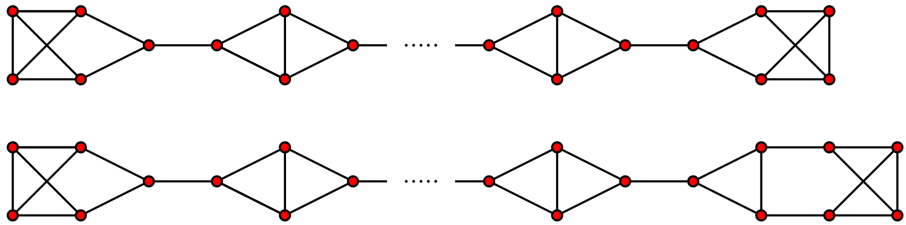

Figure 4: Graphs L_{4k+2} (above) and L_{4k+4} (below).

Conjecture 3.6. *Among all r-regular graphs on n vertices, the minimum Wiener index is attained by a graph with the minimum possible diameter.*

Finally, the following problem from [60] is of a special interest.

Problem 3.7. Find all k-regular graphs on n vertices with the smallest value of Wiener index.

As observed in [60], Problem 3.7 is surprisingly related to the cages and the following famous degree-diameter problem (see [66] for details).

Problem 3.8 (The degree-diameter problem)**.** Given positive integers d and k, find the largest possible number $n(d, k)$ of vertices in a graph of maximum degree d and diameter k.

Computer results in [60] (see also [65]) showed that among graphs with the minimum Wiener index there are graphs achieving $n(k, d)$ for pairs (k, d) from $\{(3, 2), (3, 3), (4, 2)\}$. There might appear graphs achieving $n(k, d)$ also for higher values of diameter d, but for those we could not search the space of k-regular graphs of order n exhaustively. Anyway, for higher diameters the graphs achieving $n(k, d)$ do not need to be those with the smallest Wiener index. Among extremal graphs found by a computer, $n(3, 2)$ and $n(3, 3)$ are realized by the well-known Petersen graph and the Flower snark J_5. Interestingly, there appears also the Heawood graph, which is the Cage$(3, 6)$, i.e., the smallest graph of degree 3 and girth 6, see [31].

The following conjectures were proposed in [60] (probably, it suffices to choose $n_k = k + 1$ therein).

Conjecture 3.9 (The even case conjecture)**.** *Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is even, then G is k-regular.*

Conjecture 3.10 (The odd case conjecture)**.** *Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is odd, then G has a unique vertex of degree smaller than k and in that case this smaller degree is $k - 1$.*

4 Wiener index of digraphs

A *directed graph* (a *digraph*) D is given by a set of vertices $V(D)$ and a set of ordered pairs of vertices $A(D)$ called *directed edges* or *arcs*. If uv is an arc in D, we say that

u *dominates* v. The *out-degree* $d^+(u)$ of a vertex $u \in V(D)$ is the number of its *out-neighbors*, i.e. the vertices, dominated by u. A *(directed) path* in D is a sequence of vertices $v_0, v_1, \ldots, v_k$ such that $v_{i-1}v_i$ is an arc of D for each $i \in \{1, 2, \ldots, k\}$, and by adding the arc $v_k v_0$ we obtain a *directed cycle*. An orientation of a graph G is said to be *acyclic* if it has no directed cycles. The *distance* $d(u, v)$ between vertices $u, v \in V(D)$ is the length of a shortest path from u to v. Notice that $d(u, v)$ is usually distinct from $d(v, u)$.

Early studies of Wiener index of digraphs were limited to *strongly connected* digraphs, i.e. digraphs in which a directed path between every pair of vertices exists. However, in the studies of real directed networks it is possible that there is no directed path connecting some pairs of vertices, thus the convention $d(u, v) = 0$ is used if there is no directed path from u to v [11, 12]. Under this assumption, in analogy to graphs, the Wiener index $W(D)$ of a digraph D is defined as the sum of all distances, where each ordered pair of vertices is taken into account. Hence,

$$W(D) = \sum_{(u,v)\in V(D)\times V(D)} d(u, v).$$

Let $W_{\max}(G)$ and $W_{\min}(G)$ be the maximum possible and the minimum possible, respectively, Wiener index among all digraphs obtained by orienting the edges of a graph G. If an orientation of G achieves the minimum Wiener index $W_{\min}(G)$, we call this orientation a *minimum Wiener index orientation* of G.

Problem 4.1. For a given graph G find $W_{\max}(G)$ and $W_{\min}(G)$.

In [58] there was posed a question if it is NP-hard to find an orientation of a given graph which maximizes the Wiener index. Dankelmann [19] answered it affirmatively. Plesník [69] proved that finding a strongly connected orientation of a given graph G that minimizes the Wiener index is NP-hard too, but the case for non-necessarily strongly connected digraphs is unsolved [58] in general. However, it can be decided in polynomial time if a given graph with m edges has an orientation for which the Wiener index is precisely m (note that it cannot be less).

Problem 4.2. What is the complexity of finding $W_{\min}(G)$ for an input graph G?

The following conjecture from [58] remains unsolved as well, but it is known to hold for bipartite graphs, unicyclic graphs, the Petersen graph and prisms.

Conjecture 4.3. *For every graph G, the value $W_{\min}(G)$ is achieved by some acyclic orientation of G.*

In [67, 69] Plesník and Moon found strongly connected tournaments (orientations of K_n) with the maximum and the second maximum Wiener index. In [57] it was shown that the same tournaments solve the problem if we drop out the requirement that the digraph should be strongly connected. In the same paper oriented Θ-graphs are studied. By $\Theta_{a,b,c}$ we denote a graph obtained when two distinct vertices u_1 and u_2 are connected by three internally vertex-disjoint paths of lengths $a + 1$, $b + 1$ and $c + 1$, respectively, where $a \geq b \geq c$ and $b \geq 1$ (see Figure 5 where a non-strongly connected orientation of $\Theta_{3,2,1}$ is depicted). Although intuitively one may expect that $W_{\max}$ is attained for some strongly connected orientation, this is not the case. Namely, in [57] it is shown that the orientation of $\Theta_{a,b,c}$ which achieves the maximum Wiener index is not strongly connected if $c \geq 1$.

For strongly connected orientations of $\Theta_{a,b,c}$, it was shown that the maximum Wiener index is achieved by the one in which the union of the u_1, u_2-paths of lengths $a+1$ and $b+1$ forms a directed cycle. Li and Wu [61] confirmed the conjecture from [57], that the same holds if we drop the assumption that orientations are strongly connected.

Theorem 4.4. *Let $a \geq b \geq c$. Then $W_{\max}(\Theta_{a,b,c})$ is attained by an orientation of $\Theta_{a,b,c}$ in which the union of the paths of lengths $a+1$ and $b+1$ forms a directed cycle.*

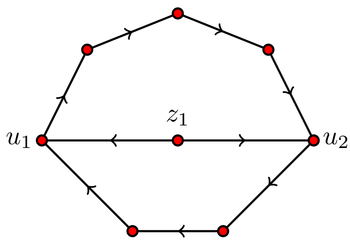

Figure 5: An orientation of $\Theta_{3,2,1}$.

However, the following conjecture remains open.

Conjecture 4.5. *Let G be a 2-connected chordal graph. Then $W_{\max}(G)$ is attained by an orientation which is strongly connected.*

Among digraphs on n vertices, the directed cycle $\overrightarrow{C}_n$ (in which all edges are directed in the same way, say clockwise) achieves the maximum Wiener index. In [55] digraphs with the second maximum Wiener index were investigated. In [58] the Wiener theorem was generalized to directed graphs, as well as a relation between the Wiener index and betweenness centrality.

An orientation of a graph G is called *k-coloring-induced*, if it is obtained from a proper k-coloring of G such that each edge is oriented from the end-vertex with the bigger color to the end-vertex with the smaller color. In [58] it was proved that graphs with at most one cycle and prisms attain the minimum Wiener index for k-coloring-induced orientation with k being the chromatic number $\chi(G)$. The same holds for bipartite graphs, complete graphs, Petersen graph and others. These observations lead to the conjecture that $W_{\min}(G)$ of an arbitrary graph is achieved for a $\chi(G)$-coloring-induced orientation, which Fang and Gao [32] showed to be false. They expressed the Wiener index of a digraph D as $W(D) = \sum_{u \in V(D)} w(u)$ where $w(u) = \sum_{v \in V(D)} d(u,v)$, and defined the notion of Wiener increment. For $u \in V(D)$ the *Wiener increment of u* is defined as $\Delta w(u) = w(u) - d^+(u)$. The *Wiener increment of D*, $\Delta W(D)$, is the sum of Wiener increments of all vertices of D. Fang and Gao observed that the comparison of Wiener indices of two different orientations of a graph is equal to the comparison of their Wiener increments. Using this observation they found that for the graph G in Figure 6, $W_{\min}(G)$ cannot be achieved for any $\chi(G)$-coloring-induced orientation of G, and this is not the only counterexample. Moreover, their investigations lead them to pose the following two conjectures.

Conjecture 4.6. *For any given constant $k \geq 3$, there exists a 3-colorable graph G such that any minimum Wiener index orientation of G has a directed path of length k.*

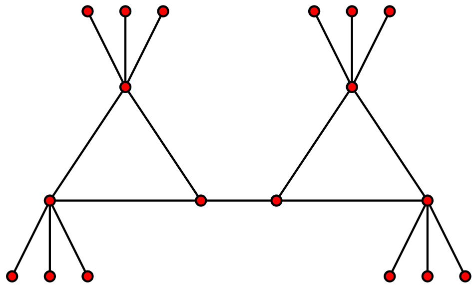

Figure 6: A graph G, for which $W_{\min}(G)$ is not achieved for any $\chi(G)$-coloring-induced orientation of G.

Conjecture 4.7. *For any given constant $k \geq 3$, there exists a 3-colorable graph G such that $W_{\min}(G)$ cannot be achieved by any k-coloring-induced orientation.*

Figure 7: A no-zig-zag path (left) and a zig-zag path (right) on six vertices.

In [58] orientations of trees with the maximum Wiener index were considered. An orientation of a tree is called *zig-zag* if there is a subpath in which edges change the orientation twice. If an orientation is not zig-zag, it is *no-zig-zag*, see Figure 7. A different view on no-zig-zag trees can be described as follows. A vertex v in a directed tree T is *core*, if for every vertex u of T there exists either a directed path from u to v or a directed path from v to u, see Figure 8. Notice that then in each component C of $T - v$ all edges point in the direction towards v or all edges point in the direction from v.

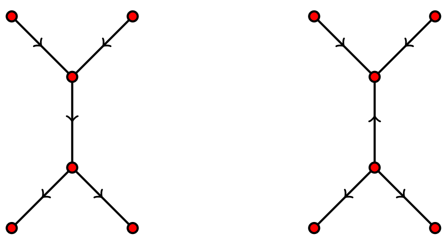

Figure 8: The graph on the left-hand side has two core vertices, while the right-hand side one has no core vertex.

In [58] the following conjecture was proposed.

Conjecture 4.8. *Let T be a tree. Then every orientation of T achieving the maximum Wiener index is no-zig-zag (i.e. has a core vertex).*

It was supported by showing that it holds for trees on at most 10 vertices, subdivision of stars, and trees constructed from two stars whose central vertices are connected by a path. Furthermore, since it is reasonable to expect that an orientation of a tree maximizing the Wiener index also maximizes the number of pairs of vertices (u, v) between which there exists a path, Conjecture 4.8 is supported also by a result of Henning and Oellermann [39]. They proved that if T is a tree and D is an orientation of T that maximizes the number of ordered pairs (u, v) of vertices of D for which there exists a (u, v)-path in D, then D contains a core vertex. However, Li and Wu [61] constructed a tree of order 85 contradicting Conjecture 4.8. Independently, Dankelmann [19] found an infinite family of counter-examples. For $k \in \mathbb{N}$, where k is a multiple of 3, let T_k be the tree obtained from a path of order k with vertices $w_1, w_2, \ldots, w_k$, by connecting vertices $u_1, u_2, \ldots, u_{k^2/9}$ to w_1, connecting x_1 from the path $x_1x_2x_3x_4x_5$ to w_2, and a single vertex y_1 to w_3. Now let D_k be the orientation of T_k such the edges of the path $w_1w_2\ldots w_k$ are oriented towards w_k, each edge u_iw_1 is oriented towards w_1, the edges of the path $x_1x_2x_3x_4x_5$ are oriented towards x_5, and the edge y_1w_3 is oriented towards w_3, see Figure 9 for an example. Observe that the edges of the (x_5, y_1)-path change their direction twice as the path is traversed, thus D_k is a zig-zag orientation. Dankelmann proved that if k is sufficiently large, then D_k and its converse (i.e., a digraph obtained by reversing the direction of every arc in D_k) are the only orientations of T_k that maximize the Wiener index, which contradicts Conjecture 4.8.

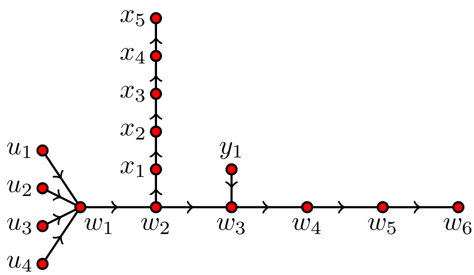

Figure 9: A no-zig-zag tree T_6.

The Cartesian product $P_m \Box P_n$ of paths on m and n vertices, respectively, is called the *grid* and is denoted by $G_{m,n}$. If $m = 2$, it is a called the ladder graph L_n. Kraner Šumenjak et al. [75] proved a conjecture from [59] by showing that the maximum Wiener index of a digraph whose underlying graph is L_n is $(8n^3 + 3n^2 - 5n + 6)/3$, and is obtained for the orientation presented in Figure 10. In addition, they proved a lower bound for $W_{\max}(G \Box H)$ for general graphs G and H, and posed a question regarding its sharpness. Let $\tau(G) = \sum_{x \in V(G)} \sigma(x)$, where $\sigma(x)$ denotes the number of vertices $x' \in V(G)$ for which there is a path from x to x' in G.

Theorem 4.9. *For any graphs G and H,*

$$W_{\max}(G \Box H) \geq W_{\max}(G)\tau(H) + W_{\max}(H)|V(G)|^2.$$

Problem 4.10. Is the bound given in Theorem 4.9 sharp? Find a sharp lower bound.

Another problem from [75] concerns a comparison of the maximum Wiener index of an orientation of G with the Wiener index of the undirected graph G.

Problem 4.11. Find functions f and g so that $f(W(G)) \leq W_{\max}(G) \leq g(W(G))$ for all graphs G. In particular, can f and g be linear functions?

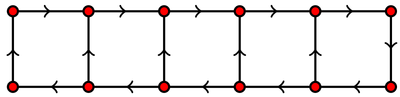

Figure 10: An orientation of the ladder $P_6 \square P_2$ with the maximum Wiener index.

Note that the orientation of L_n in Figure 10 is obtained when all layers isomorphic to one factor are directed paths directed in the same way, except one which is a directed path directed in the opposite way. Kraner Šumenjak et al. considered the following natural generalization of this orientation to general grids. Let $D_{m,n}$ be the orientation of $G_{m,n}$ with all P_m-layers oriented up except the last P_m-layer which is oriented down, and all P_n-layers oriented to the left except the first P_n-layer which is oriented to the right, see the left graph in Figure 11.

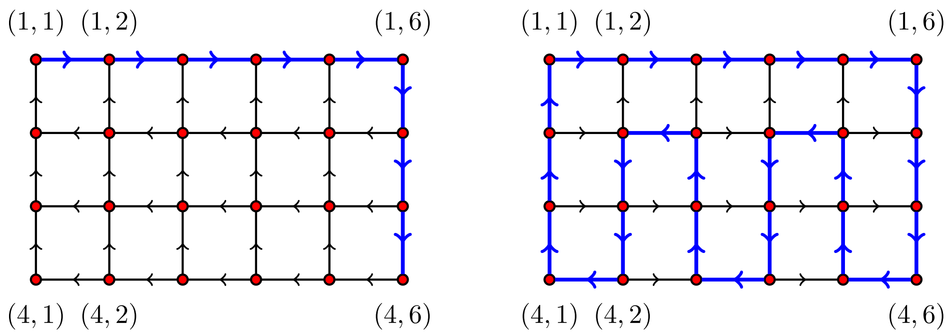

Figure 11: Two orientations, $D_{4,6}$ (left) and $C_{4,6}$ (right), of $P_4 \square P_6$.

The authors of [75] conjectured that for every $m, n \geq 2$, it holds $W_{\max}(G_{m,n}) = W(D_{m,n})$. However, it turns out that a comb-like orientation has significantly bigger Wiener index. Let $C_{m,n}$ be an orientation of $G_{m,n}$ in which the top P_n-layer is directed to the right and this layer is completed to a directed Hamiltonian cycle C in a zig-zag way as shown by blue arrows on the right graph in Figure 11. Moreover, the other edges are directed in such a way that they do not shorten directed blue path starting at the vertex $(1,1)$. Of course, $C_{m,n}$ exists only if n is even. In [53] it was shown that if $n \geq 4$ is even, and $m \geq 3$, then $W(C_{m,n}) > W(D_{m,n})$, and further observations led the authors to the following problem.

Problem 4.12. Find the biggest possible constant c, such that $W_{\max}(G_{m,n}) \geq c(mn)^3 + o\big((mn)^3\big)$.

To sum up, the following is still open.

Problem 4.13. Find an orientation of $G_{m,n}$ with the maximum Wiener index.

The authors think the above problem might be difficult as the extremal graphs in the cases $m = 3$ and $n \in \{4, 5, 6\}$ do not have any obvious simple property, but they are strongly connected. Thus they ask the following.

Question 4.14. Let $M_{m,n}$ be an orientation of $G_{m,n}$ with the maximum Wiener index. Is $M_{m,n}$ strongly connected?

5 Maximum Winer index of graphs with prescribed diameter

Recall that the *eccentricity* of a vertex in a connected graph G is the maximum distance between this vertex and any other vertex of G, and the maximum eccentricity is the graph *diameter*. Similarly, the *radius* of G, denoted by $\mathrm{rad}(G)$, is the minimum graph eccentricity. In 1984 Plesník identified graphs as well as digraphs with a given diameter that minimize the Wiener index (see also [14] for a recent alternative proof), and posed the opposite problem regarding the maximum [69].

Problem 5.1. What is the maximum Wiener index among graphs of order n and diameter d?

In general this question remains unsolved, but there has been progress and important results were obtained. First, Wang and Guo [79] determined the trees with maximum Wiener index among trees of order n and diameter d for some special values of d, $2 \leq d \leq 4$ or $n-3 \leq d \leq n-1$. Mukwembi and Vetrík [68] independently considered trees with the diameter up to 6 and gave asymptotically sharp upper bounds.

DeLaViña and Waller [22] posed a conjecture with additional restrictions in Problem 5.1.

Conjecture 5.2. *Let G be a graph with diameter $d > 2$ and order $2d+1$. Then $W(G) \leq W(C_{2d+1})$, where C_{2d+1} denotes the cycle of length $2d+1$.*

Sun et al. [76] considered general small-diameter and large-diameter graphs. They observed that if G is a graph on n vertices with diameter equal to 2, then the maximum Wiener index is attained by the star S_n. For diameter 3 they proposed a conjecture, that the extremal graph is isomorphic to K_n^c, which is a graph of order n that consists of a complete graph on c vertices and has the rest of the vertices attached to these c vertices as uniformly as possible (meaning that each of the c vertices of the complete graph has either $\lfloor (n-c)/c \rfloor$ or $\lceil (n-c)/c \rceil$ pendant vertices attached, see Figure 12 where K_4^{15} is depicted.

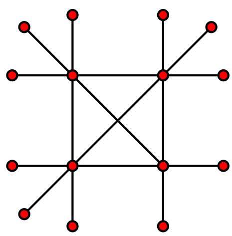

Figure 12: The graph K_4^{15}.

Conjecture 5.3. *Let G be a graph on n vertices with diameter equal to 3. Then $W(G) \leq W(K_n^c)$ where $c = \left\lfloor \sqrt{\frac{n^2}{2(n-1)}} \right\rfloor$ or $c = \left\lceil \sqrt{\frac{n^2}{2(n-1)}} \right\rceil$.*

To explain the results pertaining to trees and a conjecure on general graphs with diameter 4, we need the following definition. Let $k = \lfloor \sqrt{n-1} \rfloor$. For $k^2 + k \geq n-1$ we denote by T_n the rooted tree on n vertices in which the root has degree k, $n-k^2-1$ of its neighbours are of degree $k+1$ and the rest of them of degree k. When $k^2+k \leq n-1$ let T_n' denote the rooted tree on n vertices in which the root has degree $k+1$, $n-k^2-k-1$

of its neighbours are of degree $k+1$ and the rest of them of degree k. Wang and Guo [79] gave a complete description of trees with diameter 4 that maximize the Wiener index.

Theorem 5.4. *Let T be a tree on n vertices with diameter 4 and let $k = \lfloor \sqrt{n-1} \rfloor$. Then the following holds:*

- *if $k^2 + k > n - 1$, then $W(T) \leq W(T_n)$, with equality holding only when $T \cong T_n$;*
- *if $k^2 + k < n - 1$, then $W(T) \leq W(T'_n)$, with equality holding only when $T \cong T'_n$;*
- *if $k^2 + k = n - 1$, then $W(T) \leq W(T_n) = W(T'_n)$, with equality holding only when $T \cong T_n$ or $T \cong T'_n$.*

The authors of [76] suspect that the extremal graphs from the theorem above are extremal also for general graphs.

Conjecture 5.5. *The trees T_n and T'_n remain the unique optima in the class of graphs of diameter 4 on n vertices as it is described in* Theorem 5.4 *with the only exception of $n = 9$, in which case C_9 is also an optimal graph.*

An interested reader is referred to [76] for computer results supporting Conjectures 5.2, 5.3 and 5.5. The role of extremal graphs in the case of large-diameter graphs play the so called *double brooms* $D(n, a, b)$, i.e. graphs consisting of a path on $n - a - b$ vertices together with a leaves adjacent to one of its end-vertices and b leaves adjacent to the other end-vertex (see Figure 13 for an example).

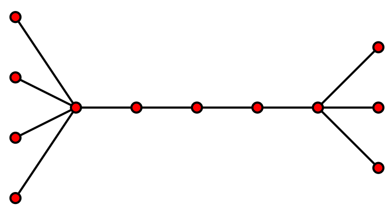

Figure 13: Double broom $D(12, 4, 3)$.

Theorem 5.6. *Let G be a graph of order n and diameter $n - c$, where $c \geq 1$ is a constant and n is large enough relative to c. Then $W(G) \leq W(D(n, \lfloor (c+1)/2 \rfloor, \lceil (c+1)/2 \rceil))$ with equality if and only if $G \cong D(n, \lfloor (c+1)/2 \rfloor, \lceil (c+1)/2 \rceil)$.*

Further details on diameters $n-3$ and $n-4$ can be found in [76]. A different approach to Problem 5.1 was recently used by Cambie [14] who gave asymptotically sharp upper bounds for Wiener index. As the main first step towards the proof of his result he constructed an almost extremal graph, in which there are many pairs of vertices which are of distance d from each other. This is achieved by having many subtrees with many leaves, and, when the diameter is even, combining them into one tree. When the diameter is odd, a central clique is used so that the distance between leaves of different subtrees are of distance d. Now if we take two vertices at random, the probability that both vertices are leaves is large since the number of leaves is large. Similarly, since we have many subtrees, the probability that both leaves are in different subtrees is large. Hence the probability that two vertices are at maximal distance is large, implying that the average distance is close to d. The above is a foundation of the following asymptotic solution to the problem of Plesník.

Theorem 5.7. *There exist positive constants c_1 and c_2 such that for any $d \geq 3$ the following holds. The maximum Wiener index among all graphs of diameter d and order n is between $d - c_1 \frac{d^{3/2}}{\sqrt{n}}$ and $d - c_2 \frac{d^{3/2}}{\sqrt{n}}$, i.e. it is of the form $d - \Theta\left(\frac{d^{3/2}}{\sqrt{n}}\right)$.*

In addition, Cambie [14] gives slightly stronger upper bound for trees, by which he extends a result of Mukwembi and Vetrík [68]. Moreover, the results he obtained lead him to the following question.

Question 5.8. For even d and large n, are the graphs of order n and diameter d with the largest Wiener index all trees?

Digraphs were considered in [14] as well, where the problem of Plesník is solved exactly if the order is large comparing to the diameter. For the sake of completeness we also mention that trees of order n and diameter d with the minimum Wiener index were presented in [63].

Having in mind the close relationship between the diameter and the radius of a connected graph, $\mathrm{rad}(G) \leq \mathrm{diam}(G) \leq 2\,\mathrm{rad}(G)$, it is natural to consider the above problems with radius instead of diameter. Chen et al. [17] posed the following question.

Problem 5.9. What is the maximum Wiener index among graphs of order n and radius r?

They succeeded to characterize graphs with the maximum Wiener index among all graphs of order n with radius 2. Das and Nadjafi-Arani [21] gave an upper bound on Wiener index of trees and graphs in terms of number of vertices n and radius r. In addition, they presented an upper bound on the Wiener index in terms of order, radius and maximum degree of trees and of graphs. The authors concluded that these results are not enough to solve Problem 5.9. Stevanović et al. [74] provide examples obtained by computer experiments, which suggest that a simple characterization of the structure of trees with maximum Wiener index among trees with a given number of vertices and radius will probably be out of our reach in some foreseeable future.

Analogous problem for the minimum Wiener index was posed by You and Liu [84].

Problem 5.10. What is the minimum Wiener index among all graphs of order n and radius r?

If $r \in \{1, 2\}$, the extremal graphs attaining the minimum total distance among all graphs of order n are easily characterized: they are complete graphs when $r = 1$, complete graphs minus a maximum matching when $r = 2$ and n is even, and complete graphs minus a maximum matching and an additional edge adjacent to the vertex not in the maximum matching, when $r = 2$ and n is odd.

A conjecture for $n \geq 3$ was posed by Chen et al. [17]. The notation $G_{n,r,s}$, where n, r and s are positive integers such that $n \geq 2r$, $r \geq 3$, and $n - 2r + 1 \geq s \geq 1$, stands for the graph obtained in the following way: let v_1, v_2, v_3 and v_4 be four consecutive vertices on a $2r$-cycle. Replace v_2 with a clique of order s, replace v_3 with a clique of order $n-2r+2-s$, join each vertex of one clique to all vertices of the other clique, join v_1 to all vertices of K_s, and join v_4 to all vertices of $K_{n-2r+2-s}$. Notice that the resulting graph has n vertices and radius r, and $W(G_{n,r,s}) = W(G_{n,r,s'})$ for any $s, s' \in \{1, \ldots, r-1\}$.

Conjecture 5.11. *Let n and r be two positive integers with $n \geq 2r$ and $r \geq 3$. For any graph G of order n with radius r, $W(G) \geq W(G_{n,r,1})$. Equality is attained if and only if $G = G_{n,r,s}$ for $s \in \{1, \ldots, r-1\}$.*

Cambie showed that the hypercube Q_3 is a counterexample to the above conjecture, so it does not hold when n is small, but he demonstrated that the conjecture is true asymptotically, i.e. if the order is sufficiently large compared to the radius [15].

Theorem 5.12. *For any $r \geq 3$, there exists a value $n_1(r)$ such that for all $n \geq n_1(r)$ it holds that any graph G of order n with radius r satisfies $W(G) \geq W(G_{n,r,1})$. Equality holds if and only if $G = G_{n,r,s}$ for $s \in \{1, \ldots, r-1\}$.*

We refer to [15] for an analog of this result for directed graphs, and to [69] for a characterization of digraphs of given order and diameter with the minimum Wiener index.

6 Šoltés problem and its relaxed variations

An interesting question regarding the Wiener index is to study how Wiener index is affected by small changes in a graph. Clearly, by removing an edge Wiener index is increased. On the other hand, the effect of deleting a vertex is far from obvious, and it was first studied by Šoltés. In his paper from 1991, Šoltés posed the following problem [71].

Problem 6.1. Find all graphs G in which the equality $W(G) = W(G - v)$ holds for all $v \in V(G)$.

Therefore, if for a vertex v in a graph G it holds that $W(G) = W(G - v)$, we say that v satisfies the *Šoltés property* in G, and a graph in which every vertex satisfies the Šoltés property is referred to as a *Šoltés graph*. The only known Šoltés graph so far is the cycle on 11 vertices. The above problem appears to be difficult, thus in subsequent studies relaxed variations were considered. The authors of [50] showed that the class of graphs for which the Wiener index does not change when a particular vertex is removed is rich, even when restricted to unicyclic graphs with fixed length of the cycle. More precisely:

- there is a unicyclic graph G on n vertices containing a vertex v with $W(G) = W(G-v)$ if and only if $n \geq 9$;
- there is a unicyclic graph G with a cycle of length c and a vertex satisfying the Šoltés property if and only if $c \geq 5$;
- for every graph G there are infinitely many graphs H such that G is an induced subgraph of H and $W(H) = W(H - v)$ for some $v \in V(H) \setminus V(G)$.

If a vertex v has degree 1 in G, then clearly $W(G) > W(G - v)$. In the construction of the above mentioned infinite class of graphs G with a vertex v satisfying the Šoltés property the vertex v is of degree 2. In [49] the authors extended their research to graphs in which v is of arbitrary degree. They showed that for a fixed positive integer $k \geq 2$ there exist infinitely many graphs G with a vertex v such that $\deg_G(v) = k$ and $W(G) = W(G-v)$. Moreover, if $n \geq 7$, there exists an n-vertex graph G with a vertex v so that $\deg_G(v) = n-2$ or $\deg_G(v) = n - 1$, and $W(G) = W(G - v)$. By proving the next theorem they showed that dense graphs cannot be a solution of Problem 6.1.

Theorem 6.2. *If G is an n-vertex graph for which $\delta(G) \geq n/2$, then $W(G) \neq W(G - v)$ for every $v \in V(G)$.*

In the results above, removal of one vertex only was considered. So the authors proposed the study of graphs G in which a given number of vertices satisfying the Šoltés property exist [49, 51].

Problem 6.3. For a given k, find (infinitely many) graphs G for which $W(G) = W(G - v_1) = W(G - v_2) = \cdots = W(G - v_k)$ for some distinct vertices $v_1, \ldots, v_k$ in G.

This problem was considered by Bok et al. [9, 10] who showed the existence of:

- infinitely many *cactus graphs* (i.e. graphs in which every edge belongs to at most one cycle) with exactly k cycles of length at least 7 that contain exactly $2k$ vertices satisfying the Šoltés property; and
- infinitely many cactus graphs with exactly k cycles of length $c \in \{5, 6\}$ that contain exactly k vertices satisfying the Šoltés property.

In addition, they proved that G contains no vertex with the Šoltés property if the length of the longest cycle in G is at most 4. Another infinite family of graphs satisfying the condition from Problem 6.3 was constructed by Hu et al. [43]. Furthermore, Hu et al. settled another problem from [49, 51] by proving that for any $k \geq 2$, there exist infinitely many graphs G such that $W(G) = W(G - \{v_1, v_2, \ldots, v_k\})$ for some distinct vertices $v_1, v_2, \ldots, v_k \in V(G)$.

Akhmejanova et. al [1] considered a relaxation of the original Šoltés problem from another point of view. They asked for graphs with a large proportion of vertices satisfying the Šoltés property. More precisely, they defined the function $\Delta_v(G) = W(G) - W(G-v)$. Then

$$\frac{|\{v \in V(G); \Delta_v(G) = 0\}|}{|V(G)|}$$

is the proportion of vertices satisfying the Šoltés property. So Akhmejanova et. al asked the following.

Problem 6.4. For a fixed $\alpha \in (0, 1]$ construct an infinite series S of graphs such that for all $G = (V(G), E(G))$ from S the following holds:

$$\frac{|\{v \in V(G); \Delta_v(G) = 0\}|}{|V(G)|} \geq \alpha.$$

Note that a solution to this problem for $\alpha = 1$ would give an infinite series of solutions to Problem 6.1. The authors noted that a slight modification of a construction from [9] yields an infinite series of graphs with the proportion of vertices satisfying the Šoltés property tending to $\frac{1}{3}$, and improved this constant by finding another two constructions. The first construction contains many 11-cycles as induced subgraphs: given $k \in \mathbb{N}, k > 1$, they defined a graph $B(k)$ on $5k + 6$ vertices by taking two vertices and connecting them with k distinct paths of length 6 and one path of length 5. It turns out that for $B(k)$ the proportion of vertices satisfying the Šoltés property equals $\frac{2k}{5k+6}$, thus this proportion tends to $\frac{2}{5}$ as k tends to infinity. Another construction of so called lily-shaped graphs involves graphs that are not 2-connected and whose proportion tends to $\frac{1}{2}$, see [1] for details. Furthermore, the authors found a graph with the proportion $\frac{2}{3}$ and expect that there exist an infinite series of graphs with a proportion $\alpha > \frac{1}{2}$, or perhaps even α tending to 1. Furthermore, they propose the following problems.

Problem 6.5. For a fixed $z \in \mathbb{Z}$, find all graphs G, for which the equality $W(G) - W(G - v) = z$ holds for all vertices v.

Problem 6.6. For a fixed $z \in \mathbb{Z}$ and $\alpha \in (0, 1]$, construct an infinite series S of graphs such that for all $G = (V(G), E(G))$ from S the following inequality takes place:

$$\frac{|\{v \in V(G); \Delta_v(G) = z\}|}{|V(G)|} \geq \alpha.$$

In [49, 51] the problem of finding k-regular connected graphs G other than C_{11} for which the equality $W(G) = W(G - v)$ holds for at least one vertex $v \in V(G)$ was posed. The answer is affirmative, see Figure 14 for 3-regular and 4-regular graphs with 4 and 2, respectively, (blue) vertices satisfying the Šoltés property. Using computer software and counting cubic graphs of orders $n \leq 26$, Bašić et al. [5] found that cubic graphs of order 12 or less do not contain Šoltés vertices. Cubic graphs with two Šoltés vertices first appear at the order 14 (there are three such graphs), and examples with three and four Šoltés vertices appear at the order 16. Moreover, they proved the following.

Theorem 6.7. *There exist infinitely many cubic* 2*-connected graphs which contain two Šoltés vertices.*

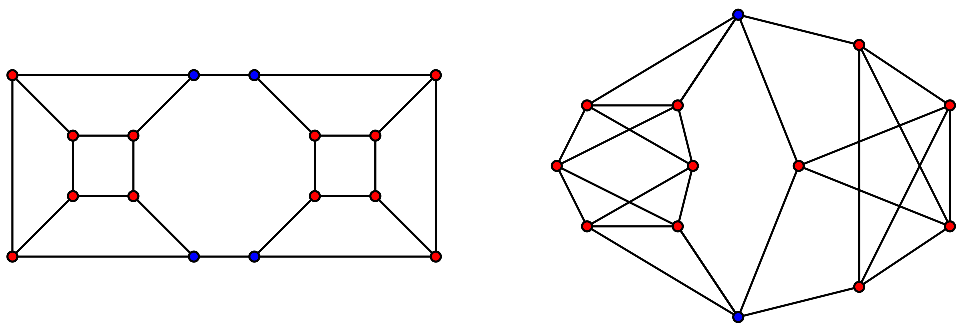

Figure 14: Regular graphs with blue vertices satisfying the Šoltés property.

In the same paper, graphs where the ratio between the number of Šoltés vertices and the order of the graph is at least α are called α-Šoltés graphs. So Problem 6.1 asks to find all 1-Šoltés graphs. The authors believe the solution to this problem should be graphs having all vertices of the same degree.

Conjecture 6.8. *If G is a Šoltés graph, then it is regular.*

For a general regular graph G, the values $W(G - u)$ and $W(G - v)$ might be significantly different for two different vertices u and v from G. It may happen that removal of one vertex increases the Wiener index, while removal of the other vertex descreases it. However, $W(G-u)$ and $W(G-v)$ are equal if vertices u and v belong to the same vertex orbit. This led the authors to believe the following.

Conjecture 6.9. *If G is a Šoltés graph, then G is vertex-transitive.*

Further, the authors report that a computer search on publicly available collections of vertex-transitive graphs did not reveal any 1-Šoltés graphs. All examples of $\frac{1}{3}$-Šoltés graphs are obtained by truncating certain cubic vertex-transitive graphs, and there are no Šoltés graphs among vertex-transitive graphs with less than 48 vertices. Recall that if v is a vertex of degree 3 adjacent to u_1, u_2 and u_3, then by *truncation* of v we mean the replacement of v by a triangle $v_1v_2v_3$, where v_i is adjacent to u_i, and by truncation of a cubic graph we mean the truncation of all its vertices. Therefore it is reasonable to consider the following conjectures and a problem.

Conjecture 6.10. *If G is a Šoltés graph, then G is a Cayley graph.*

Problem 6.11. Find an infinite family of cubic vertex-transitive graphs $\{G_i\}_{i=1}^{\infty}$, such that the truncation of G_i is a $\frac{1}{3}$-Šoltés graph for all $i \geq 1$.

Conjecture 6.12. *The cycle on eleven vertices is the only Šoltés graph.*

7 Wiener index of signed graphs

A *signed graph* is a pair (G, σ) where G is a graph and σ is a function from $E(G)$ to $\{-1, 1\}$, called a *signature function* (also called *signing* in the literature). A path P is a *uv-path* if its end-vertices are u and v. If P is a path in G and σ is a signature function of G then the notation $\sigma(P)$ stands for the sum $\sum_{e\in P} \sigma(e)$. For $u, v \in V(G)$ the *signed distance* $d_{G,\sigma}(u, v)$ equals $\min_P |\sigma(P)|$ where the minimum ranges over all uv-paths P. Spiro [72] recently introduced the Wiener index $W_\sigma(G)$ of the signed graph (G, σ) as

$$W_\sigma(G) = \sum_{\{u,v\}\subseteq V(G)} d_{G,\sigma}(u, v).$$

If σ is a constant function, then $d_{G,\sigma}(u, v) = d(u, v)$, and therefore $W_\sigma(G) = W(G)$. In particular, if $W(G) = W(G - v)$ for all $v \in V(G)$, then there exists a (constant) signature function σ of G such that $W_\sigma(G) = W_\sigma(G - v)$. In this sense the problem of finding signed graphs (G, σ) with $W_\sigma(G) = W_\sigma(G - v)$ can be viewed as a relaxation of Šoltés problem. Note that in the signed setting, it is possible to have $W_\sigma(G) = 0$. Spiro used this fact to provide many examples of signed graphs satisfying $W_\sigma(G) = W_\sigma(G - v)$ for all $v \in V(G)$, and even with $W_\sigma(G) = W_\sigma(G - S)$ for any set S of size less than some value k. To present his results, a signature function σ of a graph G is called *k-canceling* if for any set $S \subseteq V(G)$ of size less than k, we have $W_\sigma(G - S) = 0$. A graph G is *k-canceling* if there exists a k-canceling signature function σ of G, and graphs with $W_\sigma(G) = 0$ are simply referred to as *canceling graphs*. For instance, a complete graph K_n is k-canceling if $n \geq 2k + 4$. Furthermore, he proved the following.

Proposition 7.1. *Let G' be a bipartite graph with partite sets U and V, where $|U|, |V| \geq k + 2$, and minimum degree at least $k + 1$. Let G be the graph obtained from G' by adding every edge between two vertices of U and every edge between two vertices of V. Then G is k-canceling.*

Another family of examples is obtained from the blowups of odd cycles: if G is a graph on $\{v_1, \dots, v_t\}$, then the $\{n_1, \dots, n_t\}$-*blowup* of G is defined to be the t-partite graph on sets $V_1, \dots V_t$ with $|V_i| = n_i$ and with $u \in V_i$ and $w \in V_j$ adjacent if and only if v_i, v_j are adjacent in G.

Proposition 7.2. *Let G be the $(n_1, \dots, n_{2t+1})$-blowup of a cycle C_{2t+1} with $t \geq 1$. If $n_i \geq 2k$ for all i, then G is k-canceling.*

Furthermore, the following holds.

Theorem 7.3. *If n is sufficiently large and G is an n-vertex graph with minimum degree at least $\frac{2n}{3}$, then there exists a signature function σ of G such that $W_\sigma(G) = W_\sigma(G-v) = 0$ for all $v \in V(G)$.*

For necessary conditions for a graph to be canceling and several interesting open questions we refer to [72]. One of the conjectures pertains to the well known fact that in the class of n-vertex trees the star S_n and the path P_n are extremal graphs for the Wiener index. Let (T, σ) be a signed n-vertex tree and let $+$ be the constant signature function that assigns $+1$ to every edge of P_n. Then the fact that $W_\sigma(T) \le W_+(P_n)$ follows from the result for the classical Wiener index since $W_+(P_n) = W(P_n)$. It remains to prove the lower bound.

Conjecture 7.4. *If (T, σ) is a signed n-vertex tree, then*

$$W_\alpha(P_n) \le W_\sigma(T),$$

where α is the alternating signature function which assigns the first edge of the path $+1$, the second -1, the third $+1$, and so on.

Another possible direction for future study according to Spiro is the *minimum signed Wiener index* $W_*(G) = \min_\sigma(G)$, where the minimum ranges over all signature functions σ of G. Note that this concept is analogous to the minimum digraph Wiener index of all orientations of a graph G presented in Section 4. Spiro proposed a conjecture in which double stars appear as extremal graphs; a *double star* is a tree T in which there exist vertices $x, y \in V(T)$ such that every edge of T has at least one of the vertices x, y as an end-vertex. Note that by this definition a star is also a double star.

Conjecture 7.5. *If T is an n-vertex tree, then*

$$W_*(P_n) \le W_*(T) \le \max_{D \in \mathcal{D}} W_*(D),$$

where $\mathcal{D}$ is the set of all n-vertex double stars.

The conjecture was verified for $n \le 9$, and noted that it is false if one considers stars instead of double stars. We refer to [72] for more interesting questions related to the presented topic.

8 Variable Wiener index vs. variable Szeged index

For an edge uv in a graph, let $n_v(u)$ denote the number of vertices strictly closer to u than v, and analogously, let $n_u(v)$ be the number of vertices strictly closer to v than u. In his original paper [80] Wiener observed that the Wiener index of a tree can be computed as the sum of products $n_v(u) \cdot n_u(v)$ over all edges uv in the tree, but this is not the case in general graphs, owing to the fact that shortest paths are typically not unique. By relaxing the condition that the graph is a tree, the Szeged index of a graph G was defined in [34, 46] as

$$\mathrm{Sz}(G) = \sum_{uv \in E(G)} n_v(u) \cdot n_u(v).$$

Klavžar et al. [47] proved that $\mathrm{Sz}(G) \ge W(G)$ for every graph G, and in [25] all graphs for which the equality holds were classified.

Theorem 8.1. *For every graph G we have $\mathrm{Sz}(G) \geq W(G)$, and equality holds if and only if every block of G is a complete graph.*

The *variable Wiener index* (also known as the *generalized Wiener index*) of a graph G is defined as

$$W^{\alpha}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)^{\alpha},$$

and the *variable Szeged index* of a graph G is

$$\mathrm{Sz}^{\alpha}(G) = \sum_{uv \in E(G)} \left(n_v(u) \cdot n_u(v)\right)^{\alpha}.$$

Note that in [38] the quantity $\sum_{uv \in E(T)} \left(n_v(u) \cdot n_u(v)\right)^{\alpha}$ was named as the *variable Wiener index for trees*, but referring to it as the *variable Szeged index* seems to be more natural. By Theorem 8.1, for trees it holds $W(T) = \mathrm{Sz}(T)$. Using Karamata's inequality Hriňáková et al. [42] proved the following statement.

Theorem 8.2. *Let T be a tree on n vertices. Then*

(1) $W^{\alpha}(T) \leq \mathrm{Sz}^{\alpha}(T)$ *if* $\alpha > 1$,

(2) $W^{\alpha}(T) \geq \mathrm{Sz}^{\alpha}(T)$ *if* $0 \leq \alpha < 1$.

Moreover, equalities hold if and only if $n = 2$.

In the case when $\alpha > 1$, they extended this result to the class of bipartite graphs.

Theorem 8.3. *Let G be a bipartite graph on n vertices and $\alpha > 1$. Then $W^{\alpha}(G) \leq \mathrm{Sz}^{\alpha}(G)$ with equality if and only if $n = 2$.*

If G is a complete graph, we have $\mathrm{Sz}^{\alpha}(G) = \binom{|V(G)|}{2} = W^{\alpha}(G)$ for every α. Note that α is non-negative in the above results. If $\alpha < 0$ then for non-complete graphs we have the following strict inequality [42].

Proposition 8.4. *Let G be a non-complete graph. Then for every $\alpha < 0$ we have $\mathrm{Sz}^{\alpha}(G) < W^{\alpha}(G)$.*

Based on Theorem 8.2 and examples provided in [42], Hriňáková et al. proposed the following conjecture.

Conjecture 8.5. *For every non-complete graph G there is a constant $\alpha_G \in (0,1]$ such that*

$$\begin{aligned}
&\mathrm{Sz}^{\alpha}(G) > W^{\alpha}(G), \text{ if } \alpha > \alpha_G,\\
&\mathrm{Sz}^{\alpha}(G) = W^{\alpha}(G), \text{ if } \alpha = \alpha_G,\\
&\mathrm{Sz}^{\alpha}(G) < W^{\alpha}(G), \text{ if } 0 \leq \alpha < \alpha_G.
\end{aligned}$$

In other words, the conjecture states that for any non-complete graph there is a critical exponent in $(0,1]$, below which the variable Wiener index is larger and above which the variable Szeged index is larger. As seen above, this holds for trees. However, Cambie and Haslegrave [16] found infinitely many counterexamples by constructing a family of graphs $G_{k,\ell}$ as follows: take a complete graph K_k, remove a k-cycle from it, and connect all its vertices with one end-vertex of a path of length l, see Figure 15 where $G_{8,3}$ is depicted. By fixing a connected non-complete graph G, $h(\alpha) = Sz^\alpha(G) - W^\alpha(G)$ is a continuous function with $h(0) < 0$ and $h(1) \geq 0$, which by intermediate value theorem implies that there is at least one value of α for which $h(\alpha) = 0$, and at least one such value lies in $(0, 1]$. Therefore Conjecture 8.5 is equivalent to α being unique, which is not the case for many graphs of the form $G_{k,\ell}$. It turns out that if k is reasonably large, then there exist some corresponding values of ℓ having three values of α for which $Sz^\alpha(G_{k,\ell}) - W^\alpha(G_{k,\ell})$ equals 0.

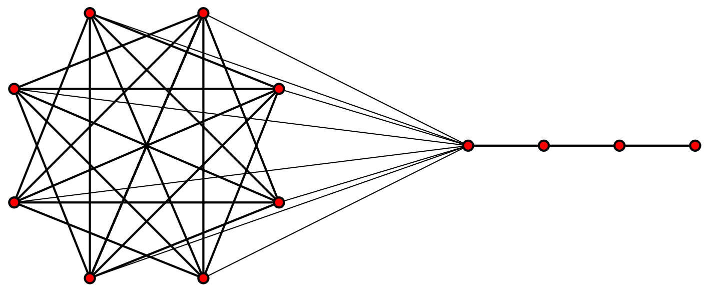

Figure 15: The graph $G_{k,\ell}$ for $k = 8$ and $\ell = 3$.

On the other hand, the authors found further families of graphs for which the statement in Conjecture 8.5 does hold. In fact, they showed its validity for almost all graphs.

Theorem 8.6. Conjecture 8.5 *holds for*

- *block graphs,*
- *edge-transitive graphs,*
- *bipartite graphs,*
- *graphs with diameter* 2*,*
- *graphs with diameter* 3*,* n *vertices and at most* $\frac{1}{2}\binom{n}{2}$ *edges,*
- *graphs with* n *vertices and* m *edges whenever* $m \leq \frac{1}{4}(n^{4/3} - n^{1/3})$.

They also proved that Conjecture 8.5 holds for almost all random graphs in 2 models of random graphs, see [16] for more detailed explanation. Anyway, it is an open problem if there exist graphs G, other than complete ones, for which $|\{\alpha; Sz^\alpha(G) - W^\alpha(G) = 0\}|$ is larger than 3. So we have the following problem.

Problem 8.7. Let $\mathcal{G}$ be the class of graphs which contain at least one block which is not complete. Is $|\{\alpha; Sz^\alpha(G) - W^\alpha(G) = 0\}|$ bounded for $G \in \mathcal{G}$? If so, what is its maximum value?

By showing that for every graph G, the sequence $(n_v(u) \cdot n_u(v))_{uv \in E(G)}$ majorizes the sequence $(d(u,v))_{u,v \in V(G)}$, Cambie and Haslegrave proved that a weaker version of Conjecture 8.5 holds. Using a different approach the same result was independently obtained by Kovijanić Vukićević and Bulatović [78].

Theorem 8.8. *For every non-complete graph G and $\alpha > 1$, we have $\mathrm{Sz}^\alpha(G) > W^\alpha(G)$.*

We conclude this section with the following question.

Question 8.9. Does Conjecture 8.5 hold for triangle-free graphs?

9 Wiener index of apex graphs

An *apex graph* is a graph that becomes planar by removal of a single vertex. Along these lines a graph G is called an *apex tree* if it contains a vertex x such that $G - x$ is a tree. Furthemore, a graph G is called an *ℓ-apex tree* if there exists a vertex subset $A \subset V(G)$ of cardinality ℓ such that $G - A$ is a tree and there is no other subset of smaller cardinality with this property [82, 83].

In [82] extremal values of (additively and multiplicatively) weighted Harary indices of apex and ℓ-apex trees were studied. Extremal values of some other topological indices of ℓ-apex trees were recently explored in [2] and [48]. In the later authors studied the generalized Wiener index and derived the following result in which $K_\ell + T$ denotes the join of a complete graph K_ℓ and a tree T on $n - \ell$ vertices.

Theorem 9.1. *Let G be an ℓ-apex tree on n vertices, where $\ell \geq 1$ and $n \geq \ell + 2$, and let $\alpha \neq 0$. Then, the following two claims hold:*

- *If $\alpha > 0$ then $W^\alpha(G)$ has the minimum value if and only if $G = K_\ell + T$, where T is any tree on $n - \ell$ vertices;*
- *If $\alpha < 0$ then $W^\alpha(G)$ has the maximum value if and only if $G = K_\ell + T$, where T is any tree on $n - \ell$ vertices.*

Moreover, in the extremal case

$$W^\alpha(G) = (n^2 - 2n\ell - 3n + \ell^2 + 3\ell + 2)\, 2^{\alpha-1} + (2n\ell + 2n - \ell^2 - 3\ell - 2)\, 2^{-1}.$$

Observe that for $\alpha = 1$ the invariant W^α is the Wiener index, and by Theorem 9.1 the extremal value is

$$W(G) = (2n^2 - 2n\ell - 4n + \ell^2 + 3\ell + 2)\, 2^{-1}.$$

Recall that a *dumbbell graph* is a graph comprised of two disjoint cliques connected by a path. More precisely, a dumbbell graph $D_c(a, b)$ is a graph obtained from a path $P_c = v_1 v_2 \cdots v_c$ and disjoint complete graphs K_a and K_b by connecting v_1 to a vertex of K_a and connecting v_c to a vertex of K_b, see Figure 16 for $D_5(3, 4)$. The order of so constructed graph is $a + b + c$. Note that without loss of generality, we can always assume that $a, b \neq 2$.

Theorem 9.2. *Let G be an apex tree on $n \geq 3$ vertices, and let $\alpha \neq 0$.*

- *If $\alpha > 0$ then $W^\alpha(G)$ has the maximum value if and only if $G = D_{n-4}(3, 1)$;*
- *If $\alpha < 0$ then $W^\alpha(G)$ has the minimum value if and only if $G = D_{n-4}(3, 1)$.*

Moreover, in the extremal case

$$W^\alpha(G) = 1 + \sum_{i=1}^{n-2} (n - i) i^\alpha.$$

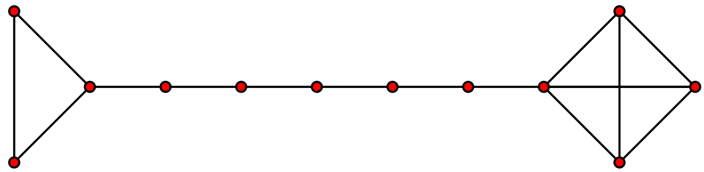

Figure 16: The graph $D_5(3, 4)$.

In [48] the following conjecture was proposed.

Conjecture 9.3. *Let G be an ℓ-apex tree on n vertices, where $\ell \geq 3$ and $n \geq \ell + 1$, such that G has maximum Wiener index. Then G is the balanced dumbbell graph, i.e. $G \cong D_c(a, b)$, where $a = \lceil \ell/2 \rceil$, $b = \lfloor \ell/2 \rfloor$, and $c = n - \ell$.*

10 Wiener index of line graphs

The *line graph* $L(G)$ of a graph G is defined as a graph whose vertex set coincides with the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are incident in G. Higher iterations of the line graph are defined recursively.

$$L^k(G) = \begin{cases} G & \text{for } k = 0, \\ L(L^{k-1}(G)) & \text{for } k > 0. \end{cases}$$

Van Rooij and Wilf [77] showed that for the sequence

$$G, L(G), L(L(G)), L(L(L(G))), \ldots$$

only four options are possible. If G is a cycle graph, then $L(G)$ and each subsequent graph in this sequence is isomorphic to G itself. If G is a claw $K_{1,3}$, then $L(G) = C_3$ and consequently the same holds for all subsequent graphs in the sequence. For a path we have $L(P_n) = P_{n-1}$, $L^2(P_n) = P_{n-2}$, …, $L^{n-1}(P_n) = P_1$ and $L^k(P_n)$ is an empty graph if $k \geq n$. In all the remaining cases the order of the graphs in the sequence increases without bound.

The following problem was proposed by Gutman [35].

Problem 10.1. Find an n-vertex graph G whose line graph $L(G)$ has maximum Wiener index.

Supported by a result from [20], we pose the following conjecture (see also [56]).

Conjecture 10.2. *Among all graphs G on n vertices, $W(L(G))$ attains maximum for some dumbbell graph on n vertices.*

Similar conjecture was proposed for bipartite graphs [56]. Let us call a graph a *barbell* graph if it is comprised of two disjoint complete bipartite graphs connected by a path.

Conjecture 10.3. *Let n be large. Among all bipartite graphs G on n vertices, $W(L(G))$ attains maximum for some barbell graph on n vertices.*

A related question we pose is the following.

Problem 10.4. For given n and k, find graphs G on n vertices with the extremal value of $W(L^k(G))$.

Dobrynin and Mel'nikov [27] proposed to estimate the extremal values for the ratio $\frac{W(L^k(G))}{W(G)}$, for a graph G on n vertices and explicitly stated the case $k = 1$ as a problem. The minimum value was given in [54].

Theorem 10.5. *Among all connected graphs on n vertices, the fraction $\frac{W(L(G))}{W(G)}$ is minimum for the star S_n, in which case $\frac{W(L(G))}{W(G)} = \frac{n-2}{2(n-1)}$.*

The problem was recently solved also for the maximal value [70] .

Theorem 10.6. *For a graph G on n vertices it holds that $\frac{W(L(G))}{W(G)} \leq \binom{n-1}{2}$ with equality if and only if $G = K_n$.*

For $k > 1$ the problem remains open.

Problem 10.7. Find n-vertex graphs G with extremal values of $\frac{W(L^k(G))}{W(G)}$ for $k \geq 2$.

Note that the line graph of K_n has the greatest number of vertices, and restricting to bipartite graphs, the (almost) balanced complete bipartite graphs have line graphs with most vertices, so $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ could be the graph attaining maximal value in this class of graphs. It is expected that the minimum value should be attained by P_n, since this is the only graph whose line graph decreases in size, see a conjecture from [56].

Conjecture 10.8. *Let $k \geq 2$ and let n be large. Among all graphs G on n vertices, $\frac{W(L^k(G))}{W(G)}$ attains the maximum for K_n, and it attains the minimum for P_n.*

The above conjecture is supported by a result from [41], where it was proved that among all trees on n vertices the path P_n has the smallest value of this ratio for $k \geq 3$, and it was conjectured that the same holds also in the case $k = 2$. Another related problem is the following.

Problem 10.9. For various ℓ and k find the extremal graphs for the ratio $\frac{W(L^k(G))}{W(L^l(G))}$.

11 Graphs with prescribed number of blocks

A graph is *non-separable* if it is connected and has no cut-vertices, i.e. either it is 2-connected or it is K_2. A *block* of G is a maximal non-separable subgraph of G. As known, the n-path P_n, which has $n - 1$ blocks, has the maximum Wiener index in the class of graphs on n vertices, and among graphs on n vertices that have just one block, the n-cycle has the largest Wiener index. The ordering of trees with respect to decreasing Wiener index is known up to the 17th maximum Wiener index [23, 64], and the increasing ordering up to the 15th maximum Wiener index [28].

Bessy et al. [8] studied the ordering of n-vertex graphs with just one block (i.e. 2-vertex connected graphs) with respect to decreasing Wiener index. Let $1 \leq p \leq q \leq n-p-q+1$ and $q > 1$. The notation $H_{n,p,q}$ stands for the graph on n vertices comprised of three internally disjoint paths with the same end-vertices, where the first path has length p, the second one has length q, and the last one has length $n - p - q + 1$. Obviously $H_{n,1,2}$ is a graph obtained from C_n by introducing a new edge connecting two vertices at distance two on the cycle, and $H_{n,2,2}$ is a graph that is obtained from a 4-cycle by connecting opposite vertices by a path of length $n-3$, see Figure 17.

In [8] it was shown that among graphs on n vertices that have just one block, $H_{n,1,2}$ has the second largest Wiener index if $n \neq 6$. If $n \geq 11$, the third extremal graph is $H_{n,2,2}$. The authors also give conjectures on the graphs with 4th and 5th greatest Wiener index in the class of 2-connected graphs. Let $H^+_{n,2,2}$ be the graph obtained from $H_{n,2,2}$ by inserting an edge between two vertices that are at distance 1 from the vertices of degree 3, see the third graph in Figure 17. Then $H^+_{n,2,2}$ has Wiener index exactly 1 less than $H_{n,2,2}$, so it is the fourth 2-connected graph by decreasing Wiener index for $n = 9$ and $n \geq 11$, but it may not be unique. However, the following can be true.

Conjecture 11.1. *For n large enough, $H^+_{n,2,2}$ is the graph with the 4th largest Wiener index among blocks on n vertices.*

Conjecture 11.2. *For n large enough, $H_{n,1,3}$ is the graph with the 5th largest Wiener index among blocks on n vertices.*

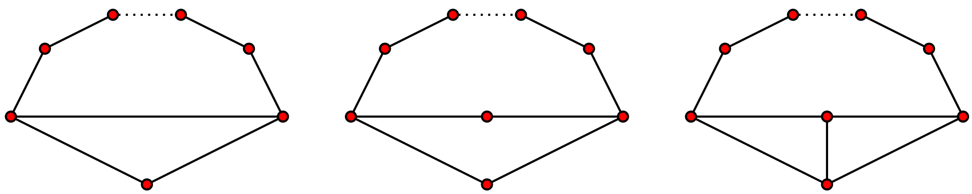

Figure 17: Graphs $H_{n,1,2}$, $H_{n,2,2}$ and $H^+_{n,2,2}$.

Bessy et al. [7] studied a general problem of finding the maximum possible value of Wiener index among graphs on n vertices with fixed number of blocks. They showed that among all graphs on n vertices which have $p \geq 2$ blocks, the maximum Wiener index is attained by a graph comprised of two cycles joined by a path, where one or both cycles can be replaced by a single edge. To be more specific, we need the following notation.

If G is a connected graph and v is a cut-vertex that partitions G into subgraphs G_1 and G_2, i.e., $G = G_1 \cup G_2$ and $G_1 \cap G_2 = \{v\}$, then we write $G = G_1 \circ_v G_2$. For simplicity reasons, by C_2 we mean the complete graph K_2.

Theorem 11.3. *Let n and p be numbers such that $n > p > 1$. Among all graphs on n vertices with p blocks, the maximum Wiener index is attained by the graph $C_a \circ_u P_{p-1} \circ_v C_b$ for some integers $a \geq 2$ and $b \geq 2$, where $a + b = n - p + 3$, and u and v are distinct end-vertices of P_{p-1}.*

Note that C_a or C_b can also be edges, and then we obtain $C_{n-p+1} \circ_u P_p$, which is a graph composed of one cycle with an attached path, or P_n if both C_a and C_b are edges.

In [6] the authors provide further details by determining the sizes of a and b in the extremal graphs for each n and p. Roughly speaking, if n is bigger than $5p - 7$, then the extremal graph is obtained for $a = 2$, i.e. the graph is a path glued to a cycle. For values $n = 5p - 8$ and $5p - 7$, there is more than one extremal graph. And when $n < 5p - 8$, the extremal graph is again unique with a and b being equal or almost equal depending on the congruence of $n - p$ modulo 4.

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On the eigenvalues of complete bipartite signed graphs*

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Abstract

Let $\Gamma = (G, \sigma)$ be a signed graph, where σ is the sign function on the edges of G. The adjacency matrix of Γ is defined canonically. Let $(K_{p,q}, \sigma)$, $p \leq q$, be a complete bipartite signed graph with bipartition (U_p, V_q), where $U_p = \{u_1, u_2, \ldots, u_p\}$ and $V_q = \{v_1, v_2, \ldots, v_q\}$. Let $(K_{p,q}, \sigma)[U_r \cup V_s]$, $r \leq p$ and $s \leq q$, be an induced signed subgraph on minimum vertices $r+s$, which contains all negative edges of the signed graph $(K_{p,q}, \sigma)$. In this paper, we show that the nullity of the signed graph $(K_{p,q}, \sigma)$ is at least $p+q-2k-2$, where $k = \min(r, s)$. The spectrum of a complete bipartite signed graph whose negative edges induce either a disjoint complete bipartite subgraphs or a path is determined. Finally, we obtain the spectrum of a complete bipartite signed graph whose negative edges (positive edges) induce a regular subgraph H. It turns out that there is a relationship between the eigenvalues of this complete bipartite signed graph and the non-negative eigenvalues of H.

Keywords: Signed graph, adjacency matrix, nullity, spectrum of complete bipartite graph.

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1 Introduction

A signed graph (or briefly sigraph) Γ is an ordered pair (G, σ), where $G = (V(G), E(G))$ is a graph (called the underlying graph), and $\sigma\colon E(G) \longrightarrow \{-1, 1\}$ is a sign function defined on the edge set of G. A signed graph is all-positive (resp. all-negative) if all of its edges are positive (resp. negative) and is denoted by $\Gamma = (G, +)$ (resp. $\Gamma = (G, -)$). The sign of a cycle in a signed graph is the product of the signs of its edges. A signed cycle is said to be positive (resp. negative) if its sign is positive (resp. negative). A signed graph is said to be balanced if none of its cycles is negative, otherwise unbalanced.

Let $A(G) = (a_{ij})$ be the adjacency matrix of G. The adjacency matrix of a signed graph $\Gamma = (G, \sigma)$ is a square matrix $A(\Gamma) = A(G, \sigma) = \left(a_{ij}^{\sigma}\right)$, where $a_{ij}^{\sigma} = \sigma(v_i v_j)\, a_{ij}$. For a matrix Z, the characteristic polynomial $|xI - Z|$ will be denoted by $\phi(Z, x)$. If Γ is a signed graph, we use $\phi(\Gamma, x)$ instead of $\phi(A(\Gamma), x)$. The eigenvalues of $A(\Gamma)$ are the eigenvalues of the signed graph Γ. The set of all distinct eigenvalues of Γ along with their multiplicities is called the spectrum of Γ. If the distinct eigenvalues of Γ are $\mu_1 > \cdots > \mu_k$, and their multiplicities are $m(\mu_1), \ldots, m(\mu_k)$, then we write

$$\operatorname{Spec}(\Gamma) = \begin{pmatrix} \mu_1 & \ldots & \mu_k \\ m(\mu_1) & \ldots & m(\mu_k) \end{pmatrix}.$$

The nullity of a signed graph Γ is the multiplicity of the eigenvalue 0 in its spectrum. It is denoted by $\eta(\Gamma)$.

Two signed graphs $\Gamma_1 = (G_1, \sigma_1)$ and $\Gamma_2 = (G_2, \sigma_2)$ are isomorphic if there is a graph isomorphism $f\colon G_1 \to G_2$ that preserves signs of the edges. If $\theta\colon V(G) \to \{+1, -1\}$ is the switching function, then switching of the signed graph $\Gamma = (G, \sigma)$ by θ means changing σ to σ^{θ} defined by

$$\sigma^{\theta}(uv) = \theta(u)\sigma(uv)\theta(v).$$

For more information about switching and recent work on signed graphs, we refer to [1, 3, 4, 5, 6, 8, 11, 12, 13, 14, 15, 16, 17].

We note that the sign function for the signed subgraph is the restriction of the original function. For $\Gamma = (G, \sigma)$ and $X \subseteq V(G)$, $\Gamma[X]$ denotes the signed subgraph induced by X, while $\Gamma - X = \Gamma[V(G) \backslash X]$. Sometimes, we also write $\Gamma - \Gamma[X]$ instead of $\Gamma - X$. Let (G, K^-) (resp. (G, K^+)) be the signed graph whose negative edges (resp. positive edges) induce a subgraph K. As usual, K_n denotes the complete graph of order n. The complete bipartite graph with two parts $U_p = \{u_1, u_2, \ldots, u_p\}$ and $V_q = \{v_1, v_2, \ldots, v_q\}$ as a partition of its vertex set is denoted by $K_{p,q}$. Also, P_n denotes the path on n vertices. $J_{r\times s}$ denotes an all-one matrix of size $r \times s$ and $O_{r\times s}$ denotes an all-zero matrix of size $r \times s$.

In the recent years, several researchers have shown interest in signed graphs, including complete bipartite signed graphs and complete signed graphs, which have a variety of applications, see [1, 2] and the references therein.

The remainder of the paper is organized as follows. In Section 2, we give some preliminary results which will be used in the sequel. In Section 3, we show that the nullity of $(K_{p,q}, \sigma)$ is at least $p + q - 2k - 2$, where $k = \min(r, s)$ and $(K_{p,q}, \sigma)[U_r \cup V_s]$, $r \leq p$ and $s \leq q$, is an induced signed subgraph on minimum vertices $r + s$, which contain all negative edges of the signed graph $(K_{p,q}, \sigma)$. In Section 4, we determine the spectrum of a complete bipartite signed graph whose negative edges (positive edges) induce (i) disjoint complete bipartite subgraphs and (ii) a path. In Section 5, we determine the spectrum of a complete bipartite signed graph whose negative edges (positive edges) induce an regular subgraph H. Also, we obtain a relation between the eigenvalues of this complete bipartite signed graph and the non-negative eigenvalues of H. For definitions and notations of graphs, we refer to [10].

2 Preliminaries

Consider $\mu_1, \mu_2, \ldots, \mu_n$ as the eigenvalues of the signed graph Γ. If for each i there exists some j such that $\mu_i + \mu_j = 0$, then we say that the spectrum is symmetric with respect to 0. It is well known that an unsigned graph which contains at least one edge is bipartite if and only if its spectrum considered as a set of points on the real axis is symmetric with respect to the origin. There exist nonbipartite signed graphs with this property as can be seen in [14]. The following result can be seen in [7].

Lemma 2.1 ([7, Theorem 2.1])**.** *Let Γ be a signed graph of order n. Then the following statements are equivalent.*

(i) *Spectrum of Γ is symmetric about the origin,*

(ii) $\phi(\Gamma, x) = x^n + \sum_{k=1}^{\lfloor \frac{n}{2} \rfloor} (-1)^k c_{2k} x^{n-2k}$, *where c_{2k} are non negative integers for all $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$,*

(iii) *Γ and $-\Gamma$ are cospectral, where $-\Gamma$ is the signed graph obtained by negating sign of each edge of Γ.*

Consider the matrix M having the block form as follows.

$$M = \begin{pmatrix} A & \beta & \cdots & \beta & \beta \\ \beta^\top & B & \cdots & C & C \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \beta^\top & C & \cdots & B & C \\ \beta^\top & C & \cdots & C & B \end{pmatrix} \tag{2.1}$$

where $A \in \mathbb{R}^{t\times t}$, $\beta \in \mathbb{R}^{t\times s}$ and $B, C \in \mathbb{R}^{s\times s}$, such that $n = t + cs$, with c being the number of copies of B. The spectrum of this matrix can be obtained as the union of the spectrum of smaller matrices using the following technique given in [9]. In the statement of the following result, $\operatorname{Spec}^{(k)}(Z)$ denotes the multi-set formed by k copies of the spectrum of Z, denoted by $\operatorname{Spec}(Z)$.

Lemma 2.2. *Let M be a matrix of the form given in* (2.1) *with $c \geq 1$ copies of the block B. Then*

(i) $\operatorname{Spec}(B - C) \subseteq \operatorname{Spec}(M)$ *with multiplicity $c - 1$,*

(ii) $\operatorname{Spec}(M) \backslash \operatorname{Spec}^{(c-1)}(B - C) = \operatorname{Spec}(M')$ *is the set of the remaining $t + s$ eigenvalues of M, where*

$$M' = \begin{pmatrix} A & \sqrt{c} \cdot \beta \\ \sqrt{c} \cdot \beta^\top & B + (c-1)C \end{pmatrix}.$$

The next two results are concerned with the spectrum of special 2×2 block matrices.

Lemma 2.3. *Let* $X = \begin{pmatrix} O_{p\times p} & A_{p\times q} \\ A^{\top}_{q\times p} & O_{q\times q} \end{pmatrix}$ *be a real symmetric matrix of order* $p+q$*,* $q \geq p$*. Then*

(i) $m(0) \geq q-p$*,*

(ii) $\pm\sqrt{\mu} \in \operatorname{Spec}(X)$*, where* μ *is an eigenvalue of a positive semidefinite square matrix* $A_{p\times q}A^{\top}_{q\times p}$*.*

Proof. By the Schur complement formula, the determinant of a 2×2 block matrix is given by

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = \left|D\right|\left|A - BD^{-1}C\right|,$$

where A and D are square blocks and D is nonsingular. So, we have

$$\begin{aligned} \phi(X,x) &= \begin{vmatrix} xI_p & -A_{p\times q} \\ -A^{\top}_{q\times p} & xI_q \end{vmatrix} = x^q \left|(xI_p) - A_{p\times q}\left(xI_q\right)^{-1} A^{\top}_{q\times p}\right| \\ &= x^q \left|\frac{1}{x}\left(x^2 I_p - A_{p\times q}A^{\top}_{q\times p}\right)\right| \\ &= x^{q-p}\phi\left(A_{p\times q}A^{\top}_{q\times p}, x^2\right). \end{aligned}$$

This completes the proof. □

Corollary 2.4. *Let* $X = \begin{pmatrix} O_{p\times p} & A_{p\times p} \\ A_{p\times p} & O_{p\times p} \end{pmatrix}$ *be a real symmetric matrix of order* $2p$*. Then* $\pm\mu \in \operatorname{Spec}(X)$*, where* μ *is an eigenvalue of the square matrix* $A_{p\times p}$*.*

We conclude this section with the following remark.

Remark 2.5. Let $(K_{p,q},\sigma)$ be a complete bipartite signed graph with bipartition (U_p, V_q), where $U_p = \{u_1, u_2, \dots, u_p\}$ and $V_q = \{v_1, v_2, \dots, v_q\}$. Then with a suitable labelling of the vertices of $(K_{p,q},\sigma)$, its adjacency matrix is given by

$$A(K_{p,q},\sigma) = \begin{pmatrix} O_{p\times p} & B_{p\times q} \\ B^{\top}_{q\times p} & O_{q\times q} \end{pmatrix}.$$

In view of Lemma 2.3, we observe that the spectrum of $(K_{p,q},\sigma)$ is related with the spectrum of the matrix $B_{p\times q}B^{\top}_{q\times p}$. Thus from here onwards, we focus on the matrix $B_{p\times q}$ and we call it as the spectral block of the adjacency matrix of the signed graph $(K_{p,q},\sigma)$.

3 Nullity of the signed graph $(K_{p,q},\sigma)$

In this section, we obtain a lower bound for the nullity of $\Gamma = (K_{p,q},\sigma)$ for any sign function σ, subject to the given condition.

Theorem 3.1. *Let* $(K_{p,q},\sigma)$*,* $p \leq q$*, be a complete bipartite signed graph and let* $(K_{p,q},\sigma)[U_r \cup V_s]$*,* $r \leq p$ *and* $s \leq q$*, be its induced signed subgraph on minimum vertices* $r+s$*, which contains all negative edges of the signed graph* $(K_{p,q},\sigma)$*. Then* $\eta((K_{p,q},\sigma)) \geq p+q-2k-2$*, where* $k = \min(r,s)$*.*

Proof. Note that the order of $(K_{p,q},\sigma)[U_r \cup V_s]$ is $r+s$. With a suitable labelling of the vertices of $(K_{p,q},\sigma)$, the adjacency matrix is given by

$$A(K_{p,q},\sigma) = \begin{pmatrix} O_{p\times p} & B_{p\times q} \\ B^\top_{q\times p} & O_{q\times q} \end{pmatrix},$$

where $B_{p\times q}$ is the spectral block of the adjacency matrix of the signed graph $(K_{p,q},\sigma)$. By Lemma 2.3, we get

$$\phi(A(K_{p,q},\sigma),x) = x^{q-p}\phi\left(B_{p\times q}B^\top_{q\times p},x^2\right). \tag{3.1}$$

Without loss of generality, we may assume that $r<p$ and $s<q$. As $(K_{p,q},\sigma)[U_r \cup V_s]$ is an induced signed subgraph on minimum vertices $r+s$, which contain all negative edges of the signed graph $(K_{p,q},\sigma)$, we have

$$B_{p\times q} = \begin{pmatrix} X_{r\times s} & J_{r\times q-s} \\ J_{p-r\times s} & J_{p-r\times q-s} \end{pmatrix},$$

where $X_{r\times s}$ is the spectral block of the adjacency matrix of the signed graph $(K_{p,q},\sigma)[U_r \cup V_s]$. The transpose of a 2×2 block matrix is given by

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^\top = \begin{pmatrix} A^\top & C^\top \\ B^\top & D^\top \end{pmatrix}.$$

Together with the fact that $J_{m\times n}J_{n\times m} = nJ_{m\times m}$, this yields

$$\begin{aligned} B_{p\times q}B^\top_{q\times p} &= \begin{pmatrix} X_{r\times s} & J_{r\times q-s} \\ J_{p-r\times s} & J_{p-r\times q-s} \end{pmatrix} \times \begin{pmatrix} X^\top_{s\times r} & J_{s\times p-r} \\ J_{q-s\times r} & J_{q-s\times p-r} \end{pmatrix} \\ &= \begin{pmatrix} X_{r\times s}X^\top_{s\times r} + (q-s)J_{r\times r} & X_{r\times s}J_{s\times p-r} + (q-s)J_{r\times p-r} \\ J_{p-r\times s}X^\top_{s\times r} + (q-s)J_{p-r\times r} & sJ_{p-r\times p-r} + (q-s)J_{p-r\times p-r} \end{pmatrix} \\ &= \begin{pmatrix} X_{r\times s}X^\top_{s\times r} + (q-s)J_{r\times r} & X_{r\times s}J_{s\times p-r} + (q-s)J_{r\times p-r} \\ J_{p-r\times s}X^\top_{s\times r} + (q-s)J_{p-r\times r} & qJ_{p-r\times p-r} \end{pmatrix}. \end{aligned}$$

Now, it is easy to see that $X_{r\times s}J_{s\times 1} + (q-s)J_{r\times 1} = Y + (q-s)J_{r\times 1}$, where Y is the column vector of the row sums of the matrix $X_{r\times s}$. Let $Z = [Y+(q-s)J_{r\times 1}\ Y + (q-s)J_{r\times 1} \ \cdots \ Y+(q-s)J_{r\times 1}] \in \mathbb{R}^{r\times p-r}$ be a matrix of order $r\times p-r$. Then, we have

$$B_{p\times q}B^\top_{q\times p} = \begin{pmatrix} X_{r\times s}X^\top_{s\times r} + (q-s)J_{r\times r} & Z \\ Z^\top & qJ_{p-r\times p-r} \end{pmatrix}. \tag{3.2}$$

The matrix $B_{p\times q}B^\top_{q\times p}$ has a special kind of symmetry. Taking $A = X_{r\times s}X^\top_{s\times r} + (q-s)J_{r\times r}$, $\beta = Y + (q-s)J_{r\times 1}$, $B=[q]$ and $C=[q]$ in (2.1), from Lemma 2.2, we get $\mathrm{Spec}^{p-r-1}(B-C) = \mathrm{Spec}^{p-r-1}([0]) \subseteq \mathrm{Spec}(B_{p\times q}B^\top_{q\times p})$. Again by Equation (3.1), Equation (3.2) and Lemma 2.2, we obtain

$$\phi(A(K_{p,q},\sigma),x) = x^{\alpha}\phi\left(Z_1,x^2\right), \tag{3.3}$$

where $\alpha = q+p-2r-2$ and

$$Z_1 = \begin{pmatrix} X_{r\times s}X^\top_{s\times r} + (q-s)J_{r\times r} & \sqrt{p-r}(Y+(q-s)J_{r\times 1}) \\ \sqrt{p-r}(Y+(q-s)J_{r\times 1})^\top & q(p-r) \end{pmatrix}.$$

Also, we have

$$B^{\top}_{q\times p}B_{p\times q} = \begin{pmatrix} X^{\top}_{s\times r}X_{r\times s} + (p-r)J_{s\times s} & X^{\top}_{s\times r}J_{r\times q-s} + (p-r)J_{s\times q-s} \\ J_{q-s\times r}X_{r\times s} + (p-r)J_{q-s\times s} & pJ_{q-s\times q-s} \end{pmatrix}.$$

Now, $X^{\top}_{s\times r}J_{r\times 1} + (p-r)J_{s\times 1} = Y' + (p-r)J_{s\times 1}$, where Y' is the column vector of the column sums of the matrix $X_{r\times s}$. Let $Z' = [Y' + (p-r)J_{s\times 1} \;\; Y' + (p-r)J_{s\times 1} \;\; \cdots \;\; Y' + (p-r)J_{s\times 1}] \in \mathbb{R}^{s\times q-s}$ be a matrix of order $s\times q-s$. Then,

$$B^{\top}_{q\times p}B_{p\times q} = \begin{pmatrix} X^{\top}_{s\times r}X_{r\times s} + (p-r)J_{s\times s} & Z' \\ Z'^{\top} & pJ_{q-s\times q-s} \end{pmatrix}. \tag{3.4}$$

Taking $A = X^{\top}_{s\times r}X_{r\times s} + (p-r)J_{s\times s}$, $\beta = Y' + (p-r)J_{s\times 1}$, $B = [p]$ and $C = [p]$ in (2.1), from Lemma 2.2, we get $\mathrm{Spec}^{q-s-1}(B-C) = \mathrm{Spec}^{q-s-1}([0]) \subseteq \mathrm{Spec}(B^{\top}_{p\times q}B_{p\times q})$. Note that the eigenvalues of $B^{\top}_{q\times p}B_{p\times q}$ are given by the eigenvalues of $B_{p\times q}B^{\top}_{q\times p}$, together with the eigenvalue 0 of multiplicity $q-p$. Therefore, by Equation (3.1), Equation (3.4) and Lemma 2.2, we obtain

$$\phi(A(K_{p,q},\sigma),x) = x^{\zeta}\phi\left(Z_2, x^2\right), \tag{3.5}$$

where $\zeta = q + p - 2s - 2$ and

$$Z_2 = \begin{pmatrix} X^{\top}_{s\times r}X_{r\times s} + (p-r)J_{s\times s} & \sqrt{q-s}(Y' + (p-r)J_{s\times 1}) \\ \sqrt{q-s}(Y' + (p-r)J_{s\times 1})^{\top} & p(q-s) \end{pmatrix}.$$

Hence the result follows by Equation (3.3) and Equation (3.5). □

As $(K_{p,q},\sigma)$ is a bipartite signed graph, therefore its spectrum is symmetric about the origin. Thus, the following is an immediate consequence of Theorem 3.1 and Lemma 2.1.

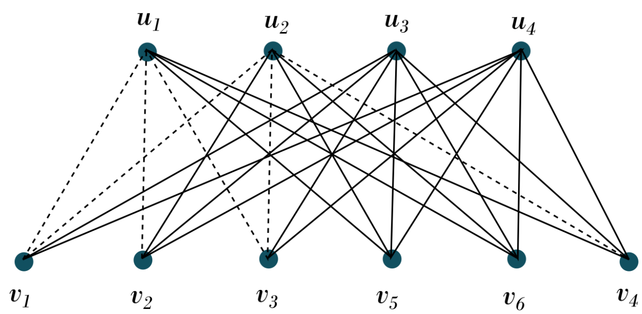

Figure 1: The signed graph $(K_{4,6},\sigma)$.

Corollary 3.2. *Let $(K_{p,q},\sigma)$, $p \leq q$, be a complete bipartite signed graph and let $(K_{p,q},\sigma)[U_r \cup V_s]$, $r \leq p$ and $s \leq q$, be its induced subgraph on minimum vertices $r+s$, which contains all positive edges of the signed graph $(K_{p,q},\sigma)$. Then $\eta((K_{p,q},\sigma)) \geq p + q - 2k - 2$, where $k = \min(r,s)$.*

We end this section with an example which shows that the lower bound for the nullity, given in Theorem 3.1, of $(K_{p,q},\sigma)$ is best possible.

Example 3.3. Consider the complete bipartite signed graph $(K_{4,6},\sigma)$ as shown in Figure 1. Plain lines denote the positive edges and dashed lines denote the negative edges. It contains an induced signed subgraph $(K_{4,6},\sigma)[U_2,V_4]$ on 6 vertices which contains all negative edges of $(K_{4,6},\sigma)$. Here, we have $p=4$, $q=6$ and $k=2$. Therefore, by Theorem 3.1, $\eta((K_{4,6},\sigma))\geq 4$. The spectral block of the adjacency matrix of the induced signed subgraph $(K_{4,6},\sigma)[U_2,V_4]$ is given as

$$X_{2\times 4}=\begin{pmatrix} -1 & -1 & -1 & 1 \\ -1 & 1 & -1 & -1 \end{pmatrix}.$$

Therefore, by Equation (3.3), we get

$$\phi(A(K_{4,6},\sigma),x)=x^4\phi\left(\begin{pmatrix} 6 & 2 & 0 \\ 2 & 6 & 0 \\ 0 & 0 & 12 \end{pmatrix},x^2\right).$$

Thus, it is easy to see that

$$\operatorname{Spec}((K_{4,6},\sigma))=\begin{pmatrix} 2\sqrt{3} & 2\sqrt{2} & 2 & 0 & -2 & -2\sqrt{2} & -2\sqrt{3} \\ 1 & 1 & 1 & 4 & 1 & 1 & 1 \end{pmatrix}.$$

4 Spectrum of $(K_{p,q},\sigma)$ when negative edges induce either a disjoint complete bipartite subgraphs or a path

We begin this section with the computation of the spectrum of the complete bipartite signed graph $\left(K_{p,q},K^-_{r,s}\right)$ whose negative edges induce a subgraph $K_{r,s}$.

Theorem 4.1. *Let $\left(K_{p,q},K^-_{r,s}\right)$, $p\leq q$, $r\leq p$ and $s\leq q$, be a complete bipartite signed graph whose negative edges induce a subgraph $K_{r,s}$ of order $r+s$. Then the spectrum of $\left(K_{p,q},K^-_{r,s}\right)$ is given as*

$$\operatorname{Spec}(\left(K_{p,q},K^-_{r,s}\right))=\begin{pmatrix} \mu_1 & \mu_2 & 0 & -\mu_2 & -\mu_1 \\ 1 & 1 & p+q-4 & 1 & 1 \end{pmatrix},$$

where

$$\mu_1,\mu_2=\sqrt{\frac{pq\pm\sqrt{p^2q^2-16rs(p-r)(q-s)}}{2}}.$$

Proof. By Equation (3.3), we have

$$\phi\left(\left(K_{p,q},K^-_{r,s}\right),x\right)=x^\alpha\phi\left(\begin{pmatrix} X_{r\times s}X^\top_{s\times r}+(q-s)J_{r\times r} & \sqrt{p-r}\beta \\ \sqrt{p-r}\beta^\top & q(p-r) \end{pmatrix},x^2\right), \quad (4.1)$$

where $\alpha=q+p-2r-2$, $\beta=Y+(q-s)J_{r\times 1}$, and Y is the column vector of the row sums of spectral block $X_{r\times s}$ of the adjacency matrix of an induced signed subgraph $K_{r,s}$, whose all edges are negative. Clearly, $X_{r\times s}X^\top_{s\times r}+(q-s)J_{r\times r}=-J_{r\times s}\times -J_{s\times r}+(q-s)J_{r\times r}=qJ_{r\times r}$ and $Y+(q-s)J_{r\times 1}=(q-2s)J_{r\times 1}$. Therefore, Equation (4.1) takes the form

$$\phi\left(\left(K_{p,q},K^-_{r,s}\right),x\right)=x^\alpha\phi\left(\begin{pmatrix} qJ_{r\times r} & \sqrt{p-r}(q-2s)J_{r\times 1} \\ \sqrt{p-r}(q-2s)J_{1\times r} & q(p-r) \end{pmatrix},x^2\right). \quad (4.2)$$

For $p \neq r$, it can be easily seen that the real symmetric matrix

$$Z_1 = \begin{pmatrix} qJ_{r\times r} & \sqrt{p-r}(q-2s)J_{r\times 1} \\ \sqrt{p-r}(q-2s)J_{1\times r} & q(p-r) \end{pmatrix}$$

has rank 2. Now, let x_1 and x_2 be the non zero eigenvalues of Z_1. We have

$$x_1 + x_2 = tr(Z_1) = rq + q(p-r) = pq. \tag{4.3}$$

Also,

$$x_1^2 + x_2^2 = tr(Z_1^2) = p^2q^2 - 16rs(p-r)(q-s). \tag{4.4}$$

Equations (4.3) and (4.4), imply that

$$x_1,\ x_2 = \frac{pq \pm \sqrt{p^2q^2 - 16rs(p-r)(q-s)}}{2}. \tag{4.5}$$

Thus, Equation (4.2) yields that

$$\phi\left(\left(K_{p,q}, K_{r,s}^-\right), x\right) = x^{p+q-4}(x^4 - (x_1+x_2)x^2 + x_1x_2),$$

where x_1 and x_2 are given in Equation (4.5). This proves the result. □

As a consequence, we compute the spectrum of a complete bipartite signed graph whose positive edges induce a complete bipartite subgraph.

Corollary 4.2. *Let $\left(K_{p,q}, K_{r,s}^+\right)$, $p \le q$, $r \le p$ and $s \le q$, be a complete bipartite signed graph whose positive edges induce a subgraph $K_{r,s}$ of order $r+s$. Then the spectrum of $\left(K_{p,q}, K_{r,s}^+\right)$ is given as*

$$\operatorname{Spec}(\left(K_{p,q}, K_{r,s}^+\right)) = \begin{pmatrix} \mu_1 & \mu_2 & 0 & -\mu_2 & -\mu_1 \\ 1 & 1 & p+q-4 & 1 & 1 \end{pmatrix},$$

where

$$\mu_1, \mu_2 = \sqrt{\frac{pq \pm \sqrt{p^2q^2 - 16rs(p-r)(q-s)}}{2}}.$$

Now, we obtain the characteristic polynomial of the complete bipartite signed graph $(K_{p,q}, \sigma)$ whose negative edges form the disjoint subgraphs $K_{r,s}$ of different orders.

Theorem 4.3. *Let $(K_{p,q}, \sigma)$, $p \le q$, be a complete bipartite signed graph whose negative edges induce disjoint complete bipartite subgraphs of orders r_1+s_1, r_2+s_2, …, r_k+s_k such that $\sum_{i=1}^k r_i = r$, $\sum_{i=1}^k s_i = s$, $r \le p$ and $s \le q$. Then the characteristic polynomial of $(K_{p,q}, \sigma)$ is given as*

$$\phi\left(\left(K_{p,q}, \sigma\right), x\right) = x^{p+q-2k-2}\phi\left(Z', x^2\right),$$

where

$$Z' = \begin{pmatrix} r_1c_{11} & r_2c_{12} & \cdots & r_kc_{1k} & c(q-2s_1) \\ r_1c_{21} & r_2c_{22} & \cdots & r_kc_{2k} & c(q-2s_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r_1c_{k1} & r_2c_{k2} & \cdots & r_kc_{kk} & c(q-2s_k) \\ r_1c(q-2s_1) & r_2c(q-2s_2) & \cdots & r_kc(q-2s_k) & q(p-r) \end{pmatrix}$$

is a matrix of order $k+1$, $c = \sqrt{p-r}$, $c_{ij} = q$ if $i = j$ and $c_{ij} = q - 2s_i - 2s_j$ otherwise.

Proof. Consider the matrix given in Equation (3.3)

$$Z_1 = \begin{pmatrix} X_{r\times s}X_{s\times r}^{\top} + (q-s)J_{r\times r} & \sqrt{p-r}(Y+(q-s)J_{r\times 1}) \\ \sqrt{p-r}(Y+(q-s)J_{r\times 1})^{\top} & q(p-r) \end{pmatrix}, \tag{4.6}$$

where Y is the column vector of the row sums of the spectral block $X_{r\times s}$ of the adjacency matrix of an induced signed subgraph of $(K_{p,q},\sigma)$ which contains all its negative edges. Hence, with a suitable relabelling of vertices of the induced signed subgraph, we have

$$X_{r\times s} = \begin{pmatrix} -J_{r_1\times s_1} & J_{r_1\times s_2} & \cdots & J_{r_1\times s_k} \\ J_{r_2\times s_1} & -J_{r_2\times s_2} & \cdots & J_{r_2\times s_k} \\ \vdots & \vdots & \ddots & \vdots \\ J_{r_k\times s_1} & J_{r_k\times s_2} & \cdots & -J_{r_k\times s_k} \end{pmatrix},$$

where $J_{r_i\times s_i}$ is the spectral block of the adjacency matrix of the complete bipartite subgraph K_{r_i,s_i}, $i=1,2,\ldots,k$, $\sum_{i=1}^{k} r_i = r$ and $\sum_{i=1}^{k} s_i = s$. Now, it is easy to obtain

$$X_{r\times s}X_{s\times r}^{\top} = \begin{pmatrix} b_{11}J_{r_1\times r_1} & b_{12}J_{r_1\times r_2} & \cdots & b_{1k}J_{r_1\times r_k} \\ b_{21}J_{r_2\times r_1} & b_{22}J_{r_2\times r_2} & \cdots & b_{2k}J_{r_2\times r_k} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k1}J_{r_k\times r_1} & b_{k2}J_{r_k\times r_2} & \cdots & b_{kk}J_{r_k\times r_k} \end{pmatrix},$$

where, $b_{ij} = \sum_{i=1}^{k} s_i = s$ if $i=j$ and $b_{ij} = s-2s_i-2s_j$, otherwise. As Y is the column vector of the row sums of the spectral block $X_{r\times s}$, therefore the matrix Z_1 given in (4.6) takes the form

$$Z_1 = \begin{pmatrix} c_{11}J_{r_1\times r_1} & c_{12}J_{r_1\times r_2} & \cdots & c_{1k}J_{r_1\times r_k} & c(q-2s_1)J_{r_1\times 1} \\ c_{21}J_{r_2\times r_1} & c_{22}J_{r_2\times r_2} & \cdots & c_{2k}J_{r_2\times r_k} & c(q-2s_2)J_{r_2\times 1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{k1}J_{r_k\times r_1} & c_{k2}J_{r_k\times r_2} & \cdots & c_{kk}J_{r_k\times r_k} & c(q-2s_k)J_{r_k\times 1} \\ c(q-2s_1)J_{1\times r_1} & c(q-2s_2)J_{1\times r_2} & \cdots & c(q-2s_k)J_{1\times r_k} & q(p-r)J_{1\times 1} \end{pmatrix},$$

where $c=\sqrt{p-r}$, $c_{ij}=q$ if $i=j$ and $c_{ij}=q-2s_i-2s_j$ otherwise. Clearly, the matrix Z_1 has equitable quotient matrix Z', where

$$Z' = \begin{pmatrix} r_1c_{11} & r_2c_{12} & \cdots & r_kc_{1k} & c(q-2s_1) \\ r_1c_{21} & r_2c_{22} & \cdots & r_kc_{2k} & c(q-2s_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r_1c_{k1} & r_2c_{k2} & \cdots & r_kc_{kk} & c(q-2s_k) \\ r_1c(q-2s_1) & r_2c(q-2s_2) & \cdots & r_kc(q-2s_k) & q(p-r) \end{pmatrix}.$$

Now by [18, Theorem 3.1], $\mathrm{Spec}(Z_1) = \mathrm{Spec}(Z') \cup \begin{pmatrix} 0 \\ r-k \end{pmatrix}$, where Z' is equitable quotient matrix of Z_1 and is given as

$$Z' = \begin{pmatrix} r_1c_{11} & r_2c_{12} & \cdots & r_kc_{1k} & c(q-2s_1) \\ r_1c_{21} & r_2c_{22} & \cdots & r_kc_{2k} & c(q-2s_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r_1c_{k1} & r_2c_{k2} & \cdots & r_kc_{kk} & c(q-2s_k) \\ r_1c(q-2s_1) & r_2c(q-2s_2) & \cdots & r_kc(q-2s_k) & q(p-r) \end{pmatrix},$$

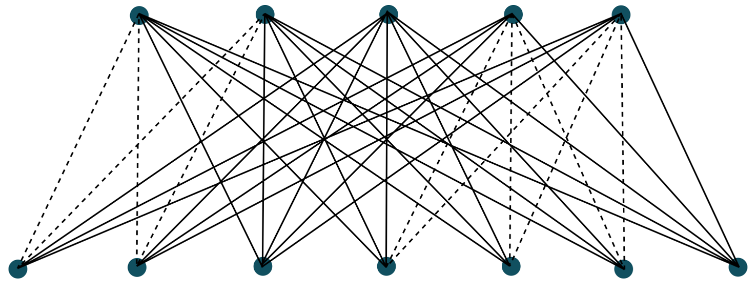

Figure 2: Signed graph whose negative edges induce two disjoint complete bipartite subgraphs.

where $c = \sqrt{p-r}$, $c_{ij} = q$ if $i = j$ and $c_{ij} = q - 2s_i - 2s_j$ otherwise. As $\operatorname{Spec}(Z_1) = \operatorname{Spec}(Z') \cup \begin{pmatrix} 0 \\ r-k \end{pmatrix}$, therefore the result follows by Equation (3.3) and Equation (4.6). □

An application of Theorem 4.3 can be seen in the following example.

Example 4.4. Consider the complete bipartite signed graph $(K_{5,7}, \sigma)$ as shown in Figure 2. Here, we have $p = 5$, $q = 7$, $r_1 = 2$, $s_1 = 2$, $r_2 = 2$, $s_2 = 3$, $r = r_1 + r_2 = 4$ and $s = s_1 + s_2 = 5$. Therefore, by Theorem 4.3, we get

$$\phi(A(K_{5,7}, \sigma), x) = x^6 \phi\left(\begin{pmatrix} 14 & -6 & 3 \\ -6 & 14 & 1 \\ 6 & 2 & 7 \end{pmatrix}, x^2\right).$$

Thus, it is easy to see that

$$\operatorname{Spec}((K_{5,7}, \sigma)) = \begin{pmatrix} 4.50 & 3.37 & 1.82 & 0 & -1.82 & -3.37 & -4.50 \\ 1 & 1 & 1 & 6 & 1 & 1 & 1 \end{pmatrix}.$$

The next corollary follows from Lemma 2.1 and Theorem 4.3 which gives the spectrum of a complete bipartite signed graph whose positive edges induce the disjoint complete bipartite subgraphs of different orders.

Corollary 4.5. *Let $(K_{p,q}, \sigma)$, $p \le q$, be a complete bipartite signed graph whose positive edges induce disjoint complete bipartite subgraphs of orders $r_1 + s_1$, $r_2 + s_2$, …, $r_k + s_k$ such that $\sum_{i=1}^{k} r_i = r$, $\sum_{i=1}^{k} s_i = s$, $r \le p$ and $s \le q$. Then the characteristic polynomial of $(K_{p,q}, \sigma)$ is given as*

$$\phi\left((K_{p,q}, \sigma), x\right) = x^{p+q-2k-2} \phi\left(Z', x^2\right),$$

where

$$Z' = \begin{pmatrix} r_1 c_{11} & r_2 c_{12} & \cdots & r_k c_{1k} & c(q-2s_1) \\ r_1 c_{21} & r_2 c_{22} & \cdots & r_k c_{2k} & c(q-2s_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r_1 c_{k1} & r_2 c_{k2} & \cdots & r_k c_{kk} & c(q-2s_k) \\ r_1 c(q-2s_1) & r_2 c(q-2s_2) & \cdots & r_k c(q-2s_k) & q(p-r) \end{pmatrix}$$

is a matrix of order $k+1$, $c = \sqrt{p-r}$, $c_{ij} = q$ if $i = j$ and $c_{ij} = q - 2s_i - 2s_j$ otherwise.

We conclude this section with the following result whose proof can be obtained in a similar way as in Theorem 4.3.

Theorem 4.6. (i) *Let* $(K_{p,q}, P_{2r}^-)$*,* $p \leq q$ *and* $r \geq 1$*, be a complete bipartite signed graph whose negative edges induce a path on* $2r$ *vertices. Then the characteristic polynomial of* $(K_{p,q}, P_{2r}^-)$ *is given as*

$$\phi\left(\left(K_{p,q}, P_{2r}^-\right), x\right) = x^{p+q-2r-2}\phi\left(Z', x^2\right),$$

where

$$Z' = \begin{pmatrix} q & q-2 & q-6 & q-6 & \cdots & q-6 & c(q-2) \\ q-2 & q & q-4 & q-8 & \cdots & q-8 & c(q-4) \\ q-6 & q-4 & q & q-4 & \ddots & \vdots & \vdots \\ q-6 & q-8 & q-4 & q & \ddots & q-8 & c(q-4) \\ \vdots & \vdots & \ddots & \ddots & \ddots & q-4 & c(q-4) \\ q-6 & q-8 & \cdots & q-8 & q-4 & q & c(q-4) \\ c(q-2) & c(q-4) & \cdots & c(q-4) & c(q-4) & c(q-4) & q(p-r-1) \end{pmatrix}$$

is a positive semidefinite matrix of order $r+1$ *and* $c = \sqrt{p-r-1}$*.*
(ii) *Let* $(K_{p,q}, P_{2r+1}^-)$*,* $p \leq q$ *and* $r \geq 1$*, be a complete bipartite signed graph whose negative edges induce a path on* $2r+1$ *vertices with both pendent vertices of the path* P_{2r+1} *in* U_p*. Then the characteristic polynomial of* $(K_{p,q}, P_{2r+1}^-)$ *is given as*

$$\phi\left(\left(K_{p,q}, P_{2r+1}^-\right), x\right) = x^{p+q-2r-4}\phi\left(Z', x^2\right),$$

where

$$Z' = \begin{pmatrix} q & q-2 & q-6 & q-6 & \cdots & q-6 & q-4 & c(q-2) \\ q-2 & q & q-4 & q-8 & \cdots & q-8 & q-6 & c(q-4) \\ q-6 & q-4 & q & q-4 & \ddots & \vdots & \vdots & \vdots \\ q-6 & q-8 & q-4 & q & \ddots & q-8 & q-6 & c(q-4) \\ \vdots & \vdots & \ddots & \ddots & \ddots & q-4 & q-6 & c(q-4) \\ q-6 & q-8 & \cdots & q-8 & q-4 & q & q-2 & c(q-4) \\ q-4 & q-6 & \cdots & q-6 & q-6 & q-2 & q & c(q-2) \\ c(q-2) & c(q-4) & \cdots & c(q-4) & c(q-4) & c(q-4) & c(q-2) & q(p-r) \end{pmatrix}$$

is a positive semidefinite matrix of order $r+2$ *and* $c = \sqrt{p-r}$*.*
(iii) *Let* $(K_{p,q}, P_{2r+1}^-)$*,* $p \leq q$ *and* $r \geq 1$*, be a complete bipartite signed graph whose negative edges induce a path on* $2r+1$ *vertices with both pendent vertices of the path* P_{2r+1} *in* V_q*. Then the characteristic polynomial of* $(K_{p,q}, P_{2r+1}^-)$ *is given as*

$$\phi\left(\left(K_{p,q}, P_{2r+1}^-\right), x\right) = x^{p+q-2r-2}\phi\left(Z', x^2\right),$$

where

$$Z' = \begin{pmatrix} q & q-4 & q-8 & q-8 & \cdots & q-8 & c(q-4) \\ q-4 & q & q-4 & q-8 & \cdots & q-8 & c(q-4) \\ q-8 & q-4 & q & q-4 & \ddots & \vdots & \vdots \\ q-8 & q-8 & q-4 & q & \ddots & q-8 & c(q-4) \\ \vdots & \vdots & \ddots & \ddots & \ddots & q-4 & c(q-4) \\ q-8 & q-8 & \dots & q-8 & q-4 & q & c(q-4) \\ c(q-4) & c(q-4) & \dots & c(q-4) & c(q-4) & c(q-4) & q(p-r) \end{pmatrix}$$

is a positive semidefnite matrix of order $r+1$ *and* $c = \sqrt{p-r}$.

The next example gives the spectrum of a complete bipartite signed graph whose negative edges induce a path on 5 vertices.

Example 4.7. Let $\left(K_{p,q}, P_5^-\right)$, $p \leq q$, be a complete bipartite signed graph whose negative edges induce a path on 5 vertices with both pendent vertices of the path P_5 in V_q. By Theorem 4.6 (Part (iii)), the characteristic polynomial of $\left(K_{p,q}, P_5^-\right)$ is given by

$$\phi\left(\left(K_{p,q}, P_5^-\right), x\right) = x^{p+q-6}\phi\left(\begin{pmatrix} q & q-4 & c(q-4) \\ q-4 & q & c(q-4) \\ c(q-4) & c(q-4) & q(p-2) \end{pmatrix}, x^2\right),$$

where $c = \sqrt{p-2}$. To determine the spectrum of $(K_{p,q}, P_5^-)$, it is enough to consider the matrix

$$Z' = \begin{pmatrix} q & q-4 & c(q-4) \\ q-4 & q & c(q-4) \\ c(q-4) & c(q-4) & q(p-2) \end{pmatrix}.$$

Clearly, 4 is an eigenvalue of the matriz Z' corresponding to an eigenvector $(1, -1, 0)^\top$. To compute the other two eigenvalues of Z', we use the fact that the sum and product of the eigenvalues of Z' are equal to the trace and determinant, respectively. Then, we obtain the eigenvalues as

$$\frac{pq - 4 \pm \sqrt{p^2q^2 - 56pq + 128p + 96q - 240}}{2}.$$

Thus, the spectrum of $(K_{p,q}, P_5^-)$ is given as

$$\operatorname{Spec}((K_{p,q}, P_5^-)) = \begin{pmatrix} \mu_1 & \mu_2 & 2 & 0 & -2 & -\mu_2 & -\mu_1 \\ 1 & 1 & 1 & p+q-6 & 1 & 1 & 1 \end{pmatrix},$$

where

$$\mu_1, \mu_2 = \sqrt{\frac{pq - 4 \pm \sqrt{p^2q^2 - 56pq + 128p + 96q - 240}}{2}}.$$

5 Eigenvalues of $\left(K_{p,q}, H_{r,n}^-\right)$

The complete bipartite signed graph Γ whose negative edges induce a 1-regular graph of different orders has been studied in [2]. In this section, we consider the complete bipartite signed graph $\big(K_{p,q}, H^-_{r,n}\big)$, $p \leq q$, whose negative edges induce an r-regular subgraph H (not necessarily connected) of order n. We find a relation between the eigenvalues of this complete bipartite signed graph and the non-negative eigenvalues of H. The other eigenvalues of $\big(K_{p,q}, H^-_{r,n}\big)$ are also determined. We start with the following lemma.

Lemma 5.1. *Let $\big(K_{k,k}, H^-_{r,2k}\big)$ be a complete bipartite signed graph whose negative edges induce an r-regular subgraph H of order $2k$. If the eigenvalues of H are $\mu_1 = r \geq \mu_2 \geq \cdots \geq \mu_{2k} = -r$, then $-2\mu_i$ is an eigenvalue of $\big(K_{k,k}, H^-_{r,2k}\big)$ for $i = 2, \ldots, 2k-1$. Moreover, the other two eigenvalues of $\big(K_{k,k}, H^-_{r,2k}\big)$ are $k-2r$ and $-k+2r$.*

Proof. Let $A(H,-) = -A(H)$ be the adjacency matrix of $(H,-)$. Therefore, with a suitable labelling of the vertices of $\big(K_{k,k}, H^-_{r,2k}\big)$, we observe that

$$A\big(K_{k,k}, H^-_{r,2k}\big) = \begin{pmatrix} O_{k\times k} & A_{k\times k} \\ A_{k\times k} & O_{k\times k} \end{pmatrix} = A(K_{k,k}) - 2A(H), \tag{5.1}$$

where the $(k-2r)$-regular symmetric matrix $A_{k\times k}$ is the spectral block of the adjacency matrix of the signed graph $\big(K_{k,k}, H^-_{r,2k}\big)$. As the matrices $A(K_{k,k})$ and $A(H)$ commute, therefore they are simultaneously diagonalizable. Let $\{x_1, x_2, \ldots, x_{2k}\}$ be an orthogonal basis of $\mathbb{R}^{2k}$ consisting of the eigenvectors of $A(H)$ and $A(K_{k,k})$ with $x_1 = J_{2k\times 1} = (1, \ldots, 1)^T \in \mathbb{R}^{2k}$. Then, we have

$$(A(K_{k,k}) - 2A(H))x_1 = (k-2r)x_1.$$

Thus, $(k-2r)$ is an eigenvalue of $A(K_{k,k}) - 2A(H)$. To find the other eigenvalues of $A(K_{k,k}) - 2A(H)$, we use the facts that $\mathrm{Spec}(A(K_{k,k}) - 2A(H)) \subseteq \mathrm{Spec}(A(K_{k,k})) + \mathrm{Spec}(-2A(H))$ and the spectrum of $\big(K_{k,k}, H^-_{r,2k}\big)$ is symmetric with respect to origin. Thus,

$$(A(K_{k,k}) - 2A(H))x_i = -2\mu_i x_i, \;\; i = 2, 3, \ldots, 2k-1$$

and

$$(A(K_{k,k}) - 2A(H))x_{2k} = (-k+2r)x_{2k}.$$

This proves the result. □

The eigenvalues of a complete bipartite signed graph whose negative edges induce a regular graph H is completely determined by the non-negative eigenvalues of H and can be seen in the following result.

Theorem 5.2. *Let $\big(K_{p,q}, H^-_{r,2k}\big)$, $p \leq q$, be a complete bipartite signed graph whose negative edges induce an r-regular subgraph H of order $2k$. Then the following statements hold:*

(i) $\eta(\big(K_{p,q}, H^-_{r,2k}\big)) \geq p+q-2k-2$.

(ii) *If the first k largest non-negative eigenvalues of H are $\mu_1 = r \geq \mu_2 \geq \cdots \geq \mu_k \geq 0$, then*

  (a) $\pm\, 2\mu_i$ *is an eigenvalue of $\big(K_{p,q}, H^-_{r,2k}\big)$, for $i = 2, \ldots, k$ when $p+q \geq 2k+2$.*

  (b) $\pm\, 2\mu_i$ *is an eigenvalue of $\big(K_{p,q}, H^-_{r,2k}\big)$, for $i = 2, \ldots, k-1$ when $p+q < 2k+2$.*

Moreover, the other four eigenvalues of $\left(K_{p,q}, H^-_{r,2k}\right)$ *are*

$$\pm\sqrt{\frac{pq+(k-2r)^2-k^2\pm\theta}{2}},$$

where

$$\theta=\sqrt{(pq+(k-2r)^2-k^2)^2-4((k-2r)^2+k(q-k)-\tfrac{k(q-2r)^2}{q})(q(p-k))}.$$

Proof. Consider the matrix which is given in Equation (3.3)

$$Z_1=\begin{pmatrix} X_{r\times s}X^\top_{s\times r}+(q-s)J_{r\times r} & \sqrt{p-r}(Y+(q-s)J_{r\times 1}) \\ \sqrt{p-r}(Y+(q-s)J_{r\times 1})^\top & q(p-r)\end{pmatrix}, \tag{5.2}$$

where Y is the column vector of the row sums of the spectral block $X_{r\times s}$ of the adjacency matrix of the induced signed subgraph $\left(K_{k,k}, H^-_{r,2k}\right)$ of $\left(K_{p,q}, H^-_{r,2k}\right)$ which contains all the negative edges. By Equation (5.1), it is easy to see that $r=s=k$, $X_{r\times s}X^\top_{s\times r}=A^2_{k\times k}$ and $Y=(k-2r)J_{k\times 1}$. Now, the matrix Z_1 takes the form

$$Z_1=\begin{pmatrix} A^2_{k\times k}+(q-k)J_{k\times k} & \sqrt{p-k}(q-2r)J_{k\times 1} \\ \sqrt{p-k}(q-2r)J^\top_{1\times k} & q(p-k)\end{pmatrix}.$$

The matrix $A^2_{k\times k}$ is $(k-2r)^2$-regular and hence commutes with $(q-k)J_{k\times k}$. Thus, it is easy to see that $(k-2r)^2-k(q-k)$ is an eigenvalue of $A^2_{k\times k}+(q-k)J_{k\times k}$ corresponding to an eigenvector $J_{k\times 1}$. Also, by Equation (5.1), Corollary 2.4 and Lemma 5.1, we have

$$(A^2_{k\times k}+(q-k)J_{k\times k})x_i=4\mu_i^2x_i, i=2,\dots,k,$$

where $\{x_1,x_2,\dots,x_k\}$ is an orthogonal basis of $\mathbb{R}^k$ with $x_1=J_{k\times 1}$ and μ_i is non-negative eigenvalue of H. Define $y_i=[x_i\ \ 0]^\top\in\mathbb{R}^{k+1}$, $i=2,\dots,k$. Then

$$Z_1y_i=4\mu_i^2y_i,\ i=2,\dots,k.$$

Therefore, $4\mu_i^2$, $i=2,\dots,k$ is an eigenvalue of Z_1. Let α_1 and α_2 be the other two eigenvalues of Z_1. We have

$$\alpha_1+\alpha_2+\sum_{i=2}^{k}4\mu_i^2=tr(Z_1)=k(q-2r)+q(p-k)$$

and

$$(k-2r)^2+\sum_{i=2}^{k}4\mu_i^2=tr(A^2_{k\times k})=k(k-2r).$$

This yields that

$$\alpha_1+\alpha_2=pq+(k-2r)^2-k^2. \tag{5.3}$$

By the Schur complement formula, the determinant of a 2×2 block matrix Z_1 is given by

$$\begin{vmatrix} A^2_{k\times k}+(q-k)J_{k\times k} & \sqrt{p-k}(q-2r)J_{k\times 1} \\ \sqrt{p-k}(q-2r)J^\top_{1\times k} & q(p-k)\end{vmatrix}=|q(p-k)|\,|M|,$$

where $M = A^2_{k\times k} + (q-k)J_{k\times k} - \frac{(q-2r)^2}{q}J_{k\times k}$. Now, clearly the eigenvalues of the matrix $A^2_{k\times k} + (q-k)J_{k\times k} - \frac{(q-2r)^2}{q}J_{k\times k}$ are $(k-2r)^2 + k(q-k) - \frac{k(q-2r)^2}{q}$ and $4\mu_i^2$, $i = 2, \ldots, k$, where μ_i is the non-negative eigenvalue of H. Thus, we have

$$\alpha_1\alpha_2 = ((k-2r)^2 + k(q-k) - \frac{k(q-2r)^2}{q})(q(p-k)). \tag{5.4}$$

Equations (5.3) and (5.4) imply that

$$\alpha_1, \alpha_2 = \frac{pq + (k-2r)^2 - k^2 \pm \theta}{2},$$

where $\theta = \sqrt{(pq + (k-2r)^2 - k^2)^2 - 4((k-2r)^2 + k(q-k) - \frac{k(q-2r)^2}{q})(q(p-k))}$. Hence, by Equation (3.3), we have $\eta(\big(K_{p,q}, H^-_{r,2k}\big)) \geq p + q - 2k - 2$ and with the fact that $\pm\alpha$ is an eigenvalue of $\big(K_{p,q}, H^-_{r,2k}\big)$ whenever α^2 is an eigenvalue of Z_1, the proof follows. $\square$

The eigenvalues of a complete bipartite signed graph whose positive edges induce a regular graph H is completely determined by the non-negative eigenvalues of H as can be seen in the following corollary.

Corollary 5.3. *Let $\big(K_{p,q}, H^+_{r,2k}\big)$, $p \leq q$, be a complete bipartite signed graph whose positive edges induce an r-regular subgraph H of order $2k$. Then the following statements hold:*

(i) $\eta(\big(K_{p,q}, H^+_{r,2k}\big)) \geq p + q - 2k - 2$.

(ii) *If the first k largest non-negative eigenvalues of H are $\mu_1 = r \geq \mu_2 \geq \cdots \geq \mu_k \geq 0$, then*

  (a) $\pm\, 2\mu_i$ *is an eigenvalue of* $\big(K_{p,q}, H^+_{r,2k}\big)$, *for* $i = 2, \ldots, k$ *when* $p + q \geq 2k + 2$.

  (b) $\pm\, 2\mu_i$ *is an eigenvalue of* $\big(K_{p,q}, H^+_{r,2k}\big)$, *for* $i = 2, \ldots, k-1$ *when* $p + q < 2k + 2$.

Moreover, the other four eigenvalues of $\big(K_{p,q}, H^+_{r,2k}\big)$ are

$$\pm\sqrt{\frac{pq + (k-2r)^2 - k^2 \pm \theta}{2}},$$

where

$$\theta = \sqrt{(pq + (k-2r)^2 - k^2)^2 - 4((k-2r)^2 + k(q-k) - \tfrac{k(q-2r)^2}{q})(q(p-k))}.$$

Finally, the necessary and sufficient condition for a complete bipartite signed graph whose negative edges induce a regular graph to be nonsingular is given below.

Corollary 5.4. *Let $\big(K_{p,q}, H^-_{r,2k}\big)$ $(resp.\big(K_{p,q}, H^+_{r,2k}\big))$ be a complete bipartite signed graph whose negative edges (resp. positive edges) induce an r-regular subgraph H of order $2k$. Then the signed graph $\big(K_{p,q}, H_{r,2k}\big)$ is nonsingular if and only if the graph H is nonsingular and $p = q = k \neq 2r$ or $p = q = k + 1$.*

Conclusion and future research work

In this paper, we obtained a lower bound for the nullity of a complete bipartite signed graph and proved that

$$\eta((K_{p,q},\sigma)) \geq p+q-2k-2, \tag{5.5}$$

where $k = \min(r,s)$ and $(K_{p,q},\sigma)[U_r \cup V_s]$, $r \leq p$ and $s \leq q$, is an induced signed subgraph on minimum $r+s$ vertices, which contains all the negative edges of the signed graph $(K_{p,q},\sigma)$. We showed that this lower bound is best possible for a complete bipartite signed graph as shown in Figure 1. Therefore, the following becomes interesting.

Problem 1. To characterize all complete bipartite signed graphs for which the equality holds in inequality (5.5).

Furthermore, we determine, (1) the spectrum of a complete bipartite signed graph whose negative edges induce either disjoint complete bipartite subgraphs or a path, (2) the spectrum of a complete bipartite signed graph whose negative edges (positive edges) induce a regular subgraph, along with a relation between the eigenvalues of this complete bipartite signed graph and the non-negative eigenvalues of the regular subgraph. Thus, the following becomes interesting.

Problem 2. To determine the spectrum of a complete bipartite signed graph whose negative edges induce either co-regular graph, threshold graph, tree or k-cyclic graph.

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On z-monodromies in embedded graphs

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Abstract

We characterize all permutations which occur as the z-monodromies of faces in connected simple finite graphs embedded in surfaces whose duals are also simple.

Keywords: Central circuit, chess coloring, embedded graph, zigzag, z-monodromy.

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1 Introduction

Zigzags are closed walks in embedded graphs which generalize the concept of *Petrie polygons* in regular polyhedra [2]. They were used in computer graphics [6] and in enumerating all combinatorial possibilities for fullerenes in mathematical chemistry [1, 4]. Zigzags are also closely related to *Gauss code problem*: if an embedded graph contains a single zigzag, then this zigzag is a geometrical realization of a certain Gauss code (see [5, Section 17.7] for the planar case and [3, 9] for the case when a graph is embedded in an arbitrary surface). More results on zigzags can be found in [8, 10, 13, 15].

We will consider zigzags in connected simple finite graphs embedded in surfaces whose duals are also simple. The latter condition guarantees that for any two consecutive edges on a face there is a unique zigzag containing them. This property is the crucial tool in the concept of z*-monodromy*. For a face F, the z-monodromy M_F is a permutation on the set of all oriented edges obtained by orienting each edge of F in the two possible ways. If e_0, e is a pair of consecutive edges in F, then $M_F(e)$ is the first oriented edge of F that occurs in the zigzag containing e_0, e after e.

Such z-monodromies were introduced in [12] and exploited to prove that any triangulation of an arbitrary (not necessarily oriented) closed surface can be shredded to a triangulation with a single zigzag. There are precisely 7 types of z-monodromies for triangle faces and each of them is realized. The properties and some applications of z-monodromies of

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triangle faces can be found in [11, 16]. See also [14] for a generalization of z-monodromies on pairs of edges.

Faces of embedded graph under consideration contains at least three edges. We characterize permutations that occur as z-monodromies of k-gonal faces for any $k \geq 3$. More precisely, a permutation σ on the set

$$[k]_{\pm} = \{1, \ldots, k, -k, \ldots, -1\}$$

occurs as the z-monodromy if and only if it satisfies the following conditions:

- if $\sigma(i) = j$, then $\sigma(-j) = -i$;
- $\sigma(i) \neq -i$.

In the plane case, our construction is based on the *chess coloring* of 4-regular plane graphs. For every permutation σ satisfying the above conditions there is a plane graph with a face F whose z-monodromy is σ; furthermore, this graph contains a unbounded triangle face T such that every zigzag passing through F does not pass through T. To extend the construction on the general case, we take any graph embedded in a surface with a triangle face and replace this face by the above plane graph.

We consider the case when an embedded graph and its dual both are simple. In the general case, zigzags cannot be reconstructed from pairs of consecutive edges. This shows that the concept of z-monodromy cannot be generalized in a direct way.

2 Zigzags in embedded graphs

Let S be a connected closed 2-dimensional (not necessarily orientable) surface. Let Γ be a 2-cell embedding of a connected finite graph in S, in other words, a *map* [7, Definition 1.3.6]. The difference $S \setminus \Gamma$ is a disjoint union of open disks and the closures of these disks are the *faces*. We say that a face is *k-gonal* if it contains precisely k edges. We will always assume that the following condition is satisfied:

(SS) Γ and the dual map Γ^* (see [7, p.52]) both are embeddings of simple graphs.

The fact that one of the graphs is simple does not implies that the same holds for the other graph. For example, Γ^* is not simple if Γ contains a vertex of degree 2 or two distinct faces with intersection containing more than one edge. The condition (SS) implies that each face in our graphs is k-gonal with $k \geq 3$.

A *zigzag* in Γ is a *sequence* of edges $\{e_i\}_{i \in \mathbb{N}}$ satisfying the following conditions for every $i \in \mathbb{N}$:

- e_i and e_{i+1} are distinct, they have a common vertex and belong to the same face,
- the faces containing e_i, e_{i+1} and e_{i+1}, e_{i+2} are distinct and the edges e_i and e_{i+2} are non-intersecting.

Since Γ is finite, there is a natural number $n > 1$ such that $e_{i+n} = e_i$ for every natural i. Thus, every zigzag will be represented as a cyclic sequence $e_1, \ldots, e_n$, where n is the smallest number satisfying this condition.

Any zigzag is completely determined by every pair of consecutive edges contained in this zigzag. Conversely, for every pair of distinct edges e, e' which have a common vertex and belong to the same face there is a unique zigzag containing the sequence e, e'. This property will be used in the next section.

If $Z = \{e_1, \dots, e_n\}$ is a zigzag, then the reversed sequence $Z^{-1} = \{e_n, \dots, e_1\}$ also is a zigzag. A zigzag cannot contain a sequence $e, e', \dots, e', e$ which implies that $Z \neq Z^{-1}$ for any zigzag Z. In other words, a zigzag cannot be self-reversed (see [12] for the proof for triangulations; in our case the proof is similar).

Example 2.1. Consider the cube Q_3 whose vertices are $1, \dots, 8$, see Fig. 1.

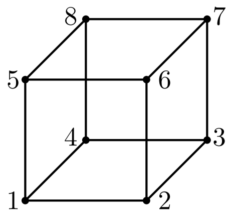

Figure 1: The cube Q_3

It contains precisely 4 zigzags up to reversing:

$$12, 23, 37, 78, 85, 51; \quad 12, 26, 67, 78, 84, 41; \quad 14, 43, 37, 76, 65, 51; \quad 23, 34, 48, 85, 56, 62.$$

Let BP_n be the n-gonal bipyramid, where $1, \dots, n$ are the consecutive vertices of the base and the remaining two vertices are a, b.

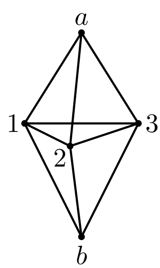

Figure 2: The bipyramid BP_3

If $n = 3$ (see Fig. 2), then it contains a single zigzag (up to reversing):

$$a1, 12, 2b, b3, 31, 1a, a2, 23, 3b, b1, 12, 2a, a3, 31, 1b, b2, 23, 3a.$$

The same holds for BP_n if n is odd. If n is even, then BP_n contains 2 or 4 zigzags up to reversing.

Every zigzag in Γ induces in a natural way a zigzag in Γ^* and vice versa.

Remark 2.2. Zigzags can be defined in maps of non-simple graphs [8]. In this case, there are simple examples showing that a zigzag cannot be determined by any pair of its consecutive edges.

3 Main result

Let Γ be as in the previous section and let F be a k-gonal face of Γ. Denote by $v_0, \dots, v_{k-1}$ the consecutive vertices of F in a fixed orientation on the boundary of this face (it is possible that $v_i = v_j$ if $|i - j| \geq 3$). Consider the set of all oriented edges of F

$$\Omega(F) = \{e_1, \dots, e_k, -e_k, \dots, -e_1\},$$

where $e_i = v_{i-1}v_i$ and $-e_i = v_i v_{i-1}$ are mutually reversed oriented edges of F (the indices are taken modulo k); it is clear that $\Omega(F)$ consists of $2k$ mutually distinct elements. Let D_F be the following permutation on $\Omega(F)$

$$D_F = (e_1, e_2, \dots, e_k)(-e_k, \dots, -e_2, -e_1).$$

In other words, D_F transfers every oriented edge of F to the next oriented edge in the corresponding orientation on the boundary.

The *z-monodromy* of F is the mapping $M_F : \Omega(F) \to \Omega(F)$ defined as follows. For any $e \in \Omega(F)$ we take $e_0 \in \Omega(F)$ such that $D_F(e_0) = e$. There is a unique zigzag, where e_0, e are consecutive edges. The first element of $\Omega(F)$ contained in this zigzag after e_0, e is denoted by $M_F(e)$.

Remark 3.1. The z-monodromy is defined when (SS) is satisfied. This concept cannot be carried out on the general case immediately.

Lemma 3.2. *The following assertions are fulfilled:*

(1) If $M_F(e) = e'$ for some $e, e' \in \Omega(F)$, then $M_F(-e') = -e$.

(2) M_F is bijective.

(3) $M_F(e) \neq -e$ for every $e \in \Omega(F)$.

Proof. (1). Let $e \in \Omega(F)$. Consider $e_0 \in \Omega(F)$ satisfying $D_F(e_0) = e$. If Z is the zigzag containing the pair e_0, e, then

$$e' = M_F(e) \text{ and } e'_0 = D_F M_F(e)$$

are the next two elements of $\Omega(F)$ in Z. Observe that $D_F(-e'_0) = -e'$. The reversed zigzag Z^{-1} contains the sequence $-e'_0, -e'$ and $-e$ is the first element of $\Omega(F)$ contained in Z^{-1} after this pair. This means that $M_F(-e') = -e$.

(2). It is sufficient to show that M_F is injective. Suppose that $M_F(e) = M_F(e') = e''$. By (1), we have $-e = M_F(-e'') = -e'$ which implies that $e = e'$.

(3). Let e and e_0 be as in the proof of (1). If $M_F(e) = -e$, then there is a zigzag Z containing the sequences e_0, e and $-e, D_F(-e)$. Since $D_F(-e) = -e_0$, Z passes through both pairs e_0, e and $-e, -e_0$. This implies that $Z = Z^{-1}$ which is impossible. □

The set $\Omega(F)$ is naturally identified with

$$[k]_\pm = [k]_+ \cup [k]_-$$

where

$$[k]_+ = \{1, \dots, k\}, \text{ and } [k]_- = \{-k, \dots, -1\}$$

(e_i and $-e_i$ correspond to i and $-i$, respectively). Then, by Lemma 3.2, the z-monodromy M_F is a permutation σ of $[k]_\pm$ satisfying the following conditions:

(M1) if $\sigma(i) = j$, then $\sigma(-j) = -i$;

(M2) $\sigma(i) \neq -i$.

Our main result is the following.

Theorem 3.3. *Let S be a connected closed 2-dimensional (not necessarily orientable) surface and let $k \geq 3$. Let also σ be a permutation of $[k]_\pm$ satisfying* (M1) *and* (M2). *There is a connected finite graph Γ embedded in S and satisfying* (SS) *which contains a k-gonal face F whose z-monodromy is σ.*

In Section 4, we prove Theorem 3.3 for plane graphs (graphs embedded in a sphere). Graphs on surfaces different from a sphere will be considered in Section 5.

4 The plane case

4.1 Preliminary

Let G be a 4-regular plane graph. The dual graph G^* is bipartite and there exists a *chess coloring* of faces of G in two colors b and w. For $c \in \{b, w\}$ we take a vertex inside every face of G assigned with the color c and join two such vertices by an edge if the corresponding faces have a common vertex at theirs boundaries. The obtained plane graph will be denoted by $\mathcal{R}_c(G)$. The graphs $\mathcal{R}_b(G)$ and $\mathcal{R}_w(G)$ are dual (see Fig. 3).

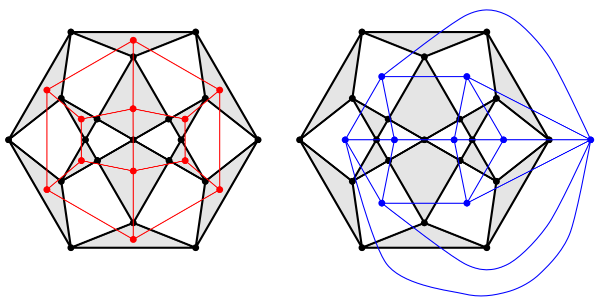

Figure 3: The chess coloring and the related graphs

Consider a plane graph Γ. The *medial graph* of Γ is the graph $\mathcal{M}(\Gamma)$ whose vertex set is the edge set of Γ and two vertices of $\mathcal{M}(\Gamma)$ are joined by an edge if they have a common vertex and belong to the same face in Γ. The graph $\mathcal{M}(\Gamma)$ is also plane. This graph is 4-regular and its face set is the union of the vertex set and the face set of Γ. Thus, $\mathcal{M}(\Gamma)$ is chess colored. Let b be the color used to coloring the faces of $\mathcal{M}(\Gamma)$ corresponding to the vertices of Γ. The remaining faces of $\mathcal{M}(\Gamma)$ (corresponding to the faces of Γ) are colored in w. Then

$$\mathcal{R}_b(\mathcal{M}(\Gamma)) = \Gamma \qquad \text{and} \qquad \mathcal{R}_w(\mathcal{M}(\Gamma)) = \Gamma^*.$$

For example, the graph marked in black in Fig. 3 is the medial graph of the graphs marked in red and blue.

A *central circuit* is a circuit in the medial graph which is obtained by starting with an edge and continuing at each vertex by the edge opposite to the entering one [4, p.5]. We will consider central circuits as cyclic sequences of vertices and distinguish each central circuit from the reversed. If Γ and Γ^* both are simple, then there is a one-to-one correspondence between zigzags in Γ and central circuits in $\mathcal{M}(\Gamma)$: a sequence formed by edges of Γ is a zigzag if and only if this sequence is a central circuit in $\mathcal{M}(\Gamma)$. In Fig. 4. the part of the zigzag is marked by the bold red line and the corresponding part of the central circuit is marked by the bold black line.

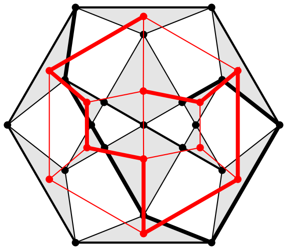

Figure 4: A zigzag and the corresponding central circuit

4.2 Main construction

Let σ be a permutation on $[k]_\pm$ satisfying (M1) and (M2). We construct a 4-regular plane graph G which is the medial graph of a plane graph, where σ occurs as the z-monodromy of a face F (this plane graph contains a k-gonal face F such that σ is M_F).

Consider a circle C embedded in the plane. We take mutually distinct points $p_1, \dots, p_k$ from C such that these points occur along C in the clockwise order; these points will be the edges of the mentioned above face F. Next, denote by C' a circle inside the part of the plane bounded by C and take mutually distinct points $a_{12}, a_{23}, \dots, a_{(k-1)k}, a_{k1}$ occurring on C' in the clockwise order. Similarly, let C'' be a circle inside the part of the plane bounded by C' and let $r_1, l_k, r_2, l_1, \dots, r_k, l_{k-1}$ be mutually distinct points that occur along C'' in the clockwise order. For every a_{ij} we take two segments that intersect precisely in a_{ij} and join p_i with l_i and p_j with r_j, respectively. Note that all such segments intersect each of C, C', C'' in precisely one point and the interiors of any two of these segments are disjoint if they contain distinct points a_{ij}. Denote by S_i the union of the segment joining r_i with p_i, the arc of C between p_i and p_{i+1} and the segment joining p_{i+1} with l_{i+1} if $i < k$; for $i = k$ we replace every index $i + 1$ by 1. See Fig. 5 for the case $k = 6$.

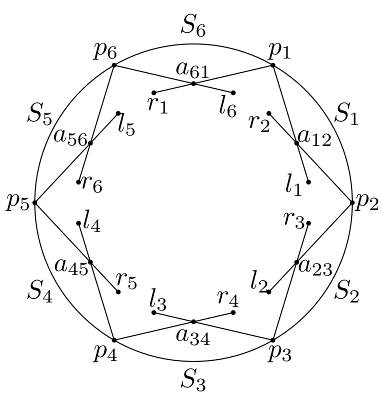

Figure 5: The beginning of construction for $k = 6$

We will work with the relation $\sim$ on the set

$$\mathcal{O} = \bigcup_{i=1}^{k} \{l_i, r_i\}$$

such that for any $i, j \in [k]_\pm$ satisfying $\sigma(i) = j$ one of the following possibilities is realized:

(1) $l_i \sim r_j$ if $i, j \in [k]_+$,

(2) $r_{-i} \sim l_{-j}$ if $i, j \in [k]_-$,

(3) $l_i \sim l_{-j}$ if $i \in [k]_+$ and $j \in [k]_-$,

(4) $r_{-i} \sim r_j$ if $i \in [k]_-$ and $j \in [k]_+$.

The relation $\sim$ is irreflexive and symmetric. Indeed, if $l_i \sim l_i$ (the case (3)) or $r_i \sim r_i$ (the case (4)), then we get $\sigma(i) = -i$ which contradicts (M2). Thus, $\sim$ is irreflexive. Now, we show that if $l_i \sim l_j$, then $l_j \sim l_i$ (the remaining three cases are similar). If $l_i \sim l_j$ with $i, j \in [k]_+$ (the case (3)), then $\sigma(i) = -j$ and, by (M1), $\sigma(j) = -i$ and $j \in [k]_+, -i \in [k]_-$; i.e. $l_j \sim l_i$. Note that for each $x \in \mathcal{O}$ there is a unique $x' \in \mathcal{O}$ such that $x \sim x'$.

If a pair of points from $\mathcal{O}$ is in the relation $\sim$, then we join them by a curve homeomorphic to the segment $[0, 1]$ inside the part of the plane bounded by C''. The following conditions must be satisfied:

• the curves have no more than finitely many intersections and self-intersections,

• for every such intersection point either there are precisely two distinct curves passing once through this point or there is a single curve passing twice through it,

• all intersections are transversal.

Let $L_1, \dots, L_k$ be the curves described above (we take an arbitrary numeration that does not depend on the endpoints from $\mathcal{O}$).

Note that each of $l_1, r_1, \dots, l_k, r_k$ is a common point of a unique S_i and a unique L_j. Thus, we obtain a family $\mathcal{C}$ of closed curves

$$S_{i_1} \cup L_{i_1} \cup S_{i_2} \cup L_{i_2} \cup \dots$$

such that every S_i and L_j is contained in precisely one of these curves. Let V be the set of all intersection and self-intersection points of curves from $\mathcal{C}$. In particular, all p_i and all a_{ij} belong to V.

Example 4.1. Let $k = 6$ and

$$\sigma = (1, -6, -4, 2)(3, -5)(5, -3)(-2, 4, 6, -1).$$

The relation $\sim$ on the set $\mathcal{O} = \{l_1 \dots, l_6, r_1, \dots, r_6\}$ is as follows

$$l_1 \sim l_6, \;\; r_6 \sim l_4, \;\; r_4 \sim r_2, \;\; l_2 \sim r_1, \;\; l_3 \sim l_5, \;\; r_5 \sim r_3.$$

One of suitable connections between points from $\mathcal{O}$ is presented in Fig. 6.

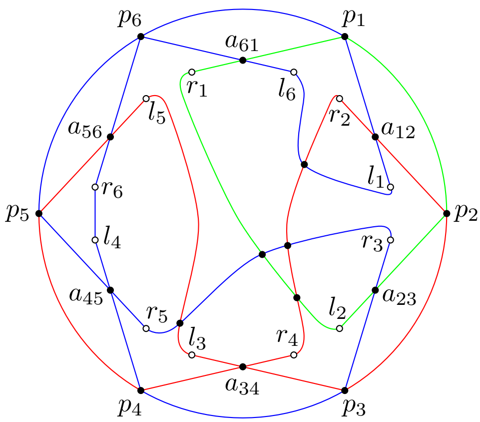

Figure 6: A suitable connection between points of $\mathcal{O}$

In this case, $\mathcal{C}$ consists of precisely 3 closed curves with 17 intersection points, i.e. $|V| = 17$.

Let $G = G(\mathcal{C})$ be the graph whose vertex set is V and two vertices are joined by an edge if they are two consecutive points on one of curves from $\mathcal{C}$. In fact, we consider G as a graph whose vertices are points on the plane and edges are parts of curves from $\mathcal{C}$ joining these points. It is easy to see that G is a 4-regular and the curves from $\mathcal{C}$ correspond to pairs of mutually reversed central circuits from G. We make the chess coloring of G and split the set of its faces into the two sets corresponding to the colors. Let b be the color of faces whose boundaries are cycles with vertices p_i, p_j, a_{ij}; as above, w is the other color.

As in Subsection 4.1, we obtain the dual graphs $\mathcal{R}_b(G)$ and $\mathcal{R}_w(G)$. These graphs are not necessarily simple; they may contain the following fragments:

(A) loops,

(B) multiple edges,

(C) edges that belong to the boundary of one face only (in particular, edges with vertices of degree 1),

(D) pairs of faces whose intersection of boundaries contains more than one edge.

If one of the cases (A) or (B) occurs in one of the graphs $\mathcal{R}_b(G), \mathcal{R}_w(G)$, then the case (C) or (D), respectively, occurs in the dual graph.

Example 4.2. Let $\mathcal{C}$ be as in Example 4.1. The graphs $\mathcal{R}_b(G)$ and $\mathcal{R}_w(G)$ are presented in Fig. 7a and Fig. 7b, respectively.

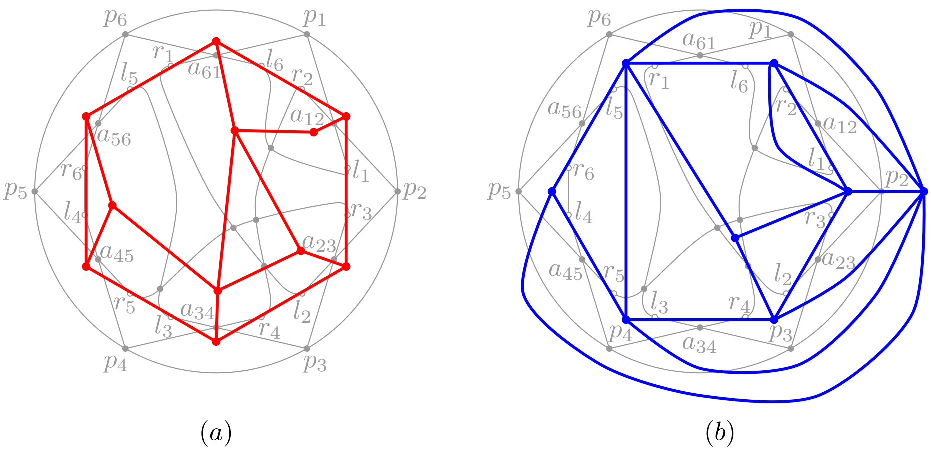

Figure 7: The dual graphs $\mathcal{R}_b(G)$ and $\mathcal{R}_w(G)$

The graph $\mathcal{R}_b(G)$ contains a pair of faces with two common edges (the case (D)) which corresponds to a double edge in $\mathcal{R}_w(G)$ (the case (B)).

Now, we show how modify the graph G such that the connections between the points from $\mathcal{O}$ induced by the relation $\sim$ do not change and the graphs $\mathcal{R}_b(G), \mathcal{R}_w(G)$ become simple.

Suppose that e is an edge joining the vertices v' and v'' in $\mathcal{R}_b(G)$ or $\mathcal{R}_w(G)$ (both the cases are similar). We consider separately the cases $v' \neq v''$ and $v' = v''$ (see Fig. 8a and 8b, respectively). If $v' \neq v''$, then we consider the following edges in the same graph ($\mathcal{R}_b(G)$ or $\mathcal{R}_w(G)$):

• e'_+ and e'_- which occur directly after e in the clockwise and the anticlockwise order on edges incident to v', respectively;

• e''_+ and e''_- which occur directly after e in the clockwise and the anticlockwise order on edges incident to v'', respectively.

If $v' = v''$, then we exclude the case when the loop e is the boundary of a face (this case will be considered separately). The edge e splits the plane into two parts and we consider the following edges:

• e'_+ and e'_- are the edges contained in one of these parts which occur directly after e in the clockwise and the anticlockwise order on edges incident to v', respectively;

• e''_+ and e''_- are the edges contained in the other part of the plane which occur directly after e in the clockwise and the anticlockwise order on edges incident to v'', respectively.

There are precisely two parts of central circuits in G (up to reversing) that pass through e (since e, e'_δ, e''_δ are vertices of G, where $\delta \in \{+,-\}$):

$$\ldots, e'_+, e, e''_+, \ldots \qquad \text{and} \qquad \ldots, e'_-, e, e''_-, \ldots$$

which are marked in blue and red in Fig. 8.

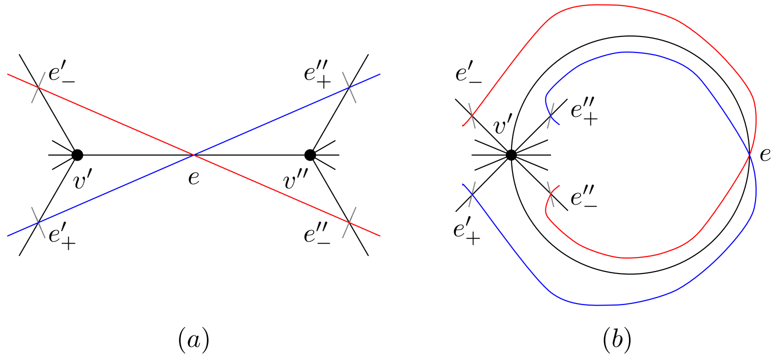

Figure 8: Parts of central circuits

For each of these cases we replace e by the graphs presented in Fig. 9a and Fig. 9b, respectively.

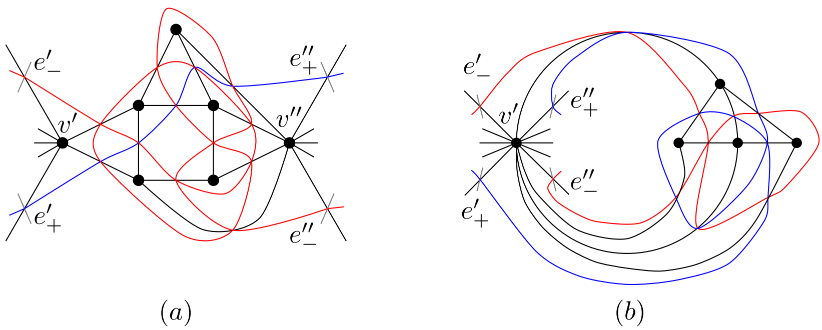

Figure 9: Two types of expansion

This operation will be called the *expansion* of e. It replaces the edge e by an intersecting trail E_δ, $\delta \in \{+,-\}$, joining e'_δ and e''_δ. So, the mentioned above parts of central circuits will be replaced by

$$\ldots, e'_+, E_+, e''_+, \ldots \qquad \text{and} \qquad \ldots, e'_-, E_-, e''_-, \ldots,$$

respectively (they are marked in blue and red in Fig. 9). Thus, central circuits do not change in a significant way.

Remark 4.3. We can obtain the same result using other pairs of graphs instead of the graphs from Fig. 9. This pair is the first which we found.

Now, we explain how transform $\mathcal{R}_b(G), \mathcal{R}_w(G)$ to simple graphs if at least one of the possibilities (A)–(D) occurs. Without loss of generality we can consider $\mathcal{R}_b(G)$. Furthermore, we restrict ourselves to the cases (A) and (B) (since (C) and (D) correspond to (A) and (B), respectively, in the dual graph). The case (A) will be decomposed in two subcases.

(A1). Suppose that $\mathcal{R}_b(G)$ contains a face whose boundary is a loop. The corresponding parts of mutually reversed central circuits from G are also loops. The loops can be removed from these graphs without changing the central circuits in a significant way (see Fig. 10).

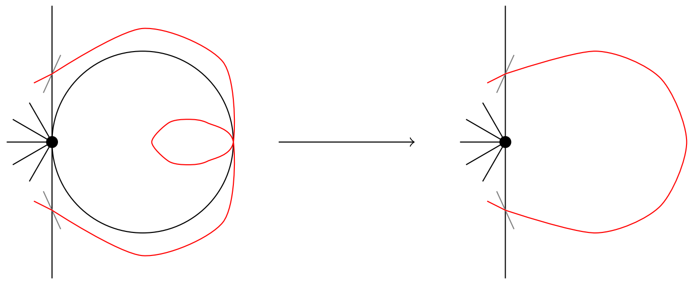

Figure 10: Removing a loop

(A2). If e is a loop in $\mathcal{R}_b(G)$ which is not a boundary of a face, then we use the expansion to e.

(B). If two distinct vertices are connected by $m \geq 2$ edges, then we expand any $m-1$ of them.

Example 4.4. Since $\mathcal{R}_w(G)$ from Example 4.2 contains two edges connecting the same pair of vertices (the case (C)), we expand one of these edges, see Fig. 11.

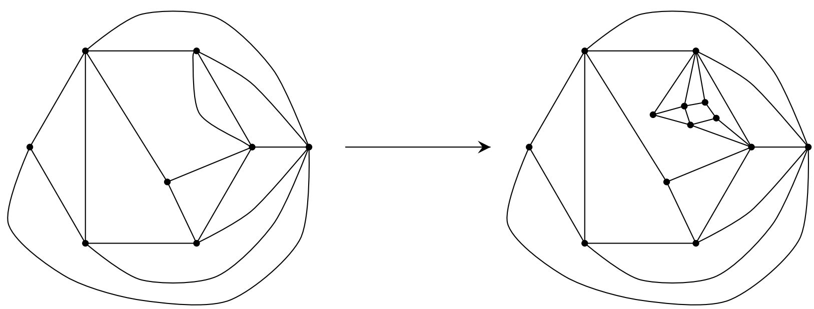

Figure 11: The expansion of an edge in $\mathcal{R}_w(G)$

This simultaneously modify $\mathcal{R}_b(G)$ and we obtain a graph without the possibility (A), see Fig. 12.

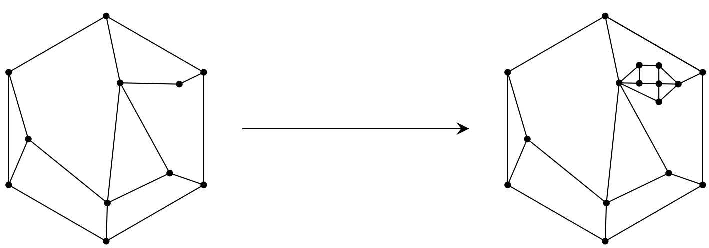

Figure 12: The corresponding modification of $\mathcal{R}_b(G)$

So, we can simultaneously transform $\mathcal{R}_b(G)$ and $\mathcal{R}_w(G)$ to simple graphs such that the relation $\sim$ on elements of $\mathcal{O}$ is not changed. In particular, we come to a new (4-regular plane) graph G and assert that $\mathcal{R}_b(G)$ contains a face for which σ occurs as the z-monodromy of one of faces.

Recall that C is a cycle in G with the vertices $p_1, \dots, p_k$ and it is the boundary of the outer face of G. This face has a common edge only with faces whose boundaries contain the vertices p_i, p_j, a_{ij}. By the definition of $\mathcal{R}_b(G)$, we have the following:

- every face with the boundary containing p_i, p_j, a_{ij} in G is a vertex in $\mathcal{R}_b(G)$ which we denote by v_{ij};
- the face bounded by C in G is a face in $\mathcal{R}_b(G)$ which will be denoted by F;
- every p_i corresponds to an edge of F.

Consider the oriented edges $e_j = v_{ij}v_{jl}$ and $-e_j = v_{jl}v_{ij}$ in $\mathcal{R}_b(G)$, where i, j, l are three consecutive elements in the cyclic sequence $1, \dots, k$. The pair of mutually reversed oriented edges $e_j, -e_j$ corresponds to the vertex p_j in G. Thus,

$$\Omega(F) = \{e_1, \dots, e_k, -e_k, \dots, -e_1\}.$$

Let $e_0, e \in \Omega(F)$ be such that $D_F(e_0) = e$. There is a unique zigzag Z in $\mathcal{R}_b(G)$ containing the pair e_0, e. The element e' which occurs in Z directly after this pair does not belong to $\Omega(F)$. The edges e_0, e, e' are three consecutive vertices in the central circuit in G corresponding to Z such that e_0, e are two consecutive vertices from the cycle C and e' is one of elements a_{ij}. Let x be the first element from $\mathcal{O}$ such that the central circuit containing e_0, e, e' passes through x (as a curve on the plane) directly after this triple (x is a point on the plane, but not a vertex of the graph). There is a unique $x' \in \mathcal{O}$ such that $x \sim x'$ and the central circuit passes through x'. Since there is no elements of $\Omega(F)$ between x and x' in the central circuit, the first element of $\Omega(F)$ that occurs after x' corresponds to $M_F(e)$. Therefore, σ occurs as M_F.

Example 4.5. Let F be the outer face of $\mathcal{R}_b(G)$ from Example 4.4 and let e_i be the oriented edge of F corresponding to p_i whose direction is defined by the clockwise orientation on the boundary of F (see Fig. 13).

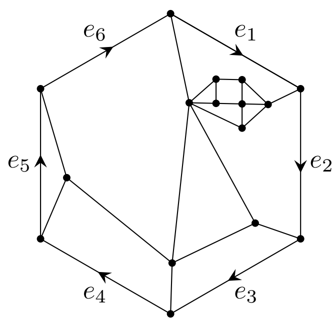

Figure 13: The new graph $\mathcal{R}_b(G)$

A direct verification shows that

$$M_F = (e_1, -e_6, -e_4, e_2)(e_3, -e_5)(e_5, -e_3)(-e_2, e_4, e_6, -e_1),$$

i.e. the permutation

$$\sigma = (1, -6, -4, 2)(3, -5)(5, -3)(-2, 4, 6, -1)$$

from Example 4.1 occurs as M_F in $\mathcal{R}_b(G)$.

5 The non-plane case

In this section, we consider an arbitrary connected closed 2-dimensional (not necessarily orientable) surface S different from a sphere. We show that any permutation σ on $[k]_\pm$ satisfying (M1) and (M2) occurs as the z-monodromy of k-gonal face in a graph embedded in S. Let Γ be a graph embedded in a sphere (a plane graph) such that σ occurs as the z-monodromy of a face F of Γ. We assume that $\Gamma = \mathcal{R}_b(G)$, where G is the 4-regular graph from Section 4.

Let e be an edge in G. It is contained in the boundaries of precisely two faces F_1, F_2 in G. We assume that F_1 and F_2 correspond to a face distinct from F and a vertex of Γ, respectively. Let us take three circles B_1, B_2, B_3 that intersect like the Borromean rings. Consider the graph G' obtained from G by adding B_1, B_2, B_3 as in Fig. 14.

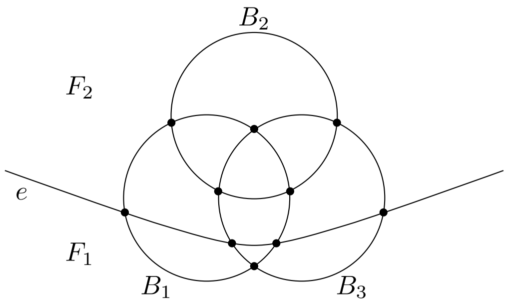

Figure 14: Constructing of G'

It must be pointed out that the circles B_1, B_2, B_3 do not intersect the remaining edges of G. The graph G' is 4-regular and $\mathcal{R}_b(G')$ is obtained from $\Gamma = \mathcal{R}_b(G)$ by adding the graph $\tilde{G}$ marked in red in Fig. 15 to the vertex v corresponding to the face F_2.

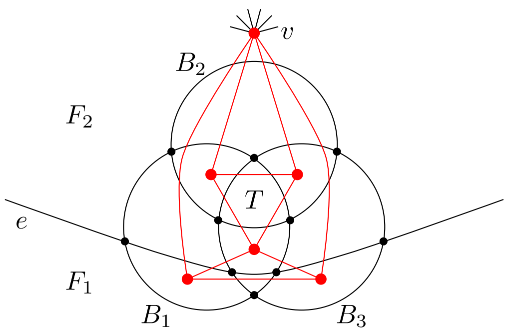

Figure 15: The graph $\tilde{G}$

It is clear that $\mathcal{R}_b(G')$ and $\mathcal{R}_w(G')$ are simple. Denote by T the face of $\tilde{G}$ which is contained in F_2 and does not contain v. Note that B_1, B_2, B_3 induce central circuits of G'. Each zigzag of $\mathcal{R}_b(G')$ passing through T corresponds to one of B_i. Observe that F is the face of $\mathcal{R}_b(G')$ and the zigzags corresponding to B_1, B_2, B_3 do not contain edges of this face. This means that the z-monodromy of F in $\mathcal{R}_b(G')$ is also σ.

Consider any graph Γ' embedded in S that contains a triangle face T'. We take the connected sum of the sphere containing $\mathcal{R}_b(G')$ and S by removing the interiors of faces

T and T' and identifying theirs boundaries by a homeomorphism that sends vertices to vertices. We come to a new graph embedded in S containing F as a face. Since every zigzag of $\mathcal{R}_b(G')$ containing an edge of F does not pass through any edge of T, the z-monodromy of F in the new graph is the same as in $\mathcal{R}_b(G')$ and, consequently, as in $\mathcal{R}_b(G)$.

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Unifying adjacency, Laplacian, and signless Laplacian theories*

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Abstract

Let G be a simple graph with associated diagonal matrix of vertex degrees $D(G)$, adjacency matrix $A(G)$, Laplacian matrix $L(G)$ and signless Laplacian matrix $Q(G)$. Recently, Nikiforov proposed the family of matrices $A_\alpha(G)$ defined for any real $\alpha \in [0,1]$ as $A_\alpha(G) := \alpha\, D(G) + (1-\alpha)\, A(G)$, and also mentioned that the matrices $A_\alpha(G)$ can underpin a unified theory of $A(G)$ and $Q(G)$. Inspired from the above definition, we introduce the B_α-matrix of G, $B_\alpha(G) := \alpha A(G) + (1-\alpha)L(G)$ for $\alpha \in [0,1]$. Note that $L(G) = B_0(G), D(G) = 2B_{\frac{1}{2}}(G), Q(G) = 3B_{\frac{2}{3}}(G), A(G) = B_1(G)$. In this article, we study several spectral properties of B_α-matrices to unify the theories of adjacency, Laplacian, and signless Laplacian matrices of graphs. In particular, we prove that each eigenvalue of $B_\alpha(G)$ is continuous on α. Using this, we characterize positive semidefinite B_α-matrices in terms of α. As a consequence, we provide an upper bound of the independence number of G. Besides, we establish some bounds for the largest and the smallest eigenvalues of $B_\alpha(G)$. As a result, we obtain a bound for the chromatic number

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of G and deduce several known results. In addition, we present a Sachs-type result for the characteristic polynomial of a B_α-matrix.

Keywords: Adjacency matrix, Laplacian matrix, signless Laplacian matrix, convex combination, B_α-matrix, A_α-matrix, chromatic number, independence number.

Math. Subj. Class. (2020): Primary: 05C50, 05C22; Secondary: 05C35.

1 Introduction

Throughout this article, we consider G to be a simple undirected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The adjacency matrix of G is a symmetric $n \times n$ matrix $A(G)$ whose (i, j)-th entry is 1 if v_i and v_j are adjacent, 0 otherwise. The degree matrix of G is a diagonal matrix $D(G)$ whose i^{th} diagonal entry is the degree of the vertex v_i. The Laplacian and the signless Laplacian matrix of G are the matrices, $L(G) := D(G) - A(G)$ and $Q(G) := D(G) + A(G)$, respectively. If graph G is clear from the context, we simply write A, L, and D instead of $A(G)$, $L(G)$, and $D(G)$, respectively. Adjacency, Laplacian, and signless Laplacian matrices are some of the matrices associated with a graph which are widely studied in the literature [8, 14, 28, 18, 13, 27, 7, 9, 10]. It can be seen that many of the spectral properties of such matrices are quite different from each other. We will thus analyze the spectral properties of the convex combinations of $A(G)$ and $L(G)$ in order to understand how uniformly the spectral behavior transforms from one matrix to another.

Definition 1.1. For $\alpha \in [0, 1]$ the B_α-matrix of G is the convex linear combination $B_\alpha(G) := \alpha A(G) + (1 - \alpha)L(G)$ (or simply $B_\alpha = \alpha A + (1 - \alpha)L$, if G is clear from the context).

Remark 1.2. Note that $L(G) = B_0(G)$, $D(G) = 2B_{\frac{1}{2}}(G)$, $Q(G) = 3B_{\frac{2}{3}}(G)$, $A(G) = B_1(G)$.

It is clear that the spectral properties of $B_{1/2}(G)$ and $B_{2/3}(G)$ are equivalent to the spectral properties of $D(G)$ and $Q(G)$, respectively. In fact, $A(G)$, $L(G)$, $Q(G)$, and $D(G)$ can be considered as the B_α-matrix of G up to proportionality. Therefore, on the one hand, the spectral properties of $B_\alpha(G)$ may reveal the common connection among the spectral properties of all such well-known matrices. On the other hand, $B_\alpha(G)$ may analyze the structural and combinatorial properties of the graph G in a better way.

Recently, Nikiforov [23] introduced a family of matrices, known as A_α-matrix, which is a convex combination of $A(G)$ and $D(G)$. The theory of A_α-matrices merges the theories of the adjacency matrix and signless Laplacian matrix of graphs. Later on, much work has been done on these matrices. We have results on the spectral radius ([1, 5, 15, 20]), the second largest eigenvalue [4], the k-th largest eigenvalue [20], the least eigenvalue ([21, 11]), the multiplicity of the eigenvalues ([3, 25]), positive semidefiniteness [24], the characteristic polynomial [22], spectral determination of graphs [19], etc. Motivated by Nikiforov's work, we consider B_α-matrices and study their spectral properties. However, unlike A_α-matrices, B_α-matrices are not always non-negative, but they obey Perron-Frobenius type

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results. In this article, we develop the theory of B_α-matrices to unify the theory of adjacency matrix, Laplacian matrix, and signless Laplacian matrix.

The paper is organized as follows. In Section 2, we list some previously known results. Section 3 discusses the positive semidefiniteness of B_α-matrices. As a consequence, we obtain an upper bound for the independence number. Then we present some bounds of eigenvalues of $B_\alpha(G)$ in terms of maximum degree and minimum degree, chromatic number, etc., in Section 4. Besides, we obtain a lower bound for chromatic number and derive several known results as consequences. Finally, we study the determinant and a Sachs-type result for the characteristic polynomial of $B_\alpha(G)$ in Section 5.

2 Preliminaries

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. If two vertices v_i and v_j are adjacent, we write $v_i \sim v_j$, and v_iv_j denotes the edge between them. The degree of a vertex v_i is the number of edges adjacent to v_i and is denoted by $d_G(v_i)$ or simply $d(v_i)$ or d_i. The minimum degree and the maximum degree of graph G are denoted by $\delta(G)$ (or simply δ) and $\Delta(G)$ (or simply Δ), respectively. The complement of a graph G is the graph $\overline{G}$ with vertex set $V(G)$ and two vertices in $\overline{G}$ are adjacent if and only if they are non-adjacent in G. The $0-1$ incidence matrix of a graph G with n vertices $\{v_1, v_2, \ldots, v_n\}$ and m edges $\{e_1, e_2, \ldots, e_m\}$ is an $n \times m$ matrix M whose (i, j)-th entry is 1 if the vertex v_i is incident on the edge e_j and 0 otherwise.

The line graph of a graph G is the graph G_ℓ with vertex set $E(G)$ and two vertices e_i and e_j in G_ℓ are adjacent if the edges e_i and e_j have a common vertex in the graph G. The identity matrix of order n is denoted by I_n (or simply I). An $a \times b$ matrix whose entries are all ones is denoted by $J_{a,b}$ (or simply J when the order is clearly understood). The transpose of a matrix M is denoted by M^t.

Lemma 2.1 ([2, Lemma 6.16])**.** *Let G be a graph with line graph G_ℓ. If M is the $0-1$ incidence matrix of G, then $M^tM = A(G_\ell) + 2I$. Moreover, if G is k-regular, then $MM^t = A(G) + kI$.*

Since the eigenvalues of any $n \times n$ symmetric matrix S are real, we denote and ordered the eigenvalues of S as follows:

$$\lambda_{max}(S) = \lambda_1(S) \geq \lambda_2(S) \geq \cdots \geq \lambda_n(S) = \lambda_{min}(S). \tag{2.1}$$

For a graph G, sometimes we denote and arrange the eigenvalues of $A(G)$, $L(G)$ and $Q(G)$ as $\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)$, $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ and $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G)$, respectively. Next, we present the well known Weyl Theorem.

Theorem 2.2 ([17, Theorem 4.3.1])**.** *If S_1 and S_2 are two Hermitian matrices of order n and their eigenvalues are ordered as in* (2.1)*. Then*

$$\lambda_{n+1-i}(S_1 + S_2) \leq \lambda_{n+1-i-j}(S_1) + \lambda_{j+1}(S_2), \quad i = 1, 2, \ldots, n; \;\; j = 0, 1, \ldots, n-i.$$

Corollary 2.3. *If S_1 and S_2 are two Hermitian matrices of order n and their eigenvalues are ordered as in* (2.1)*. Then*

$$\lambda_n(S_1) + \lambda_1(S_2) \leq \lambda_1(S_1 + S_2) \leq \lambda_1(S_1) + \lambda_1(S_2).$$

Let us recall the following upper bound of the largest eigenvalue of a Laplacian matrix.

Theorem 2.4 ([6]). *Let G be a graph with the largest Laplacian eigenvalue $\mu_1(G)$. Then*

$$\mu_1(G) \leq \max_{v_i v_j \in E(G)} (d_i + d_j).$$

Let $S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$ be a 2×2 block matrix, where S_{11} and S_{22} are square matrices. If S_{11} is nonsingular, then the Schur complement of S_{11} in S is defined to be the following matrix

$$S_{22} - S_{21} S_{11}^{-1} S_{12}. \tag{2.2}$$

Similarly, if S_{22} is nonsingular, then the Schur complement of S_{22} in S is $S_{11} - S_{12} S_{22}^{-1} S_{21}$. Let us recall the Schur complement formula for the determinant.

Theorem 2.5 ([2]). *Let $S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$ be a 2×2 block matrix, where S_{11} and S_{22} are square matrices and S_{11} is nonsingular. Then*

$$\det S = (\det S_{11}) \det(S_{22} - S_{21} S_{11}^{-1} S_{12}).$$

A matrix is irreducible if it is not similar via a permutation to a block upper triangular matrix (that has more than one block of positive size). Note that the adjacency matrix of a connected graph is always irreducible. Let $S = (s_{ij})_{n \times m}$ be a matrix, then we denote $|S| := (|s_{ij}|)_{n \times m}$.

Theorem 2.6 ([17, Theorem 6.2.24]). *A square matrix S of order n is irreducible if and only if $(I + |S|)^{n-1} > 0$, entry-wise.*

Theorem 2.7 ([17, Corollary 6.2.27]). *Let S be an irreducibly diagonally dominant matrix of order n. If S is Hermitian and every main diagonal entry is positive, then S is positive definite.*

3 Positive semidefiniteness of $B_\alpha(G)$

Let G be a graph with B_α-matrix $B_\alpha(G) := \alpha A(G) + (1 - \alpha) L(G)$. In this section we determine the values of α for which the matrix $B_\alpha(G)$ is positive semidefinite. As a consequence, we give an upper bound of the independence number. Results obtained in this section will be useful in the later sections.

For simplicity, we use the notation B_α, A, L, and D instead of $B_\alpha(G)$, $A(G)$, $L(G)$, and $D(G)$, respectively, when G is clear from the context. Some equivalent forms of B_α in terms of A, L, and D are as follows:

$$\begin{aligned} B_\alpha &= \alpha A + (1 - \alpha) L \\ &= (2\alpha - 1) A + (1 - \alpha) D \\ &= (1 - 2\alpha) L + \alpha D. \end{aligned}$$

Given two real matrices $S = (s_{ij})_{m \times n}$ and $M = (m_{ij})_{m \times n}$, we use the notation $S \geq M$ if and only if $s_{ij} \geq m_{ij}$ for all i, j. For any connected graph G with n vertices and

$\alpha\,(\neq \frac{1}{2}) \in [0,1]$, we have

$$\begin{aligned}(I+|B_\alpha|)^{n-1} &= (I+|(2\alpha-1)A+(1-\alpha)D|)^{n-1}\\ &= (I+|2\alpha-1|A+(1-\alpha)D)^{n-1}\\ &\geq I+|2\alpha-1|A+\cdots+|2\alpha-1|^{n-1}A^{n-1}.\end{aligned} \tag{3.1}$$

Since G is connected, any two vertices v_i and v_j are joined by a path with length $k \leq n-1$. Therefore (i,j)-th entry of A^k, which counts the number of walks of length k connecting v_i and v_j, is positive. Hence, from (3.1), $(I+|B_\alpha|)^{n-1} \geq I+|2\alpha-1|A+\cdots+|2\alpha-1|^{n-1}A^{n-1} > 0$. Thus, by Theorem 2.6, B_α is irreducible for $\alpha\,(\neq \frac{1}{2}) \in [0,1]$.

We begin the section with the following basic property of $B_\alpha(G)$.

Proposition 3.1. *For any $\alpha \in [0,1]$, eigenvalues of $B_\alpha(G)$ are real numbers.*

Proof. Since $A(G)$ and $L(G)$ are symmetric matrices, so $B_\alpha(G) = \alpha A(G)+(1-\alpha)L(G)$ is also a symmetric matrix. Hence, all the eigenvalues of B_α are real numbers for any $\alpha \in [0,1]$. □

For a graph G, let $\lambda_1(B_\alpha) \geq \cdots \geq \lambda_n(B_\alpha)$ be the eigenvalues of $B_\alpha(G)$. In the following theorem, we prove that $\lambda_k(B_\alpha)$ is uniformly continuous for $\alpha \in [0,1]$.

Theorem 3.2. *Let B_α be the B_α-matrix of a graph G with n vertices. Then, for $k \in \{1,2,\ldots,n\}$, the mapping $f_G : [0,1] \to \mathbb{R}$ defined as $f_G(\alpha) = \lambda_k(B_\alpha)$ is a uniformly continuous function.*

Proof. Let L and D be the Laplacian and the degree matrix of G, respectively. Then, for any $\alpha,\beta \in [0,1]$, we have $B_\alpha - B_\beta = 2(\beta-\alpha)L + (\alpha-\beta)D$. Then, for any $i \in \{1,2,\ldots,n\}$ and $j \in \{0,1,\ldots,n-i\}$, using Theorem 2.2, we obtain

$$\begin{aligned}\lambda_{n+1-i}(B_\alpha) &= \lambda_{n+1-i}(B_\alpha + B_\beta - B_\beta)\\ &\leq \lambda_{n+1-i-j}(B_\alpha + B_\beta) + \lambda_{j+1}(-B_\beta)\\ &= \lambda_{n+1-i-j}(B_\alpha + B_\beta) - \lambda_{n-j}(B_\beta).\end{aligned}$$

Thus, for any $i \in \{1,2,\ldots,n\}$ and $j \in \{0,1,\ldots,n-i\}$,

$$\lambda_{n+1-i}(B_\alpha) + \lambda_{n-j}(B_\beta) \leq \lambda_{n+1-i-j}(B_\alpha + B_\beta) \quad \text{for all } \alpha,\beta \in [0,1]. \tag{3.2}$$

Assume that $\alpha \leq \beta$. By using (3.2) and Corollary 2.3, we compute

$$\begin{aligned}\lambda_k(B_\alpha) - \lambda_k(B_\beta) &= \lambda_{n+1-k}(-B_\beta) + \lambda_{n-(n-k)}(B_\alpha)\\ &\leq \lambda_{n+1-k-(n-k)}(-B_\beta + B_\alpha)\\ &= \lambda_1(B_\alpha - B_\beta)\\ &\leq \lambda_1(2(\beta-\alpha)L) + \lambda_1((\alpha-\beta)D)\\ &= 2(\beta-\alpha)\lambda_1(L) + (\alpha-\beta)\lambda_n(D)\\ &\leq |\alpha-\beta|(2\lambda_1(L) + \lambda_1(D)).\end{aligned}$$

Also, by using (3.2) and Corollary 2.3, we obtain

$$\begin{aligned}\lambda_k(B_\beta) - \lambda_k(B_\alpha) &\leq \lambda_1(B_\beta - B_\alpha)\\ &\leq \lambda_1(2(\alpha-\beta)L) + \lambda_1((\beta-\alpha)D)\\ &= 2(\alpha-\beta)\lambda_n(L) + (\beta-\alpha)\lambda_1(D)\\ &\leq |\alpha-\beta|(2\lambda_1(L) + \lambda_1(D)).\end{aligned}$$

Thus, $|\lambda_k(B_\beta) - \lambda_k(B_\alpha)| \leq |\alpha-\beta|(2\lambda_1(L)+\lambda_1(D))$. Hence, the mapping f_G is uniformly continuous. □

Note that for a graph G (with at least an edge) on n vertices, $\lambda_n(B_{\frac{1}{2}}) = \frac{1}{2}\lambda_n(D) \geq 0$ and $\lambda_n(B_1) = \lambda_n(A) \leq 0$. By Theorem 3.2, $\lambda_n(B_\alpha)$ is continuous, so there exists a $\beta \in (0,1)$ such that $\lambda_n(B_\beta) = 0$. Therefore, for a graph G (with at least an edge) on n vertices, we define $\beta_o(G) := \max\{\beta \in (0,1) : \lambda_n(B_\beta) = 0\}$. It is simply denoted by β_o if the graph G is understood from the context.

Theorem 3.3. *If G is a connected graph with $n\,(>1)$ vertices, then B_α is positive definite for $\alpha \in (0, \frac{2}{3})$.*

Proof. First we assume that $0 < \alpha \leq \frac{1}{2}$. Since G is connected and $\lambda_n(B_\alpha) = -\lambda_1(-B_\alpha)$, by Corollary 2.3, we obtain

$$\begin{aligned}\lambda_n(B_\alpha) &= \lambda_n((1-2\alpha)L + \alpha D)\\ &\geq (1-2\alpha)\lambda_n(L) + \alpha\lambda_n(D)\\ &= \alpha\lambda_n(D) > 0.\end{aligned}$$

Thus, B_α is positive definite for $\alpha \in (0, \frac{1}{2}]$.

Next we assume that $\frac{1}{2} < \alpha < \frac{2}{3}$. Then $0 < 2\alpha - 1 < 1-\alpha$. Now $B_\alpha = (2\alpha-1)A + (1-\alpha)D$. Let $(B_\alpha)_{ij}$ be the (i,j)-th entry of B_α. Then, for $i \in \{1,2,\ldots,n\}$, we have

$$|(B_\alpha)_{ii}| = |(1-\alpha)\,d_i| = (1-\alpha)\,d_i > (2\alpha-1)\,d_i = |2\alpha-1|\,d_i = \sum_{j=1,\ j\neq i}^{n} |(B_\alpha)_{ij}|.$$

Thus, B_α is strictly diagonally dominant with positive diagonal entries. Also, B_α is irreducible. Therefore, by Theorem 2.7, B_α is positive definite for $\alpha \in (\frac{1}{2}, \frac{2}{3})$. □

Corollary 3.4. *If G is a graph with no isolated vertices, then B_α is positive definite for $\alpha \in (0, \frac{2}{3})$.*

Next corollary gives a lower bound of $\beta_o(G)$. For simplicity, we use β_o instead of $\beta_o(G)$.

Corollary 3.5. *If G is a graph with no isolated vertices, then $\beta_o \geq \frac{2}{3}$.*

Proof. By Theorem 3.2, $f_G(\alpha) := \lambda_n(B_\alpha)$ is continuous. By Corollary 3.4, $\lambda_n(B_\alpha) > 0$ for $\alpha \in (0, \frac{2}{3})$. Also, $\lambda_n(B_1) < 0$. Therefore, $\beta_o \geq \frac{2}{3}$. □

Theorem 3.6. *Let G be a graph with no isolated vertices. Then B_α is positive semidefinite if and only if $\alpha \in [0, \beta_o]$.*

Proof. Let G be a graph with n vertices $\{v_1, v_2, \ldots, v_n\}$. Set $\beta_o := \beta_o(G)$. Suppose $\alpha \in [0, \beta_o]$. For $\alpha \in (0, \frac{2}{3})$, by Corollary 3.4, B_α is positive definite. Assume that $\frac{2}{3} \leq \alpha \leq \beta_o$. Then $-\alpha \geq -\beta_o$, that is, $\alpha\,(2\beta_o - 1) \geq \beta_o\,(2\alpha - 1)$ which implies $\frac{\alpha}{2\alpha-1} \geq \frac{\beta_o}{2\beta_o-1}$. Note that for any $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t \in \mathbb{R}^n$, we obtain

$$\begin{aligned}\mathbf{x}^t\, B_\alpha\, \mathbf{x} \;&=\; \mathbf{x}^t\, \alpha D\, \mathbf{x} + \mathbf{x}^t\,(1-2\alpha) L\, \mathbf{x} \\ &=\; \alpha \sum_{i=1}^{n} d_i\, x_i^2 + (1-2\alpha) \sum_{v_j v_i \in E(G)} (x_i - x_j)^2. \end{aligned} \tag{3.3}$$

Then, for any $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t \in \mathbb{R}^n$ and using (3.3), we obtain

$$0 \leq \mathbf{x}^t B_{\beta_o} \mathbf{x} = \beta_o \sum_{i=1}^{n} d_i\, x_i^2 + (1-2\beta_o) \sum_{v_j v_i \in E(G)} (x_i - x_j)^2$$

which implies

$$\sum_{v_j v_i \in E(G)} (x_i - x_j)^2 \leq \frac{\beta_o}{2\beta_o - 1} \sum_{i=1}^{n} d_i\, x_i^2 \leq \frac{\alpha}{2\alpha - 1} \sum_{i=1}^{n} d_i\, x_i^2.$$

Thus,

$$\mathbf{x}^t B_\alpha \mathbf{x} = \alpha \sum_{i=1}^{n} d_i\, x_i^2 + (1-2\alpha) \sum_{v_j v_i \in E(G)} (x_i - x_j)^2 \geq 0 \text{ for any } \mathbf{x} \in \mathbb{R}^n.$$

Hence,

$$\lambda_n(B_\alpha) = \min\{\mathbf{x}^t B_\alpha \mathbf{x} : \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\| = 1\} \geq 0.$$

Therefore, B_α is positive semidefinite for all $\alpha \in [0, \beta_o]$.

To prove the converse, it is enough to prove that if $\alpha \in (\beta_o, 1]$, then B_α is not positive semidefinite. Suppose there exists an $\alpha \in (\beta_o, 1]$ such that $\lambda_n(B_\alpha) \geq 0$. By Theorem 3.2, the function $f_G(\alpha) := \lambda_n(B_\alpha)$ is continuous and $\lambda_n(B_1) < 0$, so there exist a $\beta \in [\alpha, 1)$ such that $\lambda_n(B_\beta) = 0$. This contradicts that β_o is the largest number in $(0, 1)$ for which $\lambda_n(B_{\beta_o}) = 0$. Hence, $\lambda_n(B_\alpha) < 0$ for all $\alpha \in (\beta_o, 1]$. □

A symmetric matrix M is called indefinite if there exist two nonzero vectors x and y such that $y^T M y > 0 > x^T M x$, where x^T denotes the transpose of x.

Corollary 3.7. *For a graph G with no isolated vertices, B_α is indefinite if and only if $\alpha \in (\beta_o, 1]$.*

Proof. First we assume that B_α is indefinite. Set $\beta_o := \beta_o(G)$. Then $\lambda_1(B_\alpha) > 0$ and $\lambda_n(B_\alpha) < 0$. Thus, $\alpha \in (\beta_o, 1]$.

Conversely, suppose $\alpha \in (\beta_o, 1]$. Then $\lambda_n(B_\alpha) < 0$. Also, $\alpha > \beta_o > \frac{1}{2}$. Hence, by Corollary 2.3, we have

$$\begin{aligned}\lambda_1(B_\alpha) &= \lambda_1((2\alpha - 1)A + (1-\alpha)D) \\ &\geq \lambda_1((2\alpha - 1)A) + \lambda_n((1-\alpha)D) \\ &= (2\alpha - 1)\lambda_1(A) + (1-\alpha)\lambda_n(D) \\ &> 0.\end{aligned}$$

Hence, B_α is indefinite. □

In the next theorem, we find β_o for regular graphs.

Theorem 3.8. *If G is an r-regular graph with smallest adjacency eigenvalue $\rho_n(G)$. Then*

$$\beta_o(G) = \frac{r - \rho_n(G)}{r - 2\rho_n(G)}.$$

Proof. Set $\beta_o := \beta_o(G)$. Then

$$\begin{aligned} 0 = \lambda_n(B_{\beta_o}) &= \lambda_n\Big((2\beta_o - 1)A + (1 - \beta_o)D\Big) \\ &= \lambda_n\Big((2\beta_o - 1)A + (1 - \beta_o)rI\Big) \\ &= (2\beta_o - 1)\lambda_n(A) + (1 - \beta_o)r. \end{aligned}$$

This gives $\beta_o = \dfrac{r - \lambda_n(A)}{r - 2\lambda_n(A)}$. □

Let us recall the following Hoffman bound of independence number $\alpha(G)$ of an r-regular graph G with n vertices in terms of $\rho_n(G)$.

$$\alpha(G) \leq -\frac{\rho_n(G)}{r - \rho_n(G)}\, n.$$

In light of the above result, we obtain a close relation between the independence number $\alpha(G)$ of a regular graph G and $\beta_o(G)$.

Proposition 3.9. *Let G be an r-regular graph of n vertices with independence number $\alpha(G)$ and $\beta_o := \beta_o(G)$. Then*

$$\alpha(G) \leq n\left(\frac{1 - \beta_o}{\beta_o}\right).$$

4 On eigenvalues

The spectral radius of a matrix is the maximum value among the absolute values of all eigenvalues of that matrix. For any B_α-matrix, we first show a partial Perron-Frobenius type result (that is, $\lambda_1(B_\alpha)$ is the spectral radius of B_α). Then we compute the eigenvalues of $B_\alpha(G)$ for complete graph and complete bipartite graph. Thereafter, we obtain some lower and upper bounds on the largest eigenvalue of $B_\alpha(G)$ of graph G in terms of Δ and δ. As a consequence, we deduce some known results. In addition, we establish an upper bound on the smallest eigenvalue of $B_\alpha(G)$ in terms of the chromatic number. Finally, we derive a bound on the chromatic number in terms of $\beta_o(G)$.

It is to be observed that B_α-matrices are not always non-negative. Therefore, Perron-Frobenius Theorem is not directly applicable. However, we can still conclude that the spectral radius of a B_α-matrix is the same as its largest eigenvalue.

Theorem 4.1. *For any $\alpha \in [0, 1]$, the spectral radius of B_α of a connected graph G is $\lambda_1(B_\alpha)$.*

Proof. For $\alpha \in [0, \frac{1}{2}]$, B_α is positive semidefinite by Theorem 3.3. Hence, $\lambda_1(B_\alpha)$ is the spectral radius of B_α. Let $\alpha \in (\frac{1}{2}, 1]$. Then $2\alpha - 1 > 0$ and hence $B_\alpha = (2\alpha - 1)A + (1 - \alpha)D$ is a non-negative matrix. Also, B_α is irreducible. Therefore, by Perron-Frobenius Theorem, $\lambda_1(B_\alpha)$ is the spectral radius of B_α. □

4.1 The spectrum of B_α-matrix for complete and complete bipartite graphs

In this subsection, we determine the eigenvalues of B_α-matrices of the complete graph and the complete bipartite graph.

Proposition 4.2. *If G is a complete graph with n vertices, then eigenvalues of $B_\alpha(G)$ are $(1-\alpha)n-\alpha$ with multiplicity $n-1$ and $(n-1)\alpha$ with multiplicity 1.*

A complete bipartite graph with vertex partition size a and b is denoted by $K_{a,b}$. Since the eigenvalues of the adjacency matrix of a complete bipartite graph are known, so we compute the eigenvalues of $B_\alpha(K_{a,b})$ for $\alpha \in [0,1)$.

Proposition 4.3. *For $\alpha \in [0,1)$, the eigenvalues of $B_\alpha(K_{a,b})$ are $(1-\alpha)a$ with multiplicity $b-1$, $(1-\alpha)b$ with multiplicity $a-1$, and*

$$\frac{(1-\alpha)(a+b) \pm \sqrt{(1-\alpha)^2(a-b)^2+4(2\alpha-1)^2ab}}{2}.$$

Proof. Let $J_{a,b}$ and $J_{b,a}$ be the square matrices of order $a \times b$ and $b \times a$, respectively, of all ones. Then

$$\begin{aligned} B_\alpha(K_{a,b}) = B_\alpha &= (2\alpha-1)A + (1-\alpha)D \\ &= (2\alpha-1)\begin{pmatrix} 0 & J_{a,b} \\ J_{b,a} & 0 \end{pmatrix} + (1-\alpha)\begin{pmatrix} bI_a & 0 \\ 0 & aI_b \end{pmatrix} \\ &= \begin{pmatrix} (1-\alpha)bI_a & (2\alpha-1)J_{a,b} \\ (2\alpha-1)J_{b,a} & (1-\alpha)aI_b \end{pmatrix}. \end{aligned}$$

For $i \in \{2,3,\dots,a\}$, let the vector $\mathbf{x^{(i)}} = (x_1^i, x_2^i, \dots, x_{a+b}^i)^t$ of order $a+b$ be defined as

$$x_j^i = \begin{cases} 1 & \text{for } j = 1, \\ -1 & \text{for } j = i, \\ 0 & \text{otherwise.} \end{cases}$$

Then $\{\mathbf{x^{(2)}}, \mathbf{x^{(3)}}, \dots, \mathbf{x^{(a)}}\}$ is a linearly independent set of eigenvectors corresponding to the eigenvalue $(1-\alpha)b$. Thus, B_α has eigenvalue $(1-\alpha)b$ with multiplicity $a-1$.

For $i \in \{a+2, a+3, \dots, a+b\}$, let the vector $\mathbf{x^{(i)}} = (x_1^i, x_2^i, \dots, x_{a+b}^i)^t$ of order $a+b$ be defined as

$$x_j^i = \begin{cases} 1 & \text{for } j = a+1, \\ -1 & \text{for } j = i, \\ 0 & \text{otherwise.} \end{cases}$$

Then $\{\mathbf{x^{(a+2)}}, \mathbf{x^{(a+3)}}, \dots, \mathbf{x^{(a+b)}}\}$ is a linearly independent set of eigenvectors corresponding to the eigenvalue $(1-\alpha)a$. Thus, B_α has eigenvalue $(1-\alpha)a$ with multiplicity $b-1$.

Let $\alpha \in [0,1)$. Then, by using Theorem 2.5, we compute

$$\det(B_\alpha) = \begin{vmatrix} (1-\alpha)\, b\, I_a & (2\alpha-1)\, J_{a,b} \\ (2\alpha-1)\, J_{b,a} & (1-\alpha)\, a\, I_b \end{vmatrix}$$

$$= \det\Big((1-\alpha)\, b\, I_a\Big) \det\Big((1-\alpha)a\, I_b - (2\alpha-1)\, J_{b,a}\Big((1-\alpha)\, b\, I_a\Big)^{-1}(2\alpha-1)\, J_{a,b}\Big)$$

$$= (1-\alpha)^a\, b^a \det\Big((1-\alpha)aI_b - (2\alpha-1)^2 J_{b,a}\frac{1}{(1-\alpha)b} I_a J_{a,b}\Big)$$

$$= (1-\alpha)^a\, b^a \det\Big((1-\alpha)aI_b - \frac{a(2\alpha-1)^2}{(1-\alpha)b} J_{b,b}\Big)$$

$$= (1-\alpha)^a\, b^a (1-\alpha)^{b-1}\, a^{b-1}\Big((1-\alpha)\, a - \frac{a\,(2\alpha-1)^2}{(1-\alpha)}\Big).$$

Let x and y be the remaining eigenvalues of $B_\alpha(K_{a,b})$. Then

$$xy\Big((1-\alpha)\, a\Big)^{b-1}\Big((1-\alpha)\, b\Big)^{a-1} =$$

$$= (1-\alpha)^a\, b^a\, (1-\alpha)^{b-1}\, a^{b-1}\Big((1-\alpha)\, a - \frac{a\,(2\alpha-1)^2}{(1-\alpha)}\Big).$$

Thus we obtain

$$\begin{aligned} xy &= b(1-\alpha)\Big((1-\alpha)a - \frac{a(2\alpha-1)^2}{(1-\alpha)}\Big) \\ &= (1-\alpha)^2 ab - (2\alpha-1)^2 ab. \end{aligned} \tag{4.1}$$

Since the sum of the eigenvalues is equal to the trace of the matrix, we obtain

$$x + y + (b-1)(1-\alpha)a + (a-1)(1-\alpha)b = (1-\alpha)ab + (1-\alpha)ab,$$

that is, $x = (1-\alpha)(a+b) - y$. Substitute the value of x in (4.1), we obtain

$$y^2 - (1-\alpha)(a+b)y + (1-\alpha)^2 ab - (2\alpha-1)^2 ab = 0.$$

This gives

$$y = \frac{(1-\alpha)(a+b) \pm \sqrt{(1-\alpha)^2(a-b)^2 + 4(2\alpha-1)^2 ab}}{2}.$$

Hence the eigenvalues of $B_\alpha(K_{a,b})$ are $(1-\alpha)a$ with multiplicity $b-1$, $(1-\alpha)b$ with multiplicity $a-1$ and $\dfrac{(1-\alpha)(a+b) \pm \sqrt{(1-\alpha)^2(a-b)^2 + 4(2\alpha-1)^2 ab}}{2}$. □

4.2 Bounds on the largest eigenvalue

For a connected graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, the distance between two vertices v_i and v_j is denoted by $d(v_i, v_j)$ and is defined to be the length of the shortest path between them. We now establish some lower and upper bounds on the largest eigenvalue of $B_\alpha(G)$ of graph G.

Theorem 4.4. *Let G be a connected graph with the minimum degree δ. Then, for any $\alpha \in [0, 1]$*

$$\lambda_1(B_\alpha) \geq \alpha\delta.$$

Proof. First we assume that $\alpha \in [0, \frac{1}{2}]$, that is, $2\alpha - 1 \leq 0$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t \in \mathbb{R}^n$ be an eigenvector of B_α corresponding to $\lambda_1(B_\alpha)$ such that $x_k = \min\limits_{1\leq i\leq n} x_i < 0$. Then

$$\begin{aligned}\lambda_1(B_\alpha)\, x_k = (2\alpha - 1) \sum_{v_j : v_k v_j \in E(G)} x_j + (1 - \alpha) d_k x_k &\leq (2\alpha - 1)\, d_k x_k + (1 - \alpha) d_k\, x_k \\ &= \alpha d_k x_k.\end{aligned}$$

Therefore, $\lambda_1(B_\alpha) \geq \alpha d_k \geq \alpha\delta$.

Next we assume that $\alpha \in (\frac{1}{2}, 1]$, that is, $2\alpha - 1 > 0$. Then B_α is irreducible and non-negative. Therefore, by Perron-Frobenius Theorem, B_α has a Perron eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t > 0$ corresponding to the eigenvalue $\lambda_1(B_\alpha)$. Let $x_k = \min\limits_{1\leq i\leq n} x_i > 0$. Then we have

$$\begin{aligned}\lambda_1(B_\alpha) x_k = (2\alpha - 1) \sum_{v_j : v_j v_k \in E(G)} x_j + (1 - \alpha) d_k x_k &\geq (2\alpha - 1) d_k x_k + (1 - \alpha) d_k x_k \\ &= \alpha d_k x_k.\end{aligned}$$

Thus, $\lambda_1(B_\alpha) \geq \alpha d_k \geq \alpha\delta$, for $\alpha \in (\frac{1}{2}, 1]$. Hence, $\lambda_1(B_\alpha) \geq \alpha\delta$ for all $\alpha \in [0, 1]$. □

Let $N_G(v_1)$ denote the set of vertices of G which are adjacent to v_1. Let $N_G[v_1] := N_G(v_1) \cup \{v_1\}$.

Theorem 4.5. *Let G be a graph with at least one edge and maximum degree Δ. Then, for any $\alpha\, (\neq \frac{1}{2}) \in [0, 1]$,*

$$\lambda_1(B_\alpha) \geq \frac{Y}{Z},$$

where Y and Z are given by

$$\begin{aligned}Y = \Big[&\alpha^2\, (3\alpha - 1)^2\, (\Delta + 1)^2\, \Big(2\alpha\, m_2 + (1 - \alpha)\, m_3\Big) + (1 - \alpha)\, (2\alpha - 1)^2 \\ &\times (2\Delta + 5\alpha - 3\alpha^2)^2\, \Delta\Big]\, P^2 + 4\, (2\alpha - 1)^2\, (\Delta + 1) \Big[(2\alpha - 1)\, \Delta\, (2\Delta + 5\alpha - 3\alpha^2) \\ &+ \alpha\, (3\alpha - 1)\, (\Delta + 1)\, m_3\Big]\, PQ + 4\, (2\alpha - 1)^2\, (\Delta + 1)^2\, \Big[2\alpha\, m_1 + (1 - \alpha)\, (\Delta + m_3)\Big]\, Q^2,\end{aligned} \tag{4.2}$$

$$Z = \Big[(2\alpha-1)^2\,(2\Delta+5\alpha-3\alpha^2)^2+\alpha^2\,(3\alpha-1)^2\,(\Delta+1)^2\,(n-\Delta-1)\Big]\,P^2 + 4\Delta\,(\Delta+1)^2\,(2\alpha-1)^2\,Q^2 \tag{4.3}$$

with

$$P=(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big) \text{ and } Q=16\alpha^2-6\alpha^3-10\alpha+2, \tag{4.4}$$

and $m_1=|E(N_G(v_1))|$, *is the number of edges in the set* $N_G(v_1)$, $m_2=|E(V(G)\backslash N_G[v_1])|$, *is the number of edges in the set* $V(G)\backslash N_G[v_1]$, m_3 *is the number of edges between* $N_G(v_1)$ *and* $V(G)\backslash N_G[v_1]$, *and the vertex* v_1 *has degree* Δ.

Proof. Let v_1 be the maximum degree vertex of degree Δ in G. Also let $S=\{v_2,v_3,\dots,v_{\Delta+1}\}$ be the set of vertices adjacent to v_1 in G. Let $\mathbf{x}=(x_1,x_2,\dots,x_n)^t$ be any non-zero vector. Using Rayleigh quotient, we obtain

$$\mathbf{x}^tB_\alpha\mathbf{x}\le\lambda_1(B_\alpha)\mathbf{x}^t\mathbf{x},\ \text{ that is, }\ \lambda_1(B_\alpha)\ge\frac{2\,\alpha\sum\limits_{v_iv_j\in E(G)}x_ix_j+(1-\alpha)\sum\limits_{v_iv_j\in E(G)}(x_i-x_j)^2}{\sum\limits_{i=1}^{n}x_i^2}. \tag{4.5}$$

We consider the following two cases:

Case 1. $(\alpha-1)\,(3\alpha-2)\,\Delta+2\neq0$. In this case $P=(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)\neq0$ as $\alpha\neq\frac{1}{2}$. Setting

$$x_i=\begin{cases}1-\dfrac{2-5\alpha+3\alpha^2}{2(\Delta+1)} & \text{for } i=1,\\[2ex] \dfrac{16\alpha^2-6\alpha^3-10\alpha+2}{(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)} & \text{for } i=2,3,\dots,\Delta+1,\\[2ex] \dfrac{\alpha(3\alpha-1)}{2(2\alpha-1)} & \text{Otherwise.}\end{cases} \tag{4.6}$$

Since $m_1=|E(N_G(v_1))|$, $m_2=|E(V(G)\backslash N_G[v_1])|$, and m_3 is the number of edges between $N_G(v_1)$ and $V(G)\backslash N_G[v_1]$, we obtain

$$\begin{aligned}\sum_{v_iv_j\in E(G)}x_ix_j &= \frac{(2\Delta+5\alpha-3\alpha^2)\,(16\alpha^2-6\alpha^3-10\alpha+2)}{2(\Delta+1)\,(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)}\,\Delta\\ &\quad+\frac{(16\alpha^2-6\alpha^3-10\alpha+2)^2}{(2\alpha-1)^2\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)^2}\,m_1+\frac{\alpha^2\,(3\alpha-1)^2}{4\,(2\alpha-1)^2}\,m_2\\ &\quad+\frac{\alpha(3\alpha-1)\,(16\alpha^2-6\alpha^3-10\alpha+2)}{2(2\alpha-1)^2\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)}\,m_3,\end{aligned}$$

$$\sum_{v_iv_j\in E(G)}(x_i-x_j)^2=\left(\frac{(2\Delta+5\alpha-3\alpha^2)}{2(\Delta+1)}-\frac{16\alpha^2-6\alpha^3-10\alpha+2}{(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)}\right)^2\Delta$$

$$+\left(\frac{16\alpha^2-6\alpha^3-10\alpha+2}{(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)}-\frac{\alpha(3\alpha-1)}{2(2\alpha-1)}\right)^2 m_3,$$

and

$$\sum_{i=1}^{n}x_i^2=\frac{(2\Delta+5\alpha-3\alpha^2)^2}{4(\Delta+1)^2}+\frac{(16\alpha^2-6\alpha^3-10\alpha+2)^2}{(2\alpha-1)^2\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)^2}\,\Delta$$

$$+\frac{\alpha^2(3\alpha-1)^2}{4(2\alpha-1)^2}\,(n-\Delta-1).$$

Using the above results in (4.5), we obtain

$$\lambda_1(B_\alpha)\geq\frac{Y}{Z}$$

as

$$2\,\alpha\sum_{v_iv_j\in E(G)}x_ix_j+(1-\alpha)\sum_{v_iv_j\in E(G)}(x_i-x_j)^2=\frac{Y}{4\,(2\alpha-1)^2\,(\Delta+1)^2\,P^2}$$

and

$$\sum_{i=1}^{n}x_i^2=\frac{Z}{4\,(2\alpha-1)^2\,(\Delta+1)^2\,P^2},$$

where Y, Z and P are given by (4.2), (4.3) and (4.4), respectively. Moreover, the equality holds if and only if $\mathbf{x}=(x_1,x_2,\ldots,x_n)^t$ is an eigenvector corresponding to the eigenvalue $\lambda_1(B_\alpha)$ of B_α, where x_i is given in (4.6).

Case 2. $(\alpha-1)\,(3\alpha-2)\,\Delta+2=0$. In this case $P=(2\alpha-1)\Big((\alpha-1)\,(3\alpha-2)\,\Delta+2\Big)=0$. Thus we obtain

$Y=4\,(2\alpha-1)^2\,(\Delta+1)^2\,\Big[2\alpha\,m_1+(1-\alpha)\,(\Delta+m_3)\Big]\,Q^2$ and $Z=4\Delta\,(\Delta+1)^2\,(2\alpha-1)^2\,Q^2$.

Setting

$$x_i=\begin{cases}0 & \text{for } i=1,\\ 1 & \text{for } i=2,3,\ldots,\Delta+1,\\ 0 & \text{Otherwise.}\end{cases}$$

Since $m_1=|E(N_G(v_1))|$, $m_2=|E(V(G)\backslash N_G[v_1])|$, and m_3 is the number of edges between $N_G(v_1)$ and $V(G)\backslash N_G[v_1]$, we obtain

$$\sum_{v_iv_j\in E(G)}x_ix_j=m_1,\quad\sum_{v_iv_j\in E(G)}(x_i-x_j)^2=\Delta+m_3\ \text{ and }\ \sum_{i=1}^{n}x_i^2=\Delta.$$

Using the above results in (4.5), we obtain

$$\lambda_1(B_\alpha) \geq \frac{2\,\alpha\, m_1 + (1-\alpha)\,(\Delta + m_3)}{\Delta} = \frac{Y}{Z}.$$

Moreover, the equality holds if and only if $\mathbf{x} = (0, \underbrace{1, \ldots, 1}_{\Delta}, \underbrace{0, \ldots, 0}_{n-\Delta-1})^t$ is an eigenvector corresponding to the eigenvalue $\lambda_1(B_\alpha)$ of B_α. $\square$

Corollary 4.6. *Let G be a graph of order n with m edges and maximum degree Δ. Then*

$$\rho_1(G) \geq \frac{2m}{n}$$

with equality if and only if G is a regular graph.

Proof. For adjacency matrix, $\alpha = 1$, that is, $B_1 = B_1(G) = A(G)$. For $\alpha = 1$, from Theorem 4.5, we obtain

$$P = 2 = Q,\ Y = 32\,(\Delta{+}1)^2\,(\Delta{+}m_1{+}m_2{+}m_3) = 32\,(\Delta{+}1)^2\, m \ \text{ and } \ Z = 16\,(\Delta{+}1)^2\, n$$

and hence

$$\rho_1(G) = \lambda_1(B_1) \geq \frac{Y}{Z} = \frac{2m}{n}.$$

Moreover, the equality holds if and only if $\mathbf{x} = (1, 1, \ldots, 1)^t$ is an eigenvector corresponding to the eigenvalue $\lambda_1(B_1)\,(= \rho_1(G))$ of B_1, that is, if and only if G is a regular graph. $\square$

Corollary 4.7. *Let G be a graph of order n with m edges and maximum degree Δ. Then*

$$\mu_1(G) \geq \Delta + 1.$$

If G is connected, then the above equality holds if and only if $\Delta = n - 1$.

Proof. For Laplacian matrix, $\alpha = 0$, that is, $B_0 = B_0(G) = L(G)$. For $\alpha = 0$, from Theorem 4.5, we obtain

$$P = -2\,(\Delta{+}1),\ Q = 2,\ Y = 16\,\Delta(\Delta{+}1)^2\left((\Delta{+}1)^2 + \frac{m_3}{\Delta}\right) \ \text{ and } \ Z = 16\,\Delta\,(\Delta{+}1)^3.$$

and hence

$$\mu_1(G) = \lambda_1(B_0) \geq \frac{Y}{Z} = \Delta + 1 + \frac{m_3}{\Delta\,(\Delta+1)} \geq \Delta + 1$$

as $m_3 \geq 0$.

Suppose that G is connected. Then the equality holds if and only if $\mathbf{x} = \left(\frac{\Delta}{\Delta+1}, \underbrace{-\frac{1}{\Delta+1}, \ldots, -\frac{1}{\Delta+1}}_{\Delta}, \underbrace{0, \ldots, 0}_{n-\Delta-1}\right)^t$ is an eigenvector corresponding to the eigenvalue $\lambda_1(B_0)\,(= \mu_1(G))$ of B_0 and $m_3 = 0$. Since G is connected, then $\Delta = n - 1$. If $\Delta = n - 1$, then one can easily see that $\mu_1(G) = n = \Delta + 1$. This completes the proof of the result. $\square$

Corollary 4.8. *Let G be a graph of order n with m edges and maximum degree Δ. Then*

$$q_1(G) \geq \frac{4m}{n}$$

with equality if and only if G is a regular graph.

Proof. For signless Laplacian matrix, $\alpha = \frac{2}{3}$, that is, $B_{2/3} = B_{2/3}(G) = \frac{1}{3}\,Q(G)$. For $\alpha = \frac{2}{3}$, from Theorem 4.5, we obtain

$$P = \frac{2}{3} = Q,\ Y = \frac{64}{243}\,(\Delta{+}1)^2\,(\Delta{+}m_1{+}m_2{+}m_3) = \frac{64}{243}\,(\Delta{+}1)^2\,m,\ Z = \frac{16}{81}\,(\Delta{+}1)^2\,n$$

and hence

$$\frac{1}{3}\,q_1(G) = \lambda_1(B_{2/3}) \geq \frac{Y}{Z} = \frac{4m}{3n}, \ \text{ that is, }\ q_1(G) \geq \frac{4m}{n}.$$

Moreover, the equality holds if and only if $\mathbf{x} = (1, 1, \ldots, 1)^t$ is an eigenvector corresponding to the eigenvalue $\lambda_1(B_{2/3})\,(= \frac{1}{3}\,q_1(G))$ of $B_{2/3}$, that is, if and only if G is a regular graph. □

The lower bounds found in Corollaries 4.6-4.8 are classical. One can find all of them in [26].

Remark 4.9. *In the following Table, we give a comparison between the exact value of $\lambda_1(B_\alpha)$ (*Proposition 4.3*) and the lower bound on $\lambda_1(B_\alpha)$ obtained in* Theorem 4.5 *for the graph $G = K_{1,24}$.*

α	*Exact value of* $\lambda_1(B_\alpha)$	$\frac{Y}{Z}$
0	25	25
0.1	22.317	22.317
0.2	19.658	19.654
0.3	17.035	16.997
0.4	14.469	13.675
0.6	9.703	1.978
0.7	7.718	0.936
0.8	6.232	0.250
0.9	5.334	0.361
1	4.899	1.92

Table 1. Comparison of the largest eigenvalue $\lambda_1(B_\alpha)$ and $\frac{Y}{Z}$.

Next, we observe that the following upper bound is continuous on α.

Theorem 4.10. *Let G be a connected graph with maximum degree Δ. Then, for any $\alpha \in [0, 1]$,*

$$\lambda_1\,(B_\alpha) \leq \begin{cases} (2 - 3\,\alpha)\,\Delta & \text{if } \alpha \in [0, \frac{1}{2}], \\ \alpha\,\Delta & \text{if } \alpha \in (\frac{1}{2}, 1]. \end{cases}$$

Proof. First we assume that $\alpha \in [0, \frac{1}{2}]$. Then, by using $\alpha \geq 0$, $(1-2\alpha) \geq 0$, Corollary 2.3, and Theorem 2.4, we have

$$\lambda_1(B_\alpha) = \lambda_1\Big(\alpha D + (1-2\alpha)L\Big) \leq \lambda_1(\alpha D) + \lambda_1\Big((1-2\alpha)L\Big) \leq \alpha\Delta + (1-2\alpha)(2\Delta).$$

That is, $\lambda_1(B_\alpha) \leq (2-3\alpha)\Delta$ for all $\alpha \in [0, \frac{1}{2}]$.

Next we assume that $\alpha \in (\frac{1}{2}, 1]$. That is, $2\alpha - 1 > 0$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ be an eigenvector of B_α corresponding to the eigenvalue $\lambda_1(B_\alpha)$ such that $x_k = \max\limits_{1\leq i\leq n} x_i > 0$. Then we obtain

$$\begin{aligned}\lambda_1(B_\alpha)\, x_k &= (2\alpha-1) \sum_{v_j : v_j v_k \in E(G)} x_j + (1-\alpha)\, d_k\, x_k \\ &\leq (2\alpha-1)\, d_k\, x_k + (1-\alpha)\, d_k\, x_k \\ &= \alpha d_k\, x_k \\ &\leq \alpha\Delta x_k.\end{aligned}$$

Therefore, $\lambda_1(B_\alpha) \leq \alpha\Delta$ for all $\alpha \in (\frac{1}{2}, 1]$. □

For $\alpha \in [0, 1]$ and non-negative integers a and b, define

$$f_\alpha(a, b) = \frac{(1-\alpha)\,(a+b) + \sqrt{(1-\alpha)^2\,(a-b)^2 + 4(2\alpha-1)^2\, ab}}{2}.$$

Theorem 4.11. *Let $G = (U, W, E)$ be a connected bipartite graph, where $|U| = a$, $|W| = b$. For $\alpha \in [0, 1]$,*

$$\lambda_1(B_\alpha) \leq f_\alpha(a, b) \tag{4.7}$$

with equality if and only if $G \cong K_{a,b}$.

Proof. Without loss of generality, assume that $a \geq b$. Now, from Proposition 4.3, we have $f_\alpha(a, b) = \lambda_1(B_\alpha(K_{a,b}))$. Since, by definition, $B_0 = B_0(G) = L(G)$ and $G \subseteq K_{a,b}$, by (edge) interlacing and Proposition 4.3,

$$\lambda_1(B_0) = \mu_1(G) \leq a + b = f_0(a, b).$$

Since $B_{\frac{1}{2}} = B_{\frac{1}{2}}(G) = \frac{1}{2}\, D(G)$, we have

$$\lambda_1(B_{\frac{1}{2}}) = \frac{1}{2}\Delta(G) \leq \frac{1}{2}\Delta(K_{a,b}) = \frac{1}{2}\, a = f_{\frac{1}{2}}(a, b).$$

As $B_1 = B_1(G) = A(G)$, by (vertex) interlacing and Proposition 4.3, we have

$$\lambda_1(B_1) = \rho_1(G) \leq \rho_1(K_{a,b}) = f_1(a, b).$$

So we have to prove the result in (4.7) for $0 < \alpha < \frac{1}{2}$ and $\frac{1}{2} < \alpha < 1$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector corresponding to the largest eigenvalue $\lambda_1(B_\alpha)$ of B_α. Then $B_\alpha \mathbf{x} = \lambda_1(B_\alpha)\mathbf{x}$. We consider two cases:

Case 1. $\frac{1}{2} < \alpha < 1$. Let $x_i = \max\limits_{1\leq k\leq n} x_k$. Without loss of generality, we can assume that $v_i \in U$. Let $x_j = \max\limits_{v_k \in W} x_k$. For $v_i \in U$, we obtain

$$\lambda_1(B_\alpha)\, x_i = (1-\alpha)\, d_i x_i + (2\alpha-1) \sum_{v_k : v_i v_k \in E(G)} x_k \leq (1-\alpha)\, d_i x_i + (2\alpha-1)\, d_i x_j,$$

that is,

$$\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_i\Big]\, x_i \leq (2\alpha - 1)\, d_i x_j. \tag{4.8}$$

Similarly, for $v_j \in W$, we obtain

$$\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_j\Big]\, x_j \leq (2\alpha - 1)\, d_j x_i. \tag{4.9}$$

From the above two results, we obtain

$$\begin{aligned}\Big[\lambda_1(B_\alpha) - &(1-\alpha)\, b\Big]\Big[\lambda_1(B_\alpha) - (1-\alpha)\, a\Big] \leq \\ &\leq \Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_i\Big]\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_j\Big] \\ &\leq (2\alpha-1)^2\, d_i\, d_j \leq (2\alpha - 1)^2\, ab. \end{aligned} \tag{4.10}$$

Thus we obtain

$$\lambda_1(B_\alpha)^2 - (1-\alpha)\,(a+b)\lambda_1(B_\alpha) + (1-\alpha)^2\, ab - (2\alpha-1)^2\, ab \leq 0,$$

that is,

$$\lambda_1(B_\alpha) \leq \frac{(1-\alpha)\,(a+b) + \sqrt{(1-\alpha)^2\,(a-b)^2 + 4(2\alpha-1)^2\, ab}}{2} = f_\alpha(a,b).$$

The first part of the proof is done.

Suppose that equality holds. Then all inequalities in the above argument must be equalities. From equalities in (4.8) and (4.9), we obtain $x_k = x_i$ for all $v_k \in N_G(v_j) \subseteq U$ and $x_\ell = x_j$ for all $v_\ell \in N_G(v_i) \subseteq W$. From equality in (4.10), we obtain $d_i = b$ and $d_j = a$. Since G is a connected bipartite graph, one can easily prove that $x_k = x_i$ for all $v_k \in U$ and $x_\ell = x_j$ for all $v_\ell \in W$. For $v_i,\, v_k \in U$, we have

$$\lambda_1(B_\alpha)\, x_i = (1-\alpha)\, d_i x_i + (2\alpha - 1) \sum_{v_k : v_i v_k \in E(G)} x_k = b\,\Big[(1-\alpha)\, x_i + (2\alpha-1)\, x_j\Big]$$

and

$$\lambda_1(B_\alpha)\, x_i = d_k\,\Big[(1-\alpha)\, x_i + (2\alpha-1)\, x_j\Big].$$

Thus we have

$$b\,\Big[(1-\alpha)\, x_i + (2\alpha-1)\, x_j\Big] = d_k\,\Big[(1-\alpha)\, x_i + (2\alpha-1)\, x_j\Big],$$

that is,

$$\Big(b - d_k\Big)\,\Big[(1-\alpha)\, x_i + (2\alpha-1)\, x_j\Big] = 0.$$

Since all the elements in B_α are non-negative, by Perron-Frobenius theorem in matrix theory, we obtain that all the eigencomponents corresponding to the spectral radius $\lambda_1(B_\alpha)$ are non-negative. Since G is connected, $x_i \geq x_j > 0$. From the above with $\frac{1}{2} < \alpha < 1$, we must have $d_k = b$ for any $v_k \in U$. Similarly, $d_\ell = a$ for any $v_\ell \in W$. Hence $G \cong K_{a,b}$.

Case 2. $0 < \alpha < \frac{1}{2}$. Let $x_i = \max_{1 \leq k \leq n}\, x_k$. Without loss of generality, we can assume that $v_i \in U$. Let $x_j = \min_{v_k : v_i v_k \in E(G)}\, x_k$. For $v_i \in U$, we obtain

$$\lambda_1(B_\alpha)\, x_i = (1-\alpha)\, d_i x_i + (2\alpha - 1) \sum_{v_k : v_i v_k \in E(G)} x_k \leq (1-\alpha)\, d_i x_i + (2\alpha-1)\, d_i x_j,$$

that is,

$$\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_i\Big]\, x_i \le (2\alpha - 1)\, d_i x_j.$$

Similarly, for $v_j \in W$, we obtain

$$\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_j\Big]\, x_j \ge (2\alpha - 1)\, d_j x_i.$$

Since $\alpha < \frac{1}{2}$, from the above two results, we obtain

$$\begin{aligned} &\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_i\Big]\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_j\Big]\, x_i \\ \le &(2\alpha - 1)\, d_i \Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_j\Big]\, x_j \\ \le &(2\alpha - 1)^2\, d_i\, d_j\, x_i, \end{aligned}$$

that is,

$$\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_i\Big]\Big[\lambda_1(B_\alpha) - (1-\alpha)\, d_j\Big] \le (2\alpha - 1)^2\, d_i\, d_j,$$

that is,

$$\Big[\lambda_1(B_\alpha) - (1-\alpha)\, b\Big]\Big[\lambda_1(B_\alpha) - (1-\alpha)\, a\Big] \le (2\alpha - 1)^2\, ab.$$

Thus we obtain

$$\lambda_1(B_\alpha)^2 - (1-\alpha)\,(a+b)\lambda_1(B_\alpha) + (1-\alpha)^2\, ab - (2\alpha-1)^2\, ab \le 0,$$

that is,

$$\lambda_1(B_\alpha) \le \frac{(1-\alpha)\,(a+b) + \sqrt{(1-\alpha)^2\,(a-b)^2 + 4(2\alpha-1)^2\, ab}}{2} = f_\alpha(a,b).$$

Suppose that equality holds. Similarly as **Case 1**, one can easily prove that $G \cong K_{a,b}$.

Conversely, let $G \cong K_{a,b}$. By Proposition 4.3, we obtain

$$\lambda_1(B_\alpha) = \frac{(1-\alpha)\,(a+b) + \sqrt{(1-\alpha)^2\,(a-b)^2 + 4(2\alpha-1)^2\, ab}}{2} = f_\alpha(a,b).$$

This completes the proof of the theorem. □

4.3 Bounds on the smallest eigenvalue

We establish an upper bound on the smallest eigenvalue of a B_α-matrix in terms of the chromatic number. Then, we characterize the extremal graphs for some cases. Finally, some known results are derived as a consequence.

Theorem 4.12. *Let G be a graph of n vertices, m (> 0) edges and chromatic number χ. Then, for any $\alpha \in [0,1]$,*

$$\lambda_n\,(B_\alpha) \le \frac{2\,m}{n}\left(\frac{\chi\,(1-\alpha) - \alpha}{\chi - 1}\right). \tag{4.11}$$

Proof. Set $B_\alpha := B_\alpha(G)$. Partition the vertex set $V(G)$ as χ number of subsets $V_1, V_2, \ldots, V_\chi$, where each subset contains the vertices having the same colour. For each $j \in \{1, 2, \ldots, \chi\}$, define a vector $\mathbf{x} := (x_1, x_2, \ldots, x_n)^t$ as follows:

$$x_i = \begin{cases} \chi - 1 & \text{for } v_i \in V_j \\ -1 & \text{otherwise.} \end{cases}$$

Then

$$||\mathbf{x}||^2 = \sum_{i=1}^{n} x_i^2 = (\chi - 1)^2 |V_j| + (n - |V_j|) = \chi(\chi - 2)|V_j| + n.$$

For $j \in \{1, 2, \ldots, \chi\}$, define $m_j = \sum_{v \in V_j} d(v)$. Now,

$$\langle B_\alpha \mathbf{x}, \mathbf{x}\rangle = \langle (2\alpha - 1) A\mathbf{x}, \mathbf{x}\rangle + \langle (1 - \alpha) D\mathbf{x}, \mathbf{x}\rangle.$$

Note that

$$\langle A\mathbf{x}, \mathbf{x}\rangle = 2 \sum_{v_i v_j \in E(G)} x_i x_j = 2(1 - \chi) m_j + 2(m - m_j)$$

and

$$\langle D\mathbf{x}, \mathbf{x}\rangle = \sum_{v_i \in V} d_i x_i^2 = (\chi - 1)^2 m_j + (2m - m_j) = \chi(\chi - 2) m_j + 2m.$$

Thus we obtain

$$\begin{aligned} \langle B_\alpha \mathbf{x}, \mathbf{x}\rangle &= (2\alpha - 1)\langle A\mathbf{x}, \mathbf{x}\rangle + (1 - \alpha)\langle D\mathbf{x}, \mathbf{x}\rangle \\ &= 2(2\alpha - 1)(1 - \chi) m_j + 2(2\alpha - 1)(m - m_j) + (1 - \alpha)\chi(\chi - 2) m_j \\ &\qquad + 2(1 - \alpha) m \\ &= 2m\alpha + \Big(\chi - \alpha(\chi + 2)\Big)\chi m_j. \end{aligned}$$

Using Rayleigh quotient, we obtain

$$\lambda_n(B_\alpha)\,||\mathbf{x}||^2 \le \langle B_\alpha \mathbf{x}, \mathbf{x}\rangle.$$

Therefore, by the above inequalities, we have

$$\lambda_n(B_\alpha)\Big(\chi(\chi - 2)|V_j| + n\Big) \le 2m\alpha + \Big(\chi - \alpha(\chi + 2)\Big)\chi m_j,$$

that is,

$$\sum_{j=1}^{\chi} \lambda_n(B_\alpha)\Big(\chi(\chi - 2)|V_j| + n\Big) \le \sum_{j=1}^{\chi}\Big(2m\alpha + \Big(\chi - \alpha(\chi + 2)\Big)\chi m_j\Big),$$

that is,

$$\lambda_n(B_\alpha)\Big((\chi^2 - 2\chi) n + n\chi\Big) \le 2\chi^2 m - 2\alpha\chi^2 m - 2m\chi\alpha.$$

Therefore,

$$\lambda_n(B_\alpha) \le \frac{2m}{n}\left(\frac{\chi(1 - \alpha) - \alpha}{\chi - 1}\right).$$

□

In the next couple of results, we partially characterize the graphs attaining the equality in (4.11) of Theorem 4.12. The proofs technique is similar to the one used in [21].

Theorem 4.13. *Let G be a bipartite graph of n vertices with m edges. Then, for any $\alpha \in [0,1]$,*

$$\lambda_n(B_\alpha) \leq \frac{2m}{n}\,(2-3\alpha). \tag{4.12}$$

Equality occurs if and only if either $\alpha = \frac{2}{3}$, or G is regular with $\alpha \geq \frac{1}{2}$.

Proof. Set $\lambda_n := \lambda_n(B_\alpha)$. For any $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t \in \mathbb{R}^n$, by Rayleigh quotient, we obtain

$$\lambda_n\,\mathbf{x}^t\,\mathbf{x} \leq \mathbf{x}^t\,B_\alpha\,\mathbf{x} \quad \text{that is,} \quad \lambda_n \sum_{i=1}^{n} x_i^2 \leq \alpha \sum_{i=1}^{n} d_i\,x_i^2 + (1-2\alpha) \sum_{v_iv_j \in E(G),\ i<j} (x_i - x_j)^2.$$

Let $V(G) = V_1 \cup V_2$ be the vertex partition of G such that no two vertices of V_1 (resp V_2) are adjacent. Take $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$, where the component $x_i = 1$ if $v_i \in V_1$, and $x_i = -1$ otherwise. Then

$$\lambda_n(B_\alpha) \leq \frac{2m}{n}\,(2-3\alpha).$$

The first part of the proof is done.

If the equality holds in (4.12), then $B_\alpha\,\mathbf{x} = \lambda_n\mathbf{x}$. Suppose $v_i \in V_1$ and $v_j \in V_2$. From the i-th and j-th equation of $B_\alpha\mathbf{x} = \lambda_n\mathbf{x}$, we obtain

$$\lambda_n = d_i(2-3\alpha) \quad \text{and} \quad \lambda_n = d_j(2-3\alpha), \quad \text{that is,} \quad (\,d_i - d_j\,)(2-3\alpha) = 0.$$

Therefore, for the arbitrariness of v_i and v_j, either $\alpha = \frac{2}{3}$ or G is regular. If G is r-regular and $\alpha < \frac{1}{2}$, then

$$\lambda_n(B_\alpha) = \lambda_n\Big((1-\alpha)D + (2\alpha-1)A\Big) = (1-\alpha)\,r + (2\alpha-1)\,\rho_1 = \alpha\,r < \frac{2m}{n}\,(2-3\alpha)$$

as $\rho_1 = r$ (G is bipartite). Hence either $\alpha = \frac{2}{3}$, or G is regular with $\alpha \geq \frac{1}{2}$.

Conversely, let $\alpha = \frac{2}{3}$. Then $Q(G) = 3B_{\frac{2}{3}}(G)$ and hence $\lambda_n(B_{\frac{2}{3}}) = \frac{1}{3}\,q_n(G) = 0 = \frac{2m}{n}\,(2-3\alpha)$ as G is bipartite.

Let G be a r-regular bipartite graph with $\alpha \geq \frac{1}{2}$. Then $\rho_n = -r$. Since $\alpha \geq \frac{1}{2}$, we obtain

$$\lambda_n(B_\alpha) = \lambda_n\Big((1-\alpha)D + (2\alpha-1)A\Big) = (1-\alpha)\,r + (2\alpha-1)\,\rho_n = (2-3\,\alpha)\,r = \frac{2m}{n}\,(2-3\alpha).$$

□

In [21], the authors defined a class of graphs Λ in the following:

Let Λ be the class of graphs $H = (V, E)$ such that H is a regular χ-partite graph ($\chi \geq 3$) with n/χ vertices in every part, where $\chi | n$, and every vertex has $\frac{d}{\chi-1}$ adjacent vertices in every other part (d is the degree of each vertex in H).

Theorem 4.14. *Let G be a graph with chromatic number χ such that*

$$\lambda_n\left(B_\alpha\right) = \frac{2\,m}{n}\left(\frac{\chi\left(1-\alpha\right)-\alpha}{\chi-1}\right). \tag{4.13}$$

where $0 \leq \alpha \leq 1$. Then

(1) *for $\alpha = \frac{1}{2}$, G is regular,*

(2) *for $\chi = 2$, G is bipartite with $\alpha = \frac{2}{3}$, or G is regular bipartite with $\alpha \geq \frac{1}{2}$.*

(3) *for $\alpha \in [0, 1]$ $\left(\alpha \neq \left\{\frac{1}{2}, \frac{\chi}{\chi+1}\right\}, \chi \geq 3\right)$, $G \in \Lambda$.*

Proof. (1) Suppose that $\alpha = \frac{1}{2}$. Then by Remark 1.1 and (4.13), we obtain $\frac{\delta}{2} = \lambda_n(B_{\frac{1}{2}}) = \frac{m}{n}$, that is, $2m = n\,\delta$, that is, $n\delta \leq \sum\limits_{i=1}^{n} d_i = 2m = n\delta$, that is, $\sum\limits_{i=1}^{n} d_i = n\delta$, that is, G is regular.

(2) Suppose $\chi = 2$. Then $\lambda_n(B_\alpha) = \frac{2m}{n}\,(2-3\alpha)$. By Theorem 4.13, G is bipartite with $\alpha = \frac{2}{3}$, or G is regular bipartite with $\alpha \geq \frac{1}{2}$.

(3) We assume that $\alpha \in [0, 1]$ and $\alpha \neq \left\{\frac{1}{2}, \frac{\chi}{\chi+1}\right\}$ with $\chi \geq 3$.

Set $\lambda_n := \lambda_n(B_\alpha)$. Let us partition the vertex set $V(G)$ into χ number of color classes $V_1, V_2, \ldots, V_\chi$. For $j \in \{1, 2\ldots, \chi\}$, define $\mathbf{x}^{(\mathbf{j})} := (x_1^j, x_2^j, \ldots, x_n^j)$ as follows:

$$x_i^j = \begin{cases} \chi - 1 & \text{for } v_i \in V_j, \\ -1 & \text{otherwise.} \end{cases}$$

Then by Theorem 4.12, $\lambda_n\left(B_\alpha\right) \leq \frac{2\,m}{n}\left(\frac{\chi\,(1-\alpha)-\alpha}{\chi-1}\right)$. Since equality occurs in the above inequality, so by Rayleigh quotient and Theorem 4.12, $\mathbf{x}^{(\mathbf{1})}, \ldots, \mathbf{x}^{(\chi)}$ are all eigenvectors of B_α corresponding to the eigenvalue λ_n.

Claim 1 : G is regular.
Let $1 \leq k \neq \ell \leq \chi$. Suppose $v_s \in V_k$ and $v_t \in V_\ell$. Comparing the s-th components of the matrix equation $B_\alpha \mathbf{x}^{(\mathbf{k})} = \lambda_n \mathbf{x}^{(\mathbf{k})}$, we obtain $\lambda_n(\chi - 1) = d_s\,(\chi - \alpha\chi - \alpha)$. Similarly, comparing the t-th components of the matrix equation $B_\alpha \mathbf{x}^{(\ell)} = \lambda_n \mathbf{x}^{(\ell)}$, we have $\lambda_n(\chi - 1) = d_t\,(\chi - \alpha\chi - \alpha)$. Then $(d_s - d_t)(\chi - \alpha\chi - \alpha) = 0$. Since $\alpha \neq \frac{\chi}{\chi+1}$ and v_s, v_t are arbitrary, so G is regular.

Claim 2 : $|V_1| = \cdots = |V_\chi| = \frac{n}{\chi}$, where $\chi|n$.
By Claim 1, G is regular, so $\mathbf{1} := (1, 1, \ldots, 1)^t$ is an eigenvector of B_α. Also, B_α is symmetric, so $\mathbf{1} \perp x^{(k)}$ for $k = 1, 2, \ldots, \chi$. Therefore, $|V_k|(\chi - 1) + (-1)(n - |V_k|) = 0$. That is, $|V_k| = \frac{n}{\chi}$, for $k = 1, 2, \ldots, \chi$.

Claim 3 : Every vertex is adjacent to $\frac{d}{\chi-1}$ vertices in every other part, where d is the regularity of G.
Suppose $v_s \in V_1$ and it is adjacent with $r_2, r_3, \ldots, r_\chi$ number of vertices in the partitions

$V_2, V_3, \ldots, V_\chi$, respectively. For $v_s \in V_1$, from $B_\alpha \mathbf{x^{(k)}} = \lambda_n \mathbf{x^{(k)}}$, we obtain

$$(-1)\lambda_n = (1-\alpha)(-1)d_s + (2\alpha-1)\left(\sum_{i=2, i\neq k}^{\chi} (-1)r_i + (\chi-1)r_k\right),$$

where $2 \leq k \leq \chi$. From this we have the following $\chi - 1$ equations:

$$\begin{aligned}
(-1)\lambda_n &= (1-\alpha)(-1)d_s + (2\alpha-1)\Big((\chi-1)r_2 + (-1)r_3 + \cdots + (-1)r_\chi\Big)\\
(-1)\lambda_n &= (1-\alpha)(-1)d_s + (2\alpha-1)\Big((-1)r_2 + (\chi-1)r_3 + \cdots + (-1)r_\chi\Big)\\
&\cdots\cdots\cdots\\
&\cdots\cdots\cdots\\
(-1)\lambda_n &= (1-\alpha)(-1)d_s + (2\alpha-1)\Big((-1)r_2 + (-1)r_3 + \cdots + (\chi-1)r_\chi\Big).
\end{aligned}$$

Since $\alpha \neq \frac{1}{2}$, so from the above, we have $r_2 = r_3 = \cdots = r_\chi = \frac{d}{\chi-1}$ as G is regular by **Claim 1**. Also v_s is arbitrary, therefore the **Claim 3** is done.

Hence $G \in \Lambda$. □

In the next result, we partially obtain the converse of the Theorem 4.14. One can verify that if $\alpha = \frac{1}{2}$ and G is regular, then the equality (4.13) holds. Moreover, the equality (4.13) holds for any bipartite graph with $\alpha = \frac{2}{3}$, or any regular bipartite graph with $\alpha \geq \frac{1}{2}$. Therefore, we consider the remaining converse part of the Theorem 4.14. Since the proof technique of the following result is similar to [21, Theorem 5.1], we omit the proof.

Theorem 4.15. *If $G \in \Lambda$ and $\alpha\,(\neq \frac{1}{2}) \in [0,1]$, then $\frac{2m}{n}\left(\frac{\chi(1-\alpha)-\alpha}{\chi-1}\right)$ is an eigenvalue of $B_\alpha(G)$ with multiplicity $\chi - 1$.*

The next result is known (see to [12]); however, it can be deduced from Theorem 4.12 by taking $\alpha = \frac{2}{3}$.

Corollary 4.16 ([12])**.** *Let G be graph of order n with m edges and chromatic number χ. Then*

$$q_n(G) \leq \frac{2m}{n}\left(\frac{\chi-2}{\chi-1}\right).$$

Corollary 4.17. *Let G be graph of order n with m edges and chromatic number χ such that*

$$q_n(G) = \frac{2m}{n}\left(\frac{\chi-2}{\chi-1}\right).$$

Then G is either bipartite or $G \in \Lambda$.

Proof. Proof follows from Theorem 4.14. □

As a consequence of Theorem 4.12, a lower bound of the chromatic number of G is deduced.

Corollary 4.18. *If G is a graph with chromatic number χ and $\beta_o := \beta_o(G)$, then*

$$\chi \geq \frac{\beta_o}{1-\beta_o}.$$

5 On the determinant

In this short section, we present the determinant and the Sachs-type formula for the coefficients of the characteristic polynomial of $B_\alpha(G)$. Then, we obtain some known results as a consequence.

A spanning elementary subgraph H of a graph G is a spanning subgraph of G such that each component of H is either a cycle or an edge. For a spanning elementary subgraph H, $p(H)$ and $c(H)$ denote the number of components and the number of cycles in H, respectively. Now, we present the well known Harary's formula [16] for the determinant of the adjacency matrix of a graph.

Proposition 5.1. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Also let $A(G)$ be the adjacency matrix of G. Then,*

$$\det\left(A(G)\right) = \sum_H (-1)^{\,n-p(H)}\, 2^{\,c(H)},$$

where summation is over all spanning elementary subgraphs H of G.

Motivated by the notion of spanning elementary subgraphs and for the purpose of the main result in this section, we define the following.

Definition 5.2. Modified Elementary Subgraph: A subgraph H of a graph G is called a modified elementary subgraph if each component of H is either a vertex, an edge, or a cycle.

Let H be a modified elementary subgraph. Denote by $c(H), c_1(H)$, and $c_2(H)$ the number of components in a subgraph H which are cycles, edges, and vertices, respectively. Let $p(H) := c(H) + c_1(H) + c_2(H)$ be the number of components in H. Also, let $\mathcal{C}_2(H)$ be the collection of isolated vertices in H. In the following result, we present a Harary-type formula [16] for the determinant of B_α-matrices. For a graph G, since $\det(L(G)) = \det(B_0(G)) = 0$, so we derive a formula of $\det(B_\alpha(G))$ for $\alpha \in (0, 1]$.

Theorem 5.3. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Then, for any $\alpha \in (0, 1]$,*

$$\det\left(B_\alpha(G)\right) = \sum_H (-1)^{\,n-p(H)}\, 2^{\,c(H)}\, (1-\alpha)^{\,c_2(H)}\, (2\alpha-1)^{\,n-c_2(H)} \left(\prod_{v_i \in \mathcal{C}_2(H)} d_G(v_i)\right), \tag{5.1}$$

where summation is over all spanning modified elementary subgraphs H of G.

Proof. Consider $B_\alpha(G) = (2\alpha - 1)A(G) + (1 - \alpha)D(G) = (b_{ij})_{n\times n}$. We have

$$\det\left(B_\alpha(G)\right) = \sum_\pi \operatorname{sgn}(\pi)\, b_{1\pi(1)}\, b_{2\pi(2)} \cdots b_{n\pi(n)}, \tag{5.2}$$

where summation is over all permutations of $1, 2, \ldots, n$. Since every permutation π has a cycle decomposition, so a cycle of length 1, 2 and more corresponds to a vertex, an edge, and a cycle, respectively in the graph G. Thus, each term $b_{1\pi(1)}b_{2\pi(2)} \cdots b_{n\pi(n)}$ corresponds to a spanning modified elementary subgraph of G.

Also, each spanning modified elementary subgraph H corresponds to $2^{c(H)}$ terms in the summation (5.2) as each cycle is associated to a cyclic permutation in two ways. If π is a permutation corresponding to a spanning modified elementary subgraph H, then

$$\begin{aligned}\operatorname{sgn}(\pi) &= (-1)^{\,n-\text{number of cycles in the cyclic decomposition of } \pi} \\ &= (-1)^{\,n-c(H)-c_1(H)-c_2(H)} = (-1)^{\,n-p(H)}\end{aligned}$$

and

$$\begin{aligned}& b_{1\pi(1)}\, b_{2\pi(2)} \cdots b_{n\pi(n)} \\ =& (1-\alpha)^{c_2(H)} \left(\prod_{v_i \in \mathcal{C}_2(H)} d_G(v_i) \right) (2\alpha-1)^{2c_1(H)} (2\alpha-1)^{n-2c_1(H)-c_2(H)} \\ =& (1-\alpha)^{c_2(H)} \left(\prod_{v_i \in \mathcal{C}_2(H)} d_G(v_i) \right) (2\alpha-1)^{n-c_2(H)}.\end{aligned}$$

Therefore,

$$\det(B_\alpha(G)) = \sum_H (-1)^{\,n-p(H)}\, 2^{\,c(H)}\, (1-\alpha)^{c_2(H)}\, (2\alpha-1)^{\,n-c_2(H)} \left(\prod_{v_i \in \mathcal{C}_2(H)} d_G(v_i) \right),$$

where summation is over all spanning modified elementary subgraphs H of G . □

In the next corollary, we obtain a Sachs-type formula for the coefficients of the characteristic polynomial of $B_\alpha(G)$.

Corollary 5.4. *Let $\phi(B_\alpha) = \lambda^n + a_1\lambda^{n-1} + a_2\lambda^{n-2} + \cdots + a_{n-1}\lambda + a_n$ be the characteristic polynomial of $B_\alpha(G)$. Then*

$$a_k = \sum_H (-1)^{\,p(H)}\, 2^{\,c(H)}\, (1-\alpha)^{c_2(H)}\, (2\alpha-1)^{\,n-c_2(H)} \left(\prod_{v_i \in \mathcal{C}_2(H)} d_G(v_i) \right),$$

where summation is over all modified elementary subgraphs H of G with k vertices.

Proof. The proof follows from Theorem 5.3 and recalling that c_k is $(-1)^k$ times the sum of $k \times k$ principal minors of $B_\alpha(G)$. □

One can observe that Proposition 5.1 can also be deduced as a consequence of the Theorem 5.3.

Corollary 5.5. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Also let $Q(G)$ be the signless Laplacian matrix of G. Then,*

$$\det(Q(G)) = \sum_H (-1)^{\,n-p(H)}\, 2^{\,c(H)} \left(\prod_{v_i \in \mathcal{C}_2(H)} d_G(v_i) \right),$$

where summation is over all spanning modified elementary subgraphs H of G.

Proof. Setting $\alpha = \frac{2}{3}$ in the formula (5.1) of Theorem 5.3, we obtain the result. □

Declaration of competing interest

There are neither conflicts of interest nor competing interests. The authors have no relevant financial interests.

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