Thank you!

We would like to thank everyone who has believed and still believes in this journal. We appreciate it because we know that it is difficult to trust a journal that is not listed in MathSciNet and zbMATH. It took us over a year to get listed by these important reviewing databases, and as of today none of the citations of our papers are counted by these databases. Nevertheless we have courageous authors who have entrusted us with their excellent research results. Our sincere thanks go to them. It would have been more professionally rewarding for them to select an established venue for their work. But they have chosen to support the birth of a new journal. It is a genuine sacrifice. We would like to thank the editors and referees for their valuable time in helping improve the quality of the published papers. What a great service to the mathematical community!

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Axiomatic characterization of transit functions of weak hierarchies*

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Abstract

Transit functions provide a unified approach to study notions of intervals, convexities, and betweenness. Recently, their scope has been extended to certain set systems associated with clustering. We characterize here the class of set systems that correspond to k-ary monotonic transit functions. Convexities form a subclass and are characterized in terms of transit functions by two additional axioms. We then focus on axiom systems associated with weak hierarchies as well as other generalizations of hierarchical set systems.

Keywords: Transit functions, convexities, weak hierarchies, axiom systems.

Math. Subj. Class.: 05C05, 05C99, 52A01

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1 Introduction

Transit functions have been introduced as unifying approach for results and ideas on intervals, convexities and betweenness in graphs and posets [25]. Formally, a *transit function* [25] on a non-empty set V is a function $R\colon V \times V \to 2^V$ satisfying the three axioms

(t1) $u \in R(u, v)$ for all $u, v \in V$.

(t2) $R(u, v) = R(v, u)$ for all $u, v \in V$.

(t3) $R(u, u) = \{u\}$ for all $u \in V$.

Transit functions capture an abstract notion of "betweenness", i.e., an element x is considered to be "between" u and v, if $x \in R(u, v)$. Several classes of interesting transit function associated with connected graphs have been studied from this perspective [15], among them the interval function [1, 24, 26], induced path function [12, 13, 23], the all paths function [11], the pre-fiber transit function [25], P_3-transit function [18]. Transit function also arose as models of recombination operators in genetics and evolutionary algorithms [16, 22, 27], where again, encapsulate the idea that offsprings are genetically "in-between" their parents.

Recently, they have also been applied to set systems naturally arising from clustering problems [9, 17]. Hierarchical structures play a key role in wide range of applications in the sciences. In [17] we considered properties of transit functions that are related to hierarchies and provided a characterization in terms of simple axioms. This begs the question whether or to what extent related systems of clusters are also within the explanatory range of transit functions. Weak hierarchies were introduced in [2, 3] as the system of "weak clusters" satisfying $s(a, b) > \min\{s(a, x), s(b, x)\}$ for all a, b within a cluster and x outside, and in [5] (with closure under pairwise intersection as additional condition). Subsequently, they have become a central structure in the theory of hierarchical clustering, see e.g. [8, 9]. They subsume a number of less general constructions such as paired hierarchies [6, 7] and pyramids [20]. In [4] systems of clusters are considered that are generated by two elements. These are, as we shall see, closely related to set systems identified by transit functions.

In particular in the context hierarchies, much of the previous work focuses the relationships of transit functions and convexities [8, 9], see also [4, 15, 25] on convexities in relation to graph-theoretical constructions. Here we take a somewhat different perspective and focus on axiom systems on transit functions giving raise to set systems such as those arising naturally in the context of clustering.

This contribution is organized as follows. We start by characterizing the set systems that are identified by transit function. Then we proceed to discussing convexities, giving a characterization of the transit functions that identify them. We then consider the transit functions arising from some hierarchy-like systems. Here we focus on weak hierarchies as well as properties discussed in our previous work [17]. We then generalize the results of Section 2 to k-ary transit functions. Finally we consider k-weak hierarchies. For $k > 2$ these are not identified by convexities but require the more general setting.

2 Set systems identified by transit functions

Throughout this contribution, V is a finite, non-empty set. Consider an arbitrary set system $\mathcal{X} \subseteq 2^V$ and the function

$$R_{\mathcal{X}}(x, y) = \bigcap\{A \in \mathcal{X} \mid x, y \in A\}. \tag{2.1}$$

We are interested here in those special classes of set systems that are *identified* by the function R, that is,

$$\mathcal{X} = \{R_{\mathcal{X}}(x, y) \mid x, y \in V\}. \tag{2.2}$$

We use the notation $\subset$ to mean proper subset, and write $\subseteq$ otherwise.

If $p, q \in R_{\mathcal{X}}(x, y)$ then by definition in every $A \in \mathcal{X}$ that contains x and y also contains p and q. Thus $R_{\mathcal{X}}$ satisfies the *monotone axiom* [13, 25]

(m) $p, q \in R(u, v)$ implies $R(p, q) \subseteq R(u, v)$.

The monotone axiom ***(m)*** can be expressed in the following equivalent form:

Lemma 2.1. *A transit function R is monotone if and only if, for all $u, v \in V$,*

$$\bigcap\{R(x, y) \mid u, v \in R(x, y)\} = R(u, v). \tag{2.3}$$

Proof. Condition ***(m)*** implies $R(u, v) \subseteq \bigcap\{R(x, y) \mid u, v \in R(x, y)\}$. By ***(t1)*** and ***(t2)*** we have $u, v \in R(u, v)$, hence $\bigcap\{R(x, y) \mid u, v \in R(x, y)\} \subseteq R(u, v)$ and thus Equation (2.3) holds. Conversely, from Equation (2.3) we immediately obtain $R(u, v) \subseteq R(x, y)$ for all x, y with $u, v \in R(x, y)$, i.e., ***(m)*** holds. □

Lemma 2.2. *A set system $\mathcal{X}$ is identified by a transit function R if and only if it satisfies the following axioms:*

(KS) $\{x\} \in \mathcal{X}$ *for all* $x \in V$.

(KR) *For every $C \in \mathcal{X}$ there are points $p, q \in C$ such that $p, q \in C'$ implies $C \subseteq C'$ for all $C' \in \mathcal{X}$.*

(KC) *For every $p, q \in V$ holds $\bigcap\{C \in \mathcal{X} \mid p, q \in C\} \in \mathcal{X}$.*

Proof. Suppose set system $\mathcal{X}$ is identified by a transit function R. Then the set system $\mathcal{X}$ satisfies ***(KS)***, since R satisfies ***(t3)***. By definition of R, $C \in \mathcal{X}$ implies $C = R(u, v) = \bigcap\{A \in \mathcal{X} \mid u, v \in A\}$ for some $u, v \in V$. Therefore, for $p, q \in V$ such that $p, q \in A$, it follows that $C \subseteq C'$, which proves that $\mathcal{X}$ satisfies ***(KR)***. Now, for every $p, q \in C \in \mathcal{X}$, $R(p, q) = \bigcap\{C \in \mathcal{X} \mid p, q \in C\}$ and hence $\mathcal{X}$ satisfies ***(KC)***.

Conversely, suppose that a set system $\mathcal{X}$ satisfies the axioms ***(KS)***, ***(KR)*** and ***(KC)***. To show that $\mathcal{X}$ is identified by a transit function, define a function $R\colon V \times V \to 2^V$ as $R_{\mathcal{X}}(x, y) = \bigcap\{A \in \mathcal{X} \mid x, y \in A\}$. Axioms ***(KS)*** and ***(KC)*** for $\mathcal{X}$ imply that this function R satisfies ***(t3)*** and ***(t1)***. Since R also satisfies ***(t2)*** by definition, we conclude that R is a transit function. Moreover, R satisfies ***(m)***. Now, we show that $\mathcal{X} = \{R_{\mathcal{X}}(x, y) \mid x, y \in V\}$. By axiom ***(KR)***, $C \in \mathcal{X}$, then there exists, $p, q \in C$ such that $p, q \in C'$ implies $C \subseteq C'$ for all $C' \in \mathcal{X}$, which implies that $C \subseteq \bigcap\{C \in \mathcal{X} \mid p, q \in C\}$, that is, $C \subseteq R_{\mathcal{X}}(p, q)$. On the other hand, $p, q \in C$ implies $R_{\mathcal{X}}(p, q) \subseteq C$, Thus every cluster C is a transit set, i.e. $\mathcal{X} \subseteq \{R_{\mathcal{X}}(p, q) \mid p, q\}$. By axiom ***(KC)***, $\{R_{\mathcal{X}}(x, y) \mid x, y \in V\} \subseteq \mathcal{X}$, which completes the proof. □

In this case R is the *canonical transit function* of $\mathcal{X}$ [25]. Condition ***(KR)*** is called 2-*arity* in [13]. If R is the *canonical transit function* of $\mathcal{X}$, then ***(KC)*** becomes

(m*) For all $u, v \in V$ there is $p, q \in V$ such that

$$\bigcap\{R(s, t) \mid s, t \in V \text{ and } u, v \in R(s, t)\} = R(p, q).$$

This can be seen as a relation of Equation (2.3), which stipulates not just the existence of $p, q \in V$ but insists that $\{p, q\} = \{u, v\}$. The example in Figure 1 shows that axiom ***(KC)*** is much weaker than closure under pairwise intersection. The set systems identified by transit functions therefore are not convexities in general. We will return to this point in the next section.

The independence of the axioms ***(KS)***, ***(KR)***, and ***(KC)*** is established by the following examples.

Example 2.3 (***(KS)*** but not ***(KR)*** or ***(KC)***)**.** For $V = \{a, b, c, d, e\}$ consider

$$\mathcal{X} = \big\{\{a\}, \{b\}, \{c\}, \{d\}, \{e\}, \{a, b, c\}, \{b, c, d\}, \{a, b, d\}, \{a, c, e\}\big\}.$$

For every pair of points $p, q \in \{a, b, c\}$ there is another set containing p and q that is not a superset of $\{a, b, c\}$:

$$a, b \in \{a, b, d\}, \quad a, c \in \{a, c, e\}, \quad \text{and} \quad b, c \in \{b, c, d\}.$$

Thus ***(KR)*** does not hold. Since $\{a, b, c\} \cap \{a, b, d\} = \{a, b\} \notin \mathcal{X}$, ***(KC)*** is not satisfied. On the other hand, all singletons are in $\mathcal{X}$, i.e., the $\mathcal{X}$ satisfies ***(KS)***.

Example 2.4 (***(KR)*** but not ***(KS)*** or ***(KC)***)**.** For $V = \{a, b, c, d, e\}$ consider

$$\mathcal{X} = \big\{\{a, b, c\}, \{a, b, d\}\big\}.$$

We can easily see that $\mathcal{X}$ satisfies ***(KR)***. Since no singleton is in $\mathcal{X}$, we can see that the set system fails to satisfy ***(KS)***. Now $\{a, b, c\}, \{a, b, d\} \in \mathcal{X}$, but $\{a, b, c\} \cap \{a, b, d\} = \{a, b\} \notin \mathcal{X}$. Hence $\mathcal{X}$ does not satisfy ***(KC)***.

Example 2.5 (***(KC*** but not ***(KS)*** or ***(KR)***)**.** For $V = \{a, b, c, d, e\}$ consider

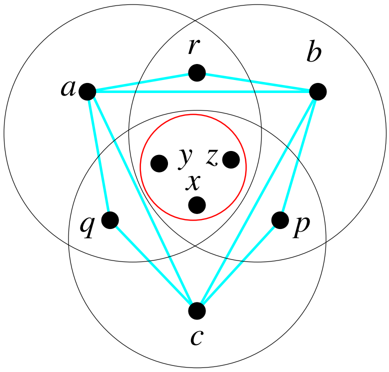
$$\mathcal{X} = \big\{\{a, b, c\}, \{b, c, d\}, \{a, b, d\}, \{a, c, e\}, \{a, b\}, \{b, c\}, \{a, c\}, \{b, d\}, \{a\}, \{b\}, \{c\}\big\}.$$

We can see that $\mathcal{X}$ satisfies ***(KC)***. For any pair of elements in $\{a, b, c\}$, there are the sets $\{b, c, d\}$, $\{a, b, d\}$, $\{a, c, e\}$ that contain a pair of $\{a, b, c\}$ but are not supersets of $\{a, b, c\}$. Hence $\mathcal{X}$ does not satisfy ***(KR)***. Also since no singleton is in $\mathcal{X}$, the set system fails to satisfy ***(KS)***.

Theorem 2.6. *There is a 1-1 correspondence between monotone transit functions R on V and set systems $\mathcal{X}$ satisfying* ***(KS)****,* ***(KR)****, and* ***(KC)*** *on V. This bijection is given by $\mathcal{X} \mapsto R_{\mathcal{X}}$ defined in Equation (2.1) and $\{R(p, q) \mid p, q \in V\} \mapsto \mathcal{X}$, respectively.*

Proof. Suppose $\mathcal{X}$ is a set system satisfying ***(KS)***, ***(KR)***, and ***(KC)*** with transit function R. By Lemma 2.2, $\mathcal{X} = \{R(u, v) \mid u, v \in V\}$. The transit function defined by Equation (2.1) satisfies ***(m)*** as argued above.

Now suppose R is a monotone transit function. Then by construction $\{R(p, q) \mid p, q \in V\}$ satisfies ***(KS)*** and ***(KR)***. Furthermore ***(m)*** implies ***(m*)***, which can be rewritten as ***(KC)*** using the fact that $\mathcal{X} = \{R(u, v) \mid u, v \in V\}$. $\square$



$\mathcal{X}$ consists of V, $\{u\}$ for $u \in V$, the nine pairs $\{a, r\}$, $\{a, q\}$, $\{b, r\}$, $\{b, p\}$, $\{c, p\}$, $\{c, q\}$, $\{a, b\}$, $\{b, c\}$, $\{a, c\}$ as well and the 18 pairs in $\{a, b, c, p, q, r\} \times \{x, y, z\}$, $A = \{a, r, q, x, y, z\}$, $B = \{b, p, r, x, y, z\}$, $C = \{c, p, q, x, y, z\}$, and $Z = \{x, y, z\}$.

Figure 1: In addition to the 27 defining pairs we have $R(a, p) = R(b, q) = R(c, r) = V$, $R(q, r) = A$, $R(r, p) = B$, $R(p, q) = C$, and $R(x, y) = R(x, z) = R(y, z) = Z$, accounting for all pairs in V. Hence it satisfies ***(KR)***. For each pair of points i, j, furthermore, the non-empty intersection of all sets containing them is again a member of $\mathcal{X}$. This is obvious for all intersections involving two-element sets in $\mathcal{X}$. In the remaining cases yield the transit sets listed above. The pairwise intersections $A \cap B$, $A \cap C$, and $B \cap C$, however, are not members of $\mathcal{X}$: any pair in these sets has as intersection of its containing sets either that pairs or Z.

Definition 2.7. A set system $\mathcal{X}$ satisfying ***(KS)***,

(K0) $\emptyset \notin \mathcal{X}$, and

(K1) $V \in \mathcal{X}$

is called a *clustering system* [4].

In the terminology of [4], a *clustering system* is *pre-binary* if, for every $u, v \in V$ the set system $\{C \in \mathcal{X} \mid u, v \in C\}$ has exactly one inclusion-minimal element, i.e., in our language, if every transit set is a cluster. The proof of Lemma 2.2 shows that this condition is equivalent to ***(KR)***. A cluster system is called *binary* if it is pre-binary and every cluster is a transit set. The latter condition is equivalent to ***(KC)***. We can summarize this discussion as

Corollary 2.8. *A set system $\mathcal{X}$ is a binary clustering system if and only if it satisfies **(K0)**, **(K1)**, **(KS)**, **(KR)**, and **(KC)**.*

Axiom ***(K1)*** can trivially be translated into the language of transit functions as

(a') There is $u, v \in V$ such that $R(u, v) = V$.

Thus we also have

Corollary 2.9. *A transit function identifies as a binary clustering system if and only if it satisfies **(m)** and **(a')**.*

3 Transit functions of convexities

A systems of sets $\mathcal{K} \subset 2^V$ that contains V and is closed under intersection is called a *convexity*. Usually, one requires the empty set $\emptyset$ to be part of a convexity. However, $\emptyset$ cannot be a transit set according to ***(t1)***. It is convenient in our context, therefore, to use a slightly modified definition, excluding the empty set and restricting closure to non-empty intersection. Furthermore, ***(t3)*** implies that $\{x\}$ is a transit set for every $x \in V$. Thus we are only interested in set systems that contain the singletons.

Definition 3.1. A *convexity* is a set system $\mathcal{X} \subseteq 2^V$ satisfying ***(K0)***, ***(K1)***, and

(K2) if $A, B \in \mathcal{X}$ and $A \cap B \neq \emptyset$ then $A \cap B \in \mathcal{X}$.

A set system is *closed (under pairwise intersection)* if it satisfies ***(K2)***. A convexity is called *grounded* if it satisfies ***(KS)***. Thus grounded convexities are the same as closed clustering systems. Closure under non-empty intersections, ***(K2)***, immediately implies ***(KC)***, but the converse is not true, as we have seen in Figure 1.

The following result from [14] is now a direct consequence of Lemma 2.2:

Proposition 3.2. *A convexity $\mathcal{X}$ is identified by a monotone transit function R if and only if it is grounded (that is, $\mathcal{X}$ satisfies **(KS)**), and satisfies **(KR)**.*

It is now easy to characterize the transit functions that identify convexities:

Lemma 3.3. *Let R be a monotone transit function. Then the transit sets $\{R(p, q) \mid p, q \in V\}$ form a convexity if and only R satisfies **(a')** and*

(m') *For all $u, v, x, y \in V$ with $R(u, v) \cap R(x, y) \neq \emptyset$, there is $p, q \in V$ such that $R(u, v) \cap R(x, y) = R(p, q)$.*

Proof. Note that by assumption there is a 1-1 correspondence between transit sets and the sets $C \in \mathcal{X}$. Thus ***(a')*** and ***(m')*** directly translate to ***(K1)*** and ***(K2)***, respectively. $\square$

Axiom ***(m')*** was introduced in [17] in the context of hierarchies. It is clear that ***(m')*** implies ***(m*)***, it does not imply ***(m)***, however. The example in Figure 1 also shows that ***(m*)*** does not imply ***(m')***.

Figure 2 gives a smaller counterexample. The interval function of a graph G with vertex set V, defined by $I(x, y) = \{z \in V \mid z \text{ lies on some shortest path between } x \text{ and } y\}$, is not monotone in general [26]. In other words, the collection of intervals is in general not sufficient to determine the "end points" of the interval.

4 Transit functions of hierarchy-like systems

Consider the following axioms for a set system $\mathcal{X} \subseteq 2^V$.

(H) $A, B \in \mathcal{X}$ implies $A \cap B \subseteq \{A, B, \emptyset\}$.

(PH) $A \in \mathcal{X}$ properly intersects at most one $B \in \mathcal{X}$.

(WH) $A, B, C \in \mathcal{X}$ implies $A \cap B \cap C \subseteq \{A \cap B, A \cap C, B \cap C\}$.

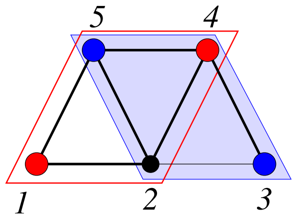


Figure 2: The interval function I of the graph G consists of singletons, a pairs with the exception of $I(1,3) = \{1,2,3\}$ (a path), $I(1,4) = \{1,2,4,5\}$ (red), and $I(3,5) = \{2,3,4,5\}$. One easily checks that I satisfies ***(m)***. For the transit sets thus ***(K0)***, ***(KS)***, ***(KR)***, and ***(KC)*** are satisfied. The pairwise intersection $I(1,4) \cap I(3,5) = \{2,4,5\}$, however is not an interval, and hence ***(K2)*** fails. Furthermore, ***(a')*** fails since $\{1,2,3,4,5\}$ is not a transit set.

A set system is called *paired hierarchical* [7] if it satisfies ***(K0)***, ***(K1)***, and ***(PH)***. If it satisfies in addition ***(WH)***, it is called a *weak hierarchy*, if ***(H)*** holds, it is a *hierarchy*. It is well known (and easy to see) that ***(H)*** implies ***(PH)*** implies ***(WH)***. Furthermore ***(H)*** implies ***(K2)***. In the following we will sometimes write $\mathfrak{W}$ instead of $\mathcal{X}$ for set systems that are weak hierarchies.

Among several hierarchy-like set systems considered in the literature, see e.g. [8, 9], the paired hierarchies are the most restrictive one, while the weak hierarchies are the most general model. In the following we show that weak hierarchies, and hence also all its more restrictive subclasses such as the paired hierarchies, are identified by transit functions if and only if they form a convexity.

Proposition 4.1 ([21]). ***(WH)*** *implies* ***(KR)***.

Lemma 4.2. *The canonical transit function R of a weak hierarchy $\mathcal{X}$ satisfies* ***(m')***.

Proof. By construction $R(p,q) = \bigcap\{C \in \mathcal{X} \mid p,q \in C\} = \bigcap_{i=1}^{h} C_i$ with $C_i \in \mathcal{X}$ for $1 \leq i \leq h$ and some $h \geq 1$. By axiom ***(WH)***, the intersection of any three sets C_i can be replaced by a pair, hence $R(p,q) = C' \cap C''$ for two not necessarily distinct sets $C', C'' \in \mathcal{X}$.

It was shown in [2] that $\mathcal{X}$ is a weak hierarchy if and only if its closure under pair-wise intersection is a weak hierarchy. Denote this weak hierarchy by $\overline{\mathcal{X}}$. Since ***(KR)*** holds for $\mathcal{X}$ it follows that $C \in \mathcal{X}$ implies $C \in \overline{\mathcal{X}}$, since every $C \in \mathcal{X}$ has points r,s that otherwise appear only in supersets of C, and thus any intersection of sets in $\mathcal{X}$ that contains r,s also contains C. Since $\mathcal{X}$ is again a weak hierarchy, all pairwise intersections $C' \cap C'' \in \overline{\mathcal{X}}$ also contain points u,v such that every set $u,v \in D \in \overline{\mathcal{X}}$ satisfies $C' \cap C'' \subseteq D$. Since all sets D are intersections of elements of $\mathcal{X}$ containing u,v, we have $C' \cap C'' = R(u,v)$. Thus all elements of $\mathcal{X}$ and their pairwise intersections are transit sets of R. In other words, $\{R(p,q) \mid p,q \in \mathcal{X}\} = \overline{\mathcal{X}}$. Thus R satisfies ***(m')***. □

Since R satisfies ***(m)***, ***(m')***, and by construction also ***(a')***, Lemma 3.3 and Lemma 4.2 together imply

Corollary 4.3. *The canonical transit function of a weak hierarchy is a convexity.*

A similar result was shown with a different approach in [9]. This is in particular also true of hierarchies [17] and paired hierarchies [9].

Because of the 1-1 correspondence between the clusters of a closed weak hierarchy $\mathcal{W}$ and the transit sets of R, we can directly translate ***(KW)*** to the language of transit sets

(w) For any six points $p, q, r, s, t, u \in V$ holds

$$R(p,q) \cap R(r,s) \cap R(t,u) \in \{R(p,q) \cap R(r,s), R(p,q) \cap R(t,u), \\ R(r,s) \cap R(t,u)\}.$$

Summarizing our discussion so far we have

Corollary 4.4. *R identifies as a closed weak hierarchy if and only if it satisfies **(m)**, **(m')**, **(a')**, and **(w)**.*

Using a different route, [9] showed that a convexity is a weak hierarchy if and only if its transit function satisfies

(w') There are not three distinct points $x_1, x_2, x_3 \in V$ such that for all $\{h, i, j\} = \{1, 2, 3\}$ holds $x_h \notin R(x_i, x_j)$.

In Section 6 we prove in the more general setting of k-ary transit functions that for a monotone transit function that ***(w')*** implies ***(a')*** (Lemma 6.4) and ***(a')*** $\wedge$ ***(w)*** implies ***(w)*** (Lemma 6.7).

Corollary 4.5. *R identifies as a closed weak hierarchy if and only if it satisfies **(m)**, **(m')**, and **(w')**.*

The independence of the axioms is established by the following examples.

Example 4.6 (***(m)***, ***(m')***, and ***(a')***, but not ***(w)***)**.** For $V = \{a, b, c, d, e\}$ consider

$$R(x,x) = \{x\} \text{ for all } x \in V, \qquad R(a,b) = V, \quad \text{and} \\ R(x,y) = \{x,y\} \text{ for all other pairs.}$$

We can easily see that R satisfies ***(m)***, ***(m')***, and ***(a')***. We have

$$R(b,c) \cap R(c,d) \cap R(b,d) = \emptyset$$

but

$$R(b,c) \cap R(c,d) = \{c\}, \\ R(b,c) \cap R(b,d) = \{b\}, \text{ and} \\ R(c,d) \cap R(b,d) = \{d\}.$$

Therefore ***(w)*** does not hold.

Example 4.7 (***(m')***, ***(a')***, and ***(w)***, but not ***(m)***)**.** For $V = \{a, b, c, d, e\}$, let

$$R(x,x) = \{x\} \text{ for all } x \in V, \qquad R(a,b) = \{a,b,c,d\}, \\ R(b,c) = \{b,c,d\}, \qquad R(b,d) = \{b,d\},$$

and for all other pair $R(x,y) = V$. We observe that R satisfies ***(m')***, ***(a')***, and ***(w)***. However, ***(m)*** fails since $c, d \in R(a,b)$ and $e \in R(c,d)$, but $e \notin R(a,b)$.

Example 4.8 (***(m)***, ***(a')***, and ***(w)***, but not ***(m')***)**.** For $V = \{a, b, c, d, e\}$ consider

$$\begin{array}{ll} R(a,c) = V, & R(a,b) = \{a,b\}, \\ R(a,d) = V - \{c\}, & R(a,e) = \{a,e\}, \\ R(b,x) = \{b,x\} \text{ for all } x \in V, & R(c,d) = \{c,d\}, \\ R(c,e) = V - \{a\}, \text{ and} & R(d,e) = \{d,e\}. \end{array}$$

It can be verified that R satisfies ***(m)***, ***(a')***, and ***(w)***. But

$$R(a,d) \cap R(c,e) = \{b,d,e\} \neq R(x,y)$$

for each pair of elements $x, y \in V$. Hence R does not satisfy ***(m')***.

Example 4.9 (***(m)***, ***(m')***, and ***(w)***, but not ***(a')***)**.** For $V = \{a, b, c, d\}$ consider

$$\begin{array}{ll} R(a,b) = \{a,b\}, & R(a,c) = \{a,b,c\}, \\ R(a,d) = \{a,b,d\}, & R(b,c) = \{b,c\}, \\ R(b,d) = \{b,d\}, \text{ and} & R(c,d) = \{c,d\}. \end{array}$$

We can easily see that R satisfies ***(m)***, ***(m')***, ***(w)***. However, there is no pair of points $x, y \in V$ such that $R(x,y) = V$; hence R does not satisfy ***(a')***.

Barthélemy and Brucker [4] call a clustering system *strongly binary* if it satisfies ***(KR)*** and

(ST) For each $S \subseteq V$, $S \neq \emptyset$, there exist $u, v \in S$ such that $S \subseteq \bigcap \{C \mid u, v \in C\}$.

and show that the strongly binary clustering systems are exactly the closed weak hierarchies. We note that ***(ST)*** implies ***(KC)*** by restricting the sets S to at most two elements.

In [9] it is shown that R is the transit function of paired hierarchy if it satisfies

(ph) For all $u, v \notin R(x,y)$ holds both $x \notin R(u,y)$ implies $y \in R(v,x)$; and $v \notin R(u,y)$ implies $x \in R(v,y)$.

We note that in [9] this condition is mistakenly stated for "pairwise distinct u, v, x, y". It is also necessary to check the implications for $u = v$, however. In addition, if $x = y$, the first precondition is always false, while the second conditions implies $x \in R(u,x)$, which is always true by ***(t1)***. This it suffices to drop the qualifier "pairwise distinct".

Corollary 4.10. *R identifies a closed paired hierarchy if and only if it satisfies* ***(m)***, ***(m')***, ***(a')***, *and* ***(ph)***.

4.1 Independence of *(m)*, *(m')*, *(a')* and *(ph)*

Example 4.11 (***(m)***, ***(m')***, and ***(a')***, but not ***(ph)***)**.** Let $V = \{a, b, c, d, e\}$ and define R on V as follows: $R(a,b) = V$, and for all other pair of elements $x, y \in V$ we set $R(x,y) = \{x,y\}$. It is not difficult to check that R satisfies ***(m)***, ***(m')***, and ***(a')***. For $R(c,d)$ we have $a, b \notin R(c,d)$ but $a \notin R(c,b)$ and $b \notin R(a,d)$; $d \notin R(c,b)$ and $a \notin R(d,b)$. Thus R does not satisfy the axiom ***(ph)***.

Example 4.12 (*(m)*, *(m')*, and *(ph)*, but not *(a')*)**.** Let $V = \{a, b, c, d\}$ and define R on V as follows:

$$R(x,x) = \{x\} \text{ for all } x \in V, \qquad R(a,b) = \{a,b,c\},$$
$$R(a,c) = \{a,c\}, \qquad R(b,c) = \{b,c\},$$
$$R(a,d) = \{a,c,d\} = R(c,d), \text{ and} \qquad R(b,d) = \{b,d\}.$$

It is easy to verify that R satisfies *(m)*, *(m')* and *(ph)*, but there is no $x, y \in V$ such that $R(x,y) = V$.

Example 4.13 (*(m)*, *(a')*, and *(ph)*, but not *(m')*)**.** For $V = \{a, b, c, d, e\}$ define $R\colon V \times V \to 2^V$ as follows:

$$R(x,x) = \{x\} \text{ for all } x \in V, \qquad R(a,b) = \{a,b\},$$
$$R(a,c) = \{a,c\}, \qquad R(a,d) = R(c,d) = \{a,b,c,d\},$$
$$R(a,e) = R(b,e) = R(c,e) = \{a,b,c,e\}, \qquad R(b,c) = \{b,c\},$$
$$R(b,d) = \{b,d\}, \text{ and} \qquad R(d,e) = V.$$

We have $R(a,d) \cap R(a,e) = \{a,b,c\}$ and $R(x,y) \neq \{a,b,c\}$ for all $x, y \in V$. Therefore R does not satisfy *(m')*. The transit sets $R(a,b)$, $R(a,c)$, $R(b,c)$, and $R(b,d)$ are subsets of $R(a,d) = R(c,d)$. Likewise, $R(a,b)$, $R(a,c)$, and $R(b,c)$ are subsets of $R(a,e) = R(b,e) = R(c,e)$. Thus R satisfies the axiom *(m)*. Furthermore, R satisfies *(a')* because $R(d,e) = V$. In order to verify *(ph)* we observe the following:
$c, d \notin R(a,b)$: we check that $a \notin R(b,c) \Rightarrow b \in R(a,d)$ and $d \notin R(b,c) \Rightarrow a \in R(b,d)$.
$c, e \notin R(a,b)$: we check that $a \notin R(b,c) \Rightarrow b \in R(a,e)$ and $d \notin R(b,c) \Rightarrow a \in R(b,e)$.
$d, e \notin R(a,b)$: we check that $a \in R(b,d)$ and $e \notin R(b,d) \Rightarrow a \in R(b,e)$.
$b, d \notin R(a,c)$: we check that $a \notin R(b,c) \Rightarrow c \in R(a,d)$ and $d \notin R(b,c) \Rightarrow a \in R(c,d)$.
$b, e \notin R(a,c)$: we check that $a \notin R(b,c) \Rightarrow c \in R(a,e)$ and $e \notin R(b,c) \Rightarrow a \in R(c,e)$.
$d, e \notin R(a,c)$: we check that $a \in R(c,d)$ and $e \notin R(c,d) \Rightarrow c \in R(d,e)$.

Example 4.14 (*(m')*, *(a')*, and *(ph)*, but not *(m)*)**.** Let $V = \{a, b, c, d\}$,

$$R(a,c) = \{a,b,c\}, \qquad R(x,x) = \{x\}$$

and $R(x,y) = V$ for all other pairs. Since $b \in R(a,c)$ and $R(a,b) = V \nsubseteq R(a,c)$, R does not satisfy axiom *(m)*. We can easily prove that the other axioms hold.

Let us now return to the convexities identified by a transit function. Condition *(a')* can be seen as a weak version of the axiom of antipodality

(a) For every $x \in V$ there is $\bar{x} \in V$ such that $R(x, \bar{x}) = V$.

It is satisfied in particular by hierarchies. Since the restriction of a (weak) hierarchy to one of its clusters is again a (weak) hierarchy, the following axiom also holds for hierarchies:

(a") For every $u, v \in V$ and $x \in R(p,q)$ there is $\bar{x} \in V$ such that $R(x, \bar{x}) = R(u,v)$.

Axiom *(a)*, and thus *(a")* does not hold for weak hierarchies in general, as the following counter-example shows. Suppose $C_1, C_2 \in \mathcal{W}$ are proper subsets of $V \in \mathcal{W}$ such that $C_1 \cup C_2 = V$ and $C_1 \cap C_2 = C_3 \in \mathcal{W}$. Choose $x \in C_3$, then $R(x,y) \subseteq C_1$ for

$y \in C_1$ and $R(x, y) \subseteq C_2$ for $y \in C_2$. Since $C_1 \cup C_2 = V$, there is no $\bar{x} \in V$ such that $R(x, \bar{x}) = V$. In fact, the set system $\mathcal{W}$ is even a paired hierarchy, since the only proper intersection is $C_1 \cap C_2$. Hence paired hierarchies, the most restrictive relaxation of a hierarchy studied in some detail in the literature [7], also do not satisfy ***(a")***.

Axiom ***(a")*** can be translated into conditions of the clusters of $\mathcal{W}$

Lemma 4.15. *Let $\mathcal{X}$ be a set system identified by a transit function R. Then R satisfies* ***(a")*** *if and only if $\mathcal{X}$ satisfies*

(KA) *For every $C \in \mathcal{X}$ and every collection $\mathcal{Q}_C \subseteq \{C' \in \mathcal{X} \mid C' \subset C\}$ with non-empty intersection $\bigcap_{C' \in \mathcal{Q}_C} C' \neq \emptyset$ holds $\bigcap_{C' \in \mathcal{Q}_C} C' \neq C$.*

Proof. Due to the correspondence of transit sets and members of $\mathcal{X}$, ***(a")*** is equivalently expressed as: For all $C \in \mathcal{X}$ and all $x \in C$, there is $\bar{x} \in C$ such that $\{x, \bar{x}\} \not\subseteq C'$ for any $C' \subset C$. Equivalently, the union of all $C' \subset C$ that contain any given x is a proper subset of C, which in turn is equivalent to ***(KA)***. □

In [17] we considered the axioms

(h') $x \in R(u, v) \Rightarrow R(u, x) = R(u, v)$ or $R(x, v) = R(u, v)$.

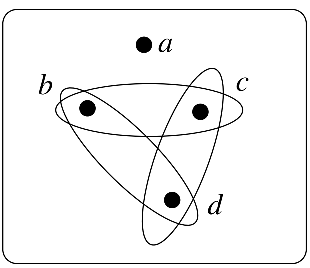
(h") $x \in R(u, v) \Rightarrow R(u, v) = R(u, x) \cup R(x, v)$.

Lemma 4.16. ***(h')*** $\wedge$ ***(m)*** *is equivalent to* ***(h")*** $\wedge$ ***(a")***.

Proof. We showed in [17] that ***(h")*** follows from ***(h')*** and monotone axiom. Furthermore, ***(h')*** implies ***(a")***: for given u, v and x we may choose $\bar{x} = u$ or $\bar{x} = v$.

Conversely, by ***(a")***, for every $x \in R(u, v)$ there is $\bar{x}$ in $R(u, v)$ such that $R(x, \bar{x}) = R(u, v)$. By ***(h")***, $R(u, x) \cup R(x, v) = R(u, v)$, hence $\bar{x} \in R(u, x)$ or $\bar{x} \in R(x, v)$, i.e., $R(u, v) \subseteq R(x, \bar{x}) \subseteq R(u, x)$ or $R(u, v) \subseteq R(x, \bar{x}) \subseteq R(x, v)$, i.e., ***(h')*** is satisfied. It was shown in [17] that ***(h")*** implies ***(m)***. □

The example in Figure 3 shows that ***(h")*** and ***(a")*** together are still insufficient to turn the transit sets into even a weak hierarchy.



R(a,b)=R(a,c)=R(a,d)={a,b,c,d}

R(b,c)={b,c}

R(c,d)={c,d}

R(b,d)={b,d}

Figure 3: The transit function R satisfies ***(m)***, ***(m')***, ***(a")***, and ***(h')***. It is not a weak hierarchy since $R(b, c) \cap R(b, d) \cap R(c, d) = \emptyset$ but the three pairwise intersection each contain a point, and thus also not a hierarchy.

5 Transit functions with arity > 2

Transit function or 2-ary functions have been generalized to k arguments to generalize convexities generated by k-ary functions [14]. For n-ary convexities, also refer [28].

Definition 5.1. A function $R\colon \underbrace{V \times V \ldots \times V}_{k \text{ times}} \to 2^V$ is a transit function of arity k (or k-ary transit function) on V if R satisfies the following axioms:

(kt1) $u_1 \in R(u_1, u_2, \ldots, u_k)$;

(kt2) $R(u_1, u_2, \ldots, u_k) = R(\pi(u_1, u_2, \ldots, u_k))$ for all $u_i \in V$, where $\pi(u_1, u_2, \ldots, u_k)$ is any permutation of $(u_1, u_2, \ldots, u_k)$;

(kt3) $R(u, u, \ldots, u) = \{u\}$ for all $u \in V$.

For an arbitrary set system $\mathcal{X}$ we define the k-ary function $R_{\mathcal{X}}\colon V^k \to 2^V$ by

$$R_{\mathcal{X}}(u_1, u_2, \ldots, u_k) = \bigcap \{A \in \mathcal{X} \mid u_1, u_2, \ldots, u_k \in A\}. \tag{5.1}$$

As in the case $k = 2$, the function R is monotone by construction, i.e., it satisfies

(km) For every $x_1, \ldots, x_k \in R(u_1, \ldots, u_k)$ holds $R(x_1, \ldots, x_k) \subseteq R(u_1, \ldots, u_k)$,

which in turn implies

(km*) For very $T = \{t_1, \ldots, t_k\}$ there is $Q = \{q_1, \ldots, q_k\}$ such that

$$\bigcap \{R(u_1, \ldots, u_k) \mid u_1, \ldots, u_k \in V \text{ and } T \in R(u_1, \ldots, u_k)\} = R(q_1, \ldots, q_k).$$

We are again interested in the case that the transit sets of R identify the set system $\mathcal{X}$, i.e.,

$$\mathcal{X} = \{R_{\mathcal{X}}(u_1, u_2, \ldots, u_k) \mid u_1, u_2, \ldots, u_k \in V\}. \tag{5.2}$$

Furthermore we consider the following generalizations of axioms ***(KR)*** and ***(KC)***:

(kKR) For all $C \in \mathcal{X}$ there is a set $T \subseteq C$ with $|T| \leq k$ such that $T \subseteq C'$ implies $C \subseteq C'$ for all $C' \in \mathcal{X}$.

(kKC) For every $T \subseteq V$ with $|T| \leq k$ holds $\bigcap \{C \in \mathcal{X} \mid T \subseteq C\} \in \mathcal{X}$.

Condition ***(kKR)*** was introduced in [14]. A necessary condition for R to explain $\mathcal{X}$ is that every set $C \in \mathcal{X}$ is identified by at most k distinct points. The following statement is a generalization of Lemma 2.2 and Theorem 2.6.

Theorem 5.2. *A set system $\mathcal{X} \subseteq 2^V$ is identified by a k-ary transit function if and only if $\mathcal{X}$ satisfies **(KS)**, **(kKC)**, and **(kKR)**. Conversely, a k-ary transit function identifies a set system if and only if R satisfies **(km)**.*

Proof. We argue in parallel with the proof of Lemma 2.2. First we note that ***(kt3)*** and ***(KS)*** ensure that $\mathcal{X}$ and the collection of transit sets both contain all singletons. As shown in [14], ***(kKR)*** is equivalent to $\mathcal{X} \subseteq \{R(u_1, \ldots, u_k) \mid u_1, \ldots, u_k \in V\}$. Property ***(km*)*** and the definition R together imply that ***(kKC)*** is equivalent to $\{R(u_1, \ldots, u_k) \mid u_1, \ldots, u_k \in V\} \subseteq \mathcal{X}$. The k-ary transit function defined by $\mathcal{X}$ is monotone. Conversely, one easily checks that the transit sets of a monotone k-ary transit function satisfy ***(KS)***, and ***(kKC)*** (by rewriting ***(km*)***), and ***(kKR)*** holds by construction. □

For a given set system $\mathcal{X}$, the minimal value of k for which ***(kKR)*** holds is called the *arity* of $\mathcal{X}$ [14].

Let $\mathcal{X}$ be a convexity on V. For a subset $S \subseteq V$, the smallest convex set containing S is the *convex hull* of S, denoted by

$$\langle S \rangle_{\mathcal{X}} = \bigcap \{C \in \mathcal{X} \mid S \subseteq C\}. \tag{5.3}$$

Basic concept from the theory of convexities can be generalized to arbitrary set systems:

Definition 5.3. Let $\mathcal{X} \subseteq 2^V$ be a set system. For every subset $S \subseteq V$, the closure of S with respect to a subset T (T-closure of S) is the set

$$\langle S \rangle_T = \bigcap \{C \in \mathcal{X} \mid S \subseteq C \text{ and } T \subseteq C\}. \tag{5.4}$$

Note that in general $\langle S \rangle_T \notin \mathcal{X}$. Interesting set systems arise by requiring $\langle S \rangle_T \in \mathcal{X}$ for all $S \subseteq V$ and certain sets T.

Definition 5.4. Let $\mathcal{X} \subseteq 2^V$. A set $S \subseteq V$ containing a subset T is $\mathcal{X}_T$*-independent* (T-independent) if $x \notin \bigcap \{C \in \mathcal{X} \mid T \subseteq (S \setminus \{x\}) \subseteq C\}$ holds for all $x \in S$. Otherwise S is T-dependent. In other words S is T-dependent if $x \in \langle S \setminus \{x\} \rangle_T$, for all $x \in S$. The T-rank $r(\mathcal{X})_T$ is the maximum cardinality of an $\mathcal{X}_T$-independent set S in V.

We can generalize the definition of well-known convexity invariants such as Carathéodory number with respect to the T-closure in a set system $\mathcal{X}$ identified with a k-ary transit function as follows.

Definition 5.5. The T*-Carathéodory number* c of a set system $\mathcal{X}$ is the smallest integer c (if it exists) such that for any finite subset F of V containing T, we have

$$\langle F \rangle_{\mathcal{X}_T} = \bigcup \{\langle S \rangle_{\mathcal{X}} \mid T \subseteq S \subseteq F, |S| \leq c\}. \tag{5.5}$$

The usual definition of the *Carathéodory number* is recovered by dropping the restrictions on T.

The *arity of a convexity* [14] is the smallest integer (which exists since V is finite in our setting) such that

$$\mathcal{X} = \{C \subseteq V \mid F \subset C, |F| \leq c \text{ implies } \langle F \rangle_{\mathcal{C}} \subseteq C\}. \tag{5.6}$$

By axiom ***(K2)***, $\langle S \rangle_{\mathcal{X}} \in \mathcal{X}$. Furthermore, ***(K2)*** implies ***(kKC)*** and every set system satisfies ***(kKR)*** for sufficiently large k. Every grounded convexity $\mathcal{X}$ is therefore identified by a transit function with sufficient arity. More precisely we have

Proposition 5.6 ([14])**.** *$\mathcal{X}$ is a grounded convexity on V of arity k if and only if $\mathcal{X}$ is identified by a k-ary transit function R on V.*

Lemma 5.7. *The k-ary transit function R identifies a convexity if and only if it satisfies **(km)** and the following two conditions:*

- ***(ka')*** *There are vertices $u_1, u_2, \ldots, u_k$ such that $R(u_1, u_2, \ldots, u_k) = V$.*
- ***(km')*** *If $R(u_1, u_2, \ldots, u_k) \cap R(v_1, v_2, \ldots, v_k) \neq \emptyset$ then there is $x_1, x_2, \ldots, x_k$ such that $R(u_1, u_2, \ldots, u_k) \cap R(v_1, v_2, \ldots, v_k) = R(x_1, x_2, \ldots, x_k)$.*

Proof. Monotonicity follows directly from the construction of R in Equation (5.1). Condition ***(km')*** states closure w.r.t. to intersection, i.e., is equivalent to ***(K2)***, and axiom ***(ka')*** is equivalent to ***(K1)***. □

6 k-weak hierarchies

We now turn to k-weak hierarchies [3, 10, 19] as a generalization of weak hierarchies.

Definition 6.1. A *k-weak hierarchy* on V is a set system $\mathcal{X} \in 2^V$ so that ***(K0)***, ***(K1)***, ***(KS)*** and one of the two equivalent conditions

(kWH) $A_1, A_2, A_3, \dots, A_{k+1} \in \mathcal{W}$ implies $\displaystyle\bigcap_{i=1}^{k+1} A_i \subseteq \left\{ \bigcap_{i=1, i\neq j}^{k} A_i \,\middle|\, 1 \le j \le k+1 \right\}$.

(kWH') There are no $k+1$ elements $x_1, \dots, x_{k+1}$ such that $x_i \in A_j$ iff $i \neq j$.

is satisfied.

The equivalence of ***(kWH)*** and ***(kWH')*** is established in [3, 19]. A k-weak hierarchy is closed (w.r.t. intersection) if in addition ***(K2)*** is satisfied. It is clear that a closed k-weak hierarchy is a convexity.

In the following we write $x_1, \dots, \widehat{x_i}, \dots, x_{k+1}$ for sequence that leaves out x_i, i.e., $x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{k+1}$.

Lemma 6.2. *If the set system $\mathcal{X}$ is a closed k-weak hierarchy, then its rank satisfies $r(\mathcal{X}) \le k$.*

Proof. Let $x_1, \dots, x_{k+1}$ be distinct $k+1$ convexly independent points. Hence $x_i \notin \langle x_1, x_2, \dots, \widehat{x_i}, \dots, x_{k+1} \rangle_{\mathcal{X}}$. Let $C_i = \langle x_1, x_2, \dots, \widehat{x_i}, \dots, x_{k+1} \rangle_{\mathcal{X}}$. Then $x_i \notin \cap C_j$ for $i = 1, \dots, k+1$. But some $x_i \in \bigcap_{i\neq j}^{k+1} C_j$. This is a contradiction to $\mathcal{X}$ being a closed k-weak hierarchy. □

It can be verified that if $\mathcal{X}$ is a closed k-weak hierarchy, then the Helly number and Carathéodory number of $\mathcal{X}$ is at most k.

Without recourse to the theory of convexities we can prove directly

Lemma 6.3. *A k-weak hierarchy satisfies **(kKR)**.*

Proof. First consider an arbitrary set system $\mathcal{X} \subseteq 2^V$ and fix a set $C \in \mathcal{X}$. Let $T \subseteq C$ be a set of minimum cardinality with the property that $T \subseteq C'$ implies $C \subseteq C'$ for all $C' \in \mathcal{X}$. Then for each $a \in T$ there is a set C_a such that $a \notin C_a$ and $T \setminus \{a\} \subseteq C_a$. This statement is a simple consequence of the minimality of T: For every $a \in T$, there must be sets $C' \in \mathcal{X}$ not containing C that do not contain a. Otherwise a could be removed from T, contradicting minimality. Now consider the set $\mathcal{X}_a$ of clusters that do not contain a. Suppose none of them contain $T \setminus \{a\}$. Then $C' \in \mathcal{X}_a$ also lacks some other element of $a' \in T$ and hence is recognizable as not containing C by virtue of a'. Thus a can be removed from T, contradicting minimality of T.

Now let $\mathcal{X}$ be a k-weak hierarchy.

Suppose there is a $C \in \mathcal{X}$ such that the minimal set T has cardinality $|T| \ge k+1$. Then there are at least $k+1$ distinct points a_i and corresponding clusters $C_i \in \mathcal{W}$ with $a_i \notin C_i$ and $T \setminus \{a_i\} \subseteq C_i$. The intersection $\bigcap_{i=1}^{k+1} C_i$ contains none of the a_i. By Axiom ***(kWH)***, however, this intersection can be written as the intersection of at most k of these clusters, and thus must contain at least one of the a_i, a contradiction. Thus the cardinality of T is at most k and the lemma follows. □

The set system defined by the transit sets is not necessarily a convexity. We can conclude, however, that every transit set of a k-weak hierarchy is the intersection of at most k others. We can generalize the notion of convex hulls and convex independence using the concept of a weak closure, we can show that for k-weak hierarchies, the axiom ***(kw')*** can be extended.

Now consider the following axioms:

(kw) For any $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{k+1} \in V^k$ holds

$$\bigcap_{i=1}^{k+1} R(\mathbf{x}_i) \subseteq \left\{ \bigcap_{i=1, i\neq j}^{k+1} R(\mathbf{x}_i) \;\middle|\; 1 \leq j \leq k+1 \right\}.$$

(kw') For every set of $k+1$ distinct points $x_1, \dots, x_{k+1} \in V$ holds

$$x_i \in R(x_1, x_2, \dots \widehat{x_i}, \dots, x_{k+1}).$$

Lemma 6.4. *Axioms **(kw')** and **(km)** imply **(a')**.*

Proof. Consider a set V with at least $k+1$ elements and let R be any k-ary transit function on V. If we have $R(x_1, \dots, x_k) = V$, we are done. Otherwise, there exists an element $x_{k+1} \in V$ that is not in $R(x_1, \dots, x_k)$. By axiom ***(kw')*** there exists i such that $x_i \in R(x_1, \dots, \widehat{x_i}, \dots, x_{k+1})$. Since R satisfies ***(km)***, we have $R(x_1, \dots, x_k) \subseteq R(x_1, \dots, \widehat{x_i}, \dots, x_{k+1})$. If $R(x_1, \dots, \widehat{x_i}, \dots, x_{k+1}) = V$, we are done. Otherwise we can find an element, say $x_{k+2} \in V \setminus R(x_1, \dots, \widehat{x_i}, \dots, x_{k+1})$. Again by the axiom ***(kw')***, there is some $x_j \in R(x_1, \dots, \widehat{x_i}, \dots, \widehat{x_j}, \dots, x_{k+1}, x_{k+2})$, and ***(km)*** implies

$$\begin{aligned} x_j \in R(x_1, \dots, \widehat{x_i}, \dots, x_j, \dots, x_{k+1}, x_{k+2}) \\ \subseteq R(x_1, \dots, \widehat{x_i}, \dots, \widehat{x_j}, \dots, x_{k+1}, x_{k+2}). \end{aligned}$$

If $R(x_1, \dots, \widehat{x_i}, \dots, \widehat{x_j}, \dots, x_{k+1}, x_{k+2}) = V$ then we are done. Otherwise we can repeat the argument. Since V contains only a finite number of elements, we eventually find a set of k elements, say $u_1, \dots, u_k$ from V so that $R(u_1, u_2, \dots, u_k) = V$, which proves the axiom ***(a')***. □

Lemma 6.5. *Let $\mathcal{X}$ be a k-weak hierarchy identified by a k-ary transit function R. Then the T-rank, $r(\mathcal{X}_T) \leq k$.*

Proof. Let $S = \{x_1, \dots, x_{k+1}\}$ be a T-independent set, i.e., for every $x_i \in S$ we have $x_i \notin \bigcap\{C \in \mathcal{X} \mid T \subseteq (S \setminus \{x_i\}) \subseteq C\}$. Let $C_i \in \mathcal{X}$ contains T and the set $S \setminus \{x_i\}$ for every i. Then $x_i \notin \cap C_j$ for $i = 1, \dots, k+1$. But some $x_i \in \bigcap_{i\neq j}^{k+1} C_j$. This is a contradiction to $\mathcal{X}$ being a k-weak hierarchy. □

Remark 6.6. If the set system $\mathcal{X}$ identified with a k-ary transit function is a k-weak hierarchy, then it can be shown easily that the T-Carathéodory number of $\mathcal{X}$ is at most k, as any set S with $|F| > k+1$ is T-dependent and hence any $x \in \langle F \rangle_{\mathcal{X}_T}$ belongs to $\langle F_i \rangle_{\mathcal{X}_T}$, where F_i is subset of F with $|F_i|$ at most k.

Lemma 6.7. *Let R be a k-ary transit function satisfying **(km)** and **(a')**. Then the axioms **(kw)** and **(kw')** are equivalent.*

Proof. Let R satisfies ***(kw)***. Then the set system $\mathcal{X}$ identified by R is a k-weak hierarchy. By definition of R, $R(x_1, \ldots, x_k) = \bigcap\{C_i \in \mathcal{X} \mid x_1, \ldots, x_k \in C_i\} = \langle x_1, \ldots, x_k\rangle_{\mathcal{X}}$. Now by Lemma 6.5, any distinct $k+1$ points, $x_1, \ldots, x_{k+1}$ are dependent with respect to some subset T contained in S. That is, $x_i \in R(x_1, \ldots, \widehat{x_i}, \ldots, x_{k+1})$ for some i. Hence R satisfies ***(kw')***.

Suppose R satisfies ***(kw')***. Proving that R satisfies ***(kw)*** is equivalent to showing that $\mathcal{X}$ is a k-weak hierarchy. Suppose this is not the case. Then we can find $k+1$ distinct elements $x_1, \ldots, x_{k+1} \in S$ and $C_1, \ldots, C_{k+1} \in \mathcal{X}$ such that $x_i \in C_j$ if and only if $i \neq j$. By axiom ***(kw')***, $x_i \in R(x_1, \ldots, \widehat{x_i}, \ldots, x_k)$ for some x_i, say x_{k+1}. Then $x_{k+1} \in C_i$ for $i = 1, \ldots, k$ and $x_{k+1} \notin C_{k+1}$. Since $x_1, \ldots, x_k \in C_{k+1}$, by definition of R, $R(x_1, \ldots, x_k) \subseteq C_{k+1}$. But $x_{k+1} \notin C_{k+1}$ and $x_{k+1} \in R(x_1, \ldots, x_k)$, a contradiction. Hence R satisfies ***(kw)***. □

Theorem 6.8. *The set system $\mathcal{X}$ induced by the k-ary transit function R on V is a closed k-weak hierarchy if and only R satisfies the axioms* **(m)**, **(m')**, *and* **(kw')**.

Proof. Suppose $\mathcal{X}$ be a closed k-weak hierarchy induced by the k-ary transit function R on V. Since a closed k weak hierarchy is a convexity, R satisfies ***(m)***, ***(m')***. By Lemma 6.7 R satisfies ***(kw')***.

Conversely suppose R satisfies ***(m)***, ***(m')***, and ***(kw')***. Since R satisfies ***(m)*** and ***(kw')***, by Lemma 6.4, R satisfies (a'). Hence the transit sets form a convexity $\mathcal{X}$. By Lemma 6.7, R satisfies ***(kw)***. Hence $\mathcal{X}$ is a closed k-weak hierarchy. □

Remark 6.9. Axiom ***(kw)*** or ***(kw')*** is a direct translation of ***(kWH)***. The condition is necessary and sufficient given that ***(m)***, ***(m')***, ***(a')*** are equivalent to the transit sets forming a convexity.

We briefly discuss the mutual dependencies between the axioms ***(km)***, ***(km')***, ***(kw)***, ***(kw')***, and ***(a')***. We already know that ***(km)*** and ***(kw')*** implies ***(a')***. Furthermore, if ***(km)*** and ***(a')*** are satisfied, then ***(kw)*** and ***(kw')*** are equivalent.

Example 6.10 (***(km)***, ***(a')***, and ***(km')***, but not ***(kw)*** and ***(kw')***)**.** Let $V = \{x_1, x_2, \ldots, x_{k+1}\}$. Define R on V as follows:

$$R(a_1, a_2, \ldots, a_k) = V,$$

for all other k-tuples

$$R(x_1, x_2, \ldots, x_k) = \{x_1, x_2, \ldots, x_k\}.$$

Example 6.11 (***(km)***, ***(a')***, ***(kw)***, and ***(kw')***, but not ***(km')***)**.** Let $V = \{x_1, x_2, \ldots, x_{k+1}\}$. Let

$$\begin{aligned}
R(x_1, x_3, x_3, \ldots, x_3) &= V,\\
R(x_1, x_4, x_4, \ldots, x_4) &= V - \{x_3\},\\
R(x_3, x_5, x_5, \ldots, x_5) &= V - \{x_1\},\\
R(x_1, x_2, x_2, \ldots, x_2) &= \{x_1, x_2\},\\
R(x_1, x_5, x_5, \ldots, x_5) &= \{x_1, x_5\},\\
R(x_2, x_2, x_2, \ldots, y) &= \{x_2, y\} \text{ for all } y \in V
\end{aligned}$$

and set $R(x_1, x_2, x_3, \ldots, x_k) = V$ for all other k-tuples. We can see that

$$R(x_1, x_4, x_4, \ldots, x_4) \cap R(x_3, x_5, x_5, \ldots, x_5) = \{x_2, x_4, \ldots, x_{k+1}\}$$

but there is no k-tuple whose R-image is $\{x_2, x_4, \ldots, x_{k+1}\}$.

Example 6.12 (***(km')***, ***(a')***, ***(kw)***, and ***(kw')***, but not ***(km)***)**.** Consider $V = \{x_1, x_2, \ldots, x_{k+1}\}$ and set

$$\begin{aligned} R(x_1, x_2, \ldots, x_2) &= \{x_1, x_2, x_3, x_4\}, \\ R(x_2, x_3, \ldots, x_3) &= \{x_2, x_3, x_4\}, \\ R(x_2, x_4, \ldots, x_4) &= \{x_2, x_4\}, \end{aligned}$$

and $R(x_1, x_2, \ldots x_k) = V$ for all other k-tuples. Since $R(x_3, x_4, \ldots x_4) = V$ we can see that R does not satisfy the axiom ***(km)***.

Example 6.13 (***(km)***, ***(km')***, and ***(kw)***, but not ***(a')***)**.** $V = \{x_1, x_2, \ldots, x_{k+1}\}$, consider R on V by

$$\begin{aligned} R(x_1, x_2, \ldots, x_2) &= \{x_1, x_2\}, \\ R(x_1, x_3, \ldots, x_3) &= \{x_1, x_2, x_3\}, \\ R(x_1, x_4, \ldots, x_4) &= \{x_1, x_2, x_4\}, \\ R(x_2, x_3, \ldots, x_3) &= \{x_2, x_3\}, \\ R(x_2, x_4, \ldots, x_4) &= \{x_2, x_4\}, \\ R(x_3, x_4, \ldots, x_4) &= \{x_3, x_4\}, \end{aligned}$$

and set $R(u_1, u_2, \ldots u_k) = \{u_1, u_2, \ldots u_k, x_3\}$ for all other k-tuples $(u_1, u_2, \ldots u_k)$.

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On König-Egerváry collections of maximum critical independent sets*

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Abstract

Let G be a simple graph with vertex set $V(G)$. A set $S \subseteq V(G)$ is *independent* if no two vertices from S are adjacent. Let $\mathrm{Ind}(G)$ denote the family of all independent sets.

The graph G is said to be *König-Egerváry* if $\alpha(G) + \mu(G) = |V(G)|$, where $\alpha(G)$ denotes the size of a maximum independent set and $\mu(G)$ is the cardinality of a maximum matching. A family $\Gamma \subseteq \mathrm{Ind}(G)$ is a *König-Egerváry collection* if $|\bigcup \Gamma| + |\bigcap \Gamma| = 2\alpha(G)$.

The number $d(X) = |X| - |N(X)|$ is the *difference* of $X \subseteq V(G)$, and a set $A \in \mathrm{Ind}(G)$ is *critical* if $d(A) = \max\{d(I) : I \in \mathrm{Ind}(G)\}$.

In this paper, we show that if the family of all maximum critical independent sets of a graph G is a König-Egerváry collection, then G is a König-Egerváry graph. This result generalizes one of our conjectures verified by Short in 2016.

Keywords: Maximum independent set, critical set, kernel, nucleus, core, corona, diadem, König-Egerváry graph.

Math. Subj. Class.: 05C69, 05C70, 05A20

1 Introduction

Throughout this paper G is a finite simple graph with vertex set $V(G)$ and edge set $E(G)$. If $X \subseteq V(G)$, then $G[X]$ is the subgraph of G induced by X. By $G - W$ we mean either the subgraph $G[V(G) - W]$, if $W \subseteq V(G)$, or the subgraph obtained by deleting the edge set W, for $W \subseteq E(G)$. In either case, we use $G - w$, whenever $W = \{w\}$.

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The *neighborhood* $N(v)$ of a vertex $v \in V(G)$ is the set $\{w : w \in V(G)$ and $vw \in E(G)\}$. The *neighborhood* $N(A)$ of $A \subseteq V(G)$ is $\{v \in V(G) : N(v) \cap A \neq \emptyset\}$, and $N[A] = N(A) \cup A$.

A set $S \subseteq V(G)$ is *independent* if no two vertices from S are adjacent, and by $\mathrm{Ind}(G)$ we mean the family of all the independent sets of G. An independent set of maximum size is a *maximum independent set* of G, and $\alpha(G) = \max\{|S| : S \in \mathrm{Ind}(G)\}$.

Let $\Omega(G)$ denote the family of all maximum independent sets,

$$\mathrm{core}(G) = \bigcap \{S : S \in \Omega(G)\} \text{ [12], and } \mathrm{corona}(G) = \bigcup \{S : S \in \Omega(G)\} \text{ [3].}$$

If $A \in \Omega(G[N[A]])$, then A is a *local maximum independent set* of G [13].

A *matching* is a set M of pairwise non-incident edges of G. A matching of maximum cardinality, denoted $\mu(G)$, is a *maximum matching*.

For $X \subseteq V(G)$, the number $|X| - |N(X)|$ is the *difference* of X, denoted $d(X)$. The *critical difference* $d(G)$ is $\max\{d(X) : X \subseteq V(G)\}$. The number $\max\{d(I) : I \in \mathrm{Ind}(G)\}$ is the *critical independence difference* of G, denoted $id(G)$. Clearly, $d(G) \geq id(G)$. It was shown in [23] that $d(G) = id(G)$ holds for every graph G. If A is an independent set in G with $d(X) = id(G)$, then A is a *critical independent set* [23].

Theorem 1.1 ([20]). *Every local maximum independent set is a subset of a maximum independent set.*

Proposition 1.2 ([15]). *Each critical independent set is a local maximum independent set.*

Combining Theorem 1.1 and Proposition 1.2 one can conclude with the following.

Corollary 1.3 ([4]). *Every critical independent set can be enlarged to a maximum independent set.*

For a graph G, let us denote

$$\begin{aligned}
\ker(G) &= \bigcap \{A : A \text{ is a critical independent set}\} \text{ [16],} \\
\mathrm{MaxCritIndep}(G) &= \{S : S \text{ is a maximum critical independent set}\}, \\
\mathrm{nucleus}(G) &= \bigcap \mathrm{MaxCritIndep}(G) \text{ [8], and} \\
\mathrm{diadem}(G) &= \bigcup \mathrm{MaxCritIndep}(G) \text{ [18].}
\end{aligned}$$

Clearly, $\ker(G) \subseteq \mathrm{nucleus}(G)$ and, by Corollary 1.3, the inclusion $\mathrm{diadem}(G) \subseteq \mathrm{corona}(G)$ is true for each graph G.

Theorem 1.4 ([16]). *For a graph G, the following assertions are true:*

(i) $\ker(G) \subseteq \mathrm{core}(G)$*;*

(ii) if A and B are critical in G, then $A \cup B$ and $A \cap B$ are critical as well.

Let us consider the graphs G_1 and G_2 from Figure 1: $\mathrm{core}(G_1) = \{a, b, c, d\}$ and it is a critical set, while $\mathrm{core}(G_2) = \{x, y, z, w\}$ and it is not critical.

Moreover,

$$\ker(G_1) = \{a, b, c\} \subset \mathrm{core}(G_1) \subset \{a, b, c, d, g\} = \mathrm{nucleus}(G_1),$$

as $\mathrm{MaxCritIndep}(G_1) = \{\{a, b, c, d, e, g\}, \{a, b, c, d, f, g\}\}$.

In addition, notice that $\mathrm{diadem}(G_1) \subsetneq \mathrm{corona}(G_1)$.

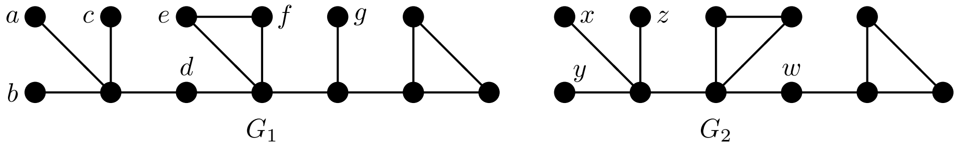

Figure 1: Both G_1 and G_2 are not König-Egerváry graphs.

Theorem 1.5 ([7]). *Let $\emptyset \neq \Gamma \subseteq \Omega(G)$. If $\bigcup \Gamma$ is critical, then $\bigcap \Gamma$ is critical as well.*

It is well known that $\alpha(G) + \mu(G) \leq |V(G)|$ holds for every graph G. Recall that if $\alpha(G) + \mu(G) = |V(G)|$, then G is a *König-Egerváry graph* [5, 22]. For example, each bipartite graph is a König-Egerváry graph. Various properties of König-Egerváry graphs can be found in [2, 6, 9, 14, 17].

Theorem 1.6 ([11, 15]). *For a graph G, the following assertions are equivalent:*

(i) *G is a König-Egerváry graph;*

(ii) *there exists some maximum independent set which is critical;*

(iii) *each of its maximum independent sets is critical.*

If Γ, Γ' are two collections of sets, we write $\Gamma' \lhd \Gamma$ if $\bigcup \Gamma' \subseteq \bigcup \Gamma$ and $\bigcap \Gamma \subseteq \bigcap \Gamma'$ [8]. Clearly, the relation $\lhd$ is a preorder. The following theorem extends and generalizes some findings from [19].

Theorem 1.7 ([8]). *Let $\emptyset \neq \Gamma \subseteq \Omega(G)$.*

(i) *If $\Gamma' \subseteq \mathrm{Ind}(G)$ is such that $\Gamma' \lhd \Gamma$, then $\left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \leq \left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right|$.*

(ii) $2\alpha(G) \leq \left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right|$.

(iii) *If, in addition, G is a König-Egerváry graph, then $\left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right| = 2\alpha(G)$, and, in particular, $|\mathrm{corona}(G)| + |\mathrm{core}(G)| = 2\alpha(G)$.*

Let us notice that if $S \in \mathrm{Ind}(G)$, then $G[N[S]]$ is not necessarily a König-Egerváry graph. For instance, consider the graph G_1 from Figure 1, and $S_1 = \{d, g\}$, $S_2 = \{d, e, g\}$. Then, $G_1[N[S_1]]$ is a König-Egerváry graph, while $G_1[N[S_2]]$ is not a König-Egerváry graph.

Theorem 1.8 ([11]). *For every graph G, there is some $X \subseteq V(G)$, such that:*

(i) *$X = N[S]$ for every $S \in \mathrm{MaxCritIndep}(G)$;*

(ii) *$G[X]$ is a König-Egerváry graph.*

In other words, Theorem 1.8*(i)* claims that $X = N[S]$ does not depend on the choice of $S \in \mathrm{MaxCritIndep}(G)$. The *critical independence number* of G is defined as $\alpha'(G) = \max\{|S| : S \in \mathrm{MaxCritIndep}(G)\}$ [11].

Recently, the following conjectures were validated in [21].

Conjecture 1.9 ([8]). *If* $|\mathrm{nucleus}(G)| + |\mathrm{diadem}(G)| = 2\alpha(G)$, *then* G *is a König-Egerváry graph.*

Conjecture 1.10 ([7]). *If* $|\mathrm{diadem}(G)| = |\mathrm{corona}(G)|$, *then* G *is a König-Egerváry graph.*

Conjecture 1.11 ([7]). $|\ker(G)| + |\mathrm{diadem}(G)| \leq 2\alpha(G)$ *for every graph* G.

An alternative proof of the inequality $|\ker(G)| + |\mathrm{diadem}(G)| \leq 2\alpha(G)$ may be found in [1].

In this paper, we involve these findings in a more general framework, where they appear as corollaries.

2 Results

Lemma 2.1. *If* $S \in \mathrm{MaxCritIndep}(G)$ *and* $X = N[S]$, *then*

$$\mathrm{MaxCritIndep}(G) \lhd \Omega\,(G[X])\,.$$

Proof. By Proposition 1.2, we get that $\alpha\,(G[X]) = |S|$. Since, in accordance with Theorem 1.8*(i)*, $X = N[A]$ for each $A \in \mathrm{MaxCritIndep}(G)$, we may conclude that $\mathrm{MaxCritIndep}(G) \subseteq \Omega\,(G[X])$. Hence, $\mathrm{MaxCritIndep}(G) \lhd \Omega\,(G[X])$. $\square$

There is a graph G with $\mathrm{MaxCritIndep}(G) \subsetneq \Omega\,(G[X])$, $S \in \mathrm{MaxCritIndep}(G)$, and $X = N[S]$. For instance, the graph G from Figure 2 has

$$\mathrm{MaxCritIndep}(G) = \{\{a,b,c,d,e,g\}, \{a,b,c,d,f,g\}\},\ X = N[\{a,b,c,d,e,g\}],$$

while $\{a,b,c,d,e,k\} \in \Omega\,(G[X]) - \mathrm{MaxCritIndep}(G)$.

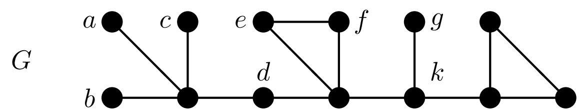

Figure 2: $d(\{a,b,c,d,e,k\}) = 1 < 2 = d(G)$.

Corollary 2.2 ([21]). *If* $S \in \mathrm{MaxCritIndep}(G)$ *and* $X = N[S]$, *then*

$$\mathrm{diadem}(G) \subseteq \mathrm{diadem}(G[X]) \quad \textit{and} \quad \mathrm{nucleus}(G[X]) \subseteq \mathrm{nucleus}(G).$$

Proof. In accordance with Theorem 1.8*(ii)*, $G[X]$ is a König-Egerváry graph. Hence, Theorem 1.6*(iii)* implies that $\mathrm{MaxCritIndep}(G[X]) = \Omega\,(G[X])$. Therefore, Lemma 2.1 ensures that $\mathrm{MaxCritIndep}(G) \lhd \mathrm{MaxCritIndep}(G[X])$, which, by definition, means $\mathrm{diadem}(G) \subseteq \mathrm{diadem}(G[X])$ and $\mathrm{nucleus}(G[X]) \subseteq \mathrm{nucleus}(G)$. $\square$

Lemma 2.3. *If* $\emptyset \neq \Gamma' \subseteq \mathrm{MaxCritIndep}(G)$ *and* $\emptyset \neq \Gamma \subseteq \Omega(G)$, *then*

$$\left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \leq 2\alpha'(G) \leq 2\alpha(G) \leq \left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right|.$$

Proof. Let $S \in \mathrm{MaxCritIndep}(G)$ and $X = N[S]$. Since $\Gamma' \subseteq \mathrm{MaxCritIndep}(G)$, and, by Lemma 2.1, $\mathrm{MaxCritIndep}(G) \lhd \Omega(G[X])$, we get $\Gamma' \lhd \Omega(G[X])$. According to Theorem 1.8*(ii)*, $G[X]$ is a König-Egerváry graph. Now, using Theorem 1.7*(ii)–(iii)*, we obtain

$$\left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \leq |\mathrm{core}(G[X])| + |\mathrm{corona}(G[X])|$$
$$= 2\alpha(G[X]) = 2\alpha'(G) \leq 2\alpha(G) \leq \left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right|,$$

as claimed. □

If $\Gamma' = \mathrm{MaxCritIndep}(G)$ and $\Gamma = \Omega(G)$, Lemma 2.3 immediately implies the following.

Corollary 2.4 ([21]). $|\mathrm{nucleus}(G)| + |\mathrm{diadem}(G)| \leq 2\alpha(G)$ *for every graph* G.

Since $\ker(G) \subseteq \mathrm{nucleus}(G)$, Corollary 2.4 validates Conjecture 1.11.

Let us recall that a family of independent sets Γ is a *König-Egerváry collection* if

$$\left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right| = 2\alpha(G) \text{ [8]}.$$

If there exists a König-Egerváry collection $\Gamma \subseteq \Omega(G)$, this does not oblige G to be a König-Egerváry graph. For instance, the graph G from Figure 3 satisfies $|\mathrm{corona}(G)| + |\mathrm{core}(G)| = 2\alpha(G)$, i.e., $\Omega(G)$ is a König-Egerváry collection, while G is not a König-Egerváry graph.

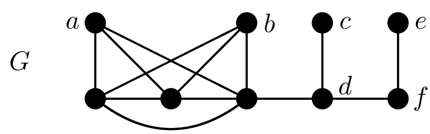

Figure 3: $\mathrm{core}(G) = \{a, b\}$ and $\mathrm{corona}(G) = \{a, b, c, d, e, f\}$.

Theorem 2.5. *For a graph G, the following assertions are equivalent:*

(i) *G is a König-Egerváry graph;*

(ii) *every non-empty family of maximum critical independent sets of G is a König-Egerváry collection;*

(iii) *there is a König-Egerváry collection of maximum critical independent sets of G.*

Proof. *(i)* $\Longrightarrow$ *(ii)*: By Theorem 1.6, we obtain $\mathrm{MaxCritIndep}(G) = \Omega(G)$. Further, in accordance with Theorem 1.7*(iii)*, each $\emptyset \neq \Gamma' \subseteq \mathrm{MaxCritIndep}(G)$ is a König-Egerváry collection.

(ii) $\Longrightarrow$ *(iii)*: Clear.

(iii) $\Longrightarrow$ *(i)*: Let $\Gamma' \subseteq \mathrm{MaxCritIndep}(G)$ be a König-Egerváry collection, $S \in \Gamma'$ and $X = N[S]$. Since, by Lemma 2.1, $\mathrm{MaxCritIndep}(G) \lhd \Omega(G[X])$, we arrive at the conclusion that $\Gamma' \lhd \Omega(G[X])$, and hence,

$$\left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \leq |\mathrm{nucleus}(G[X])| + |\mathrm{diadem}(G[X])|.$$

According to Theorem 1.8*(ii)*, $G[X]$ is a König-Egerváry graph. Using Theorem 1.7*(iii)*, we infer that

$$\begin{aligned} 2\alpha(G) &= \left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \\ &\leq |\mathrm{nucleus}(G[X])| + |\mathrm{diadem}(G[X])| = 2\alpha(G[X]) \leq 2\alpha(G). \end{aligned}$$

Consequently, we obtain $\alpha(G[X]) = \alpha(G)$, which ensures that G is a König-Egerváry graph. □

Since $|\mathrm{nucleus}(G)| + |\mathrm{diadem}(G)| = 2\alpha(G)$ means that $\mathrm{MaxCritIndep}(G)$ is a König-Egerváry collection, Theorem 2.5 immediately implies the following.

Corollary 2.6 ([21]). *If* $|\mathrm{nucleus}(G)| + |\mathrm{diadem}(G)| = 2\alpha(G)$, *then* G *is a König-Egerváry graph.*

It is worth mentioning that Corollary 2.6 validates Conjecture 1.9.

If $\emptyset \neq \Gamma \subseteq \Omega(G)$, then none of $\bigcap \Gamma$ and $\bigcup \Gamma$ is necessarily critical. For instance, consider the graph G from Figure 3, and $\Gamma = \{\{a,b,c,e\},\{a,b,c,f\}\} \subseteq \Omega(G)$.

Lemma 2.7. *Let* $\Gamma \subseteq \Omega(G)$ *and* $\emptyset \neq \Gamma' \subseteq \mathrm{MaxCritIndep}(G)$, *be such that for every* $A \in \Gamma'$ *there exists* $S \in \Gamma$ *enjoying* $A \subseteq S$. *If* $\bigcap \Gamma$ *is a critical set, then the following assertions are true:*

(i) $\bigcap \Gamma \subseteq \bigcap \Gamma'$;

(ii) $\Gamma' \lhd \Gamma$;

(iii) $\left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \leq \left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right|$;

(iv) $\bigcap \Gamma' = \bigcap \Gamma$, *if, in addition,* $\bigcup \Gamma' = \bigcup \Gamma$.

Proof.

(i) Let $A \in \Gamma'$ and $S \in \Gamma$, such that $A \subseteq S$. Since $\bigcap \Gamma \subseteq S$, it follows that $A \cup \bigcap \Gamma \subseteq S$, and hence, $A \cup \bigcap \Gamma$ is independent. By Theorem 1.4, we get that $A \cup \bigcap \Gamma$ is a critical independent set. Since $A \subseteq A \cup \bigcap \Gamma$ and A is a maximum critical independent set, we infer that $\bigcap \Gamma \subseteq A$. Thus, $\bigcap \Gamma \subseteq A$ for every $A \in \Gamma'$. Therefore, $\bigcap \Gamma \subseteq \bigcap \Gamma'$.

(ii) By Part *(i)*, we know that $\bigcap \Gamma \subseteq \bigcap \Gamma'$. According to the hypothesis, every element of Γ' is included in some element of Γ. Hence, we deduce that $\bigcup \Gamma' \subseteq \bigcup \Gamma$.

(iii) The inequality follows from Part *(ii)* and Theorem 1.7*(i)*.

(iv) Part *(iii)* implies $\left|\bigcap \Gamma'\right| \leq \left|\bigcap \Gamma\right|$, and using Part *(i)*, we obtain $\bigcap \Gamma = \bigcap \Gamma'$. □

Proposition 2.8. *Let* $\Gamma \subseteq \Omega(G)$ *and* $\emptyset \neq \Gamma' \subseteq \mathrm{MaxCritIndep}(G)$ *be such that for every* $A \in \Gamma'$ *there exists* $S \in \Gamma$ *such that* $A \subseteq S$. *If* $\bigcup \Gamma' = \bigcup \Gamma$, *then* G *is a König-Egerváry graph.*

Proof. Since, by Theorem 1.4*(ii)*, $\bigcup \Gamma'$ is critical, we get that $\bigcup \Gamma$ is critical. Hence, according to Theorem 1.5, we infer that $\bigcap \Gamma$ is critical. Applying Lemma 2.7, we obtain $\bigcap \Gamma = \bigcap \Gamma'$. Further, we have

$$\begin{aligned} 2\alpha(G) &\leq \left|\bigcap \Gamma\right| + \left|\bigcup \Gamma\right| = \left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| \\ &\leq |\mathrm{core}(G[X])| + |\mathrm{corona}(G[X])| = 2\alpha(G[X]) \leq 2\alpha(G). \end{aligned}$$

Consequently, $\left|\bigcap \Gamma'\right| + \left|\bigcup \Gamma'\right| = 2\alpha(G)$, which ensures, by Theorem 2.5, that G is a König-Egerváry graph. □

If $\Gamma' = \mathrm{MaxCritIndep}(G)$ and $\Gamma = \Omega(G)$, Proposition 2.8 immediately implies the following.

Corollary 2.9 ([21]). *If* $\mathrm{diadem}(G) = \mathrm{corona}(G)$, *then* G *is a König-Egerváry graph.*

It is worth mentioning that Corollary 2.9 validates Conjecture 1.10.

3 Conclusions

In this paper we focus on interconnections between unions and intersections of maximum critical independents sets of a graph. In [21], the question arises about polynomial-time complexity of computing the following lower bound for the independence number

$$|\mathrm{nucleus}(G)| + |\mathrm{diadem}(G)| \leq 2\alpha(G).$$

Actually, Lemma 2.3 tells us that $\alpha'(G)$ is a better lower bound, since

$$|\mathrm{nucleus}(G)| + |\mathrm{diadem}(G)| \leq 2\alpha'(G) \leq 2\alpha(G),$$

while $\alpha'(G)$ is polynomially computable [10]. It seems promising to pursue upper bounds for $\alpha(G)$ in terms of $\alpha'(G)$. Let us call G a *k-bounded graph* if $\alpha(G) \leq k \cdot \alpha'(G)$. For instance, König-Egerváry graphs are 1-bounded, in accordance with Theorem 1.6. It is worth emphasizing that the independence number can be computed in polynomial time for König-Egerváry graphs, since in this case $\alpha(G) = \alpha'(G)$.

Proposition 3.1. *If* $S \in \mathrm{MaxCritIndep}(G)$, *then* $2\alpha'(G) = d(\ker(G)) + |N[S]|$.

Proof. Since $\ker(G)$ and S are critical sets of the graph G, we obtain

$$\begin{aligned} d(\ker(G)) + |N[S]| &= |\ker(G)| - |N(\ker(G))| + |S| + |N(S)| \\ &= |S| - |N(S)| + |S| + |N(S)| = 2|S| = 2\alpha'(G), \end{aligned}$$

which completes the proof. □

By Theorem 1.6 and Proposition 3.1, if G is a König-Egerváry graph and $S \in \mathrm{MaxCritIndep}(G)$, then we get

$$2\alpha(G) = d(\ker(G)) + |N[S]|,$$

because $\alpha'(G) = \alpha(G)$, and consequently,

$$2\alpha(G) \leq |\ker(G)| + |N[S]|.$$

Proposition 3.2 ([10]). *There is a matching from $N(S)$ into S for every critical independent set S.*

Proposition 3.3. *If $2\alpha(G) \leq |\ker(G)| + |N[S]|$, where $S \in \mathrm{MaxCritIndep}(G)$, then G is $\frac{3}{2}$-bounded. More precisely,*

$$\alpha'(G) \leq \alpha(G) \leq \alpha'(G) + \frac{|N(\ker(G))|}{2} \leq \frac{3}{2}\alpha'(G).$$

Proof. According to Proposition 3.2, there is a matching from $N(S)$ into S, since S is critical. Hence, $|N[S]| \leq 2\alpha'(G)$. Therefore, taking account that $\ker(G)$ is a critical independent set, we obtain

$$2\alpha(G) \leq |\ker(G)| + |N[S]| \leq |\ker(G)| + 2\alpha'(G) \leq 3\alpha'(G).$$

In accordance with Proposition 3.1, we get

$$|\ker(G)| + |N[S]| - |N(\ker(G))| = 2\alpha'(G) \leq 2\alpha(G).$$

Thus

$$\begin{aligned} \frac{|\ker(G)| + |N[S]|}{2} - \frac{|N(\ker(G))|}{2} &= \alpha'(G) \leq \alpha(G) \\ &\leq \frac{|\ker(G)| + |N[S]|}{2} \\ &= \alpha'(G) + \frac{|N(\ker(G))|}{2} \leq \frac{3}{2}\alpha'(G), \end{aligned}$$

since, $\ker(G)$ is a critical set and, by Proposition 3.2, there exists a matching from $N(\ker(G))$ into $\ker(G)$. □

Let us emphasize that the bound $\alpha(G) \leq \alpha'(G) + \frac{|N(\ker(G))|}{2}$ is of polynomial-time complexity, since $\ker(G)$ [16] and $\alpha'(G)$ [10] can be computed polynomially.

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Maximizing general first Zagreb and sum-connectivity indices for unicyclic graphs with given independence number

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Abstract

In this paper it is shown that in the class of unicyclic graphs of order n and independence number s, the spider graph $S_\Delta(n,s)$ is the unique graph maximizing general first Zagreb index ${}^0R_\alpha(G)$ for $\alpha > 1$ and general sum-connectivity index $\chi_\alpha(G)$ for $\alpha \geq 1$.

Keywords: Unicyclic graph, independence number, general first Zagreb index, general sum-connectivity number, spider graph, Jensen inequality.

Math. Subj. Class.: 05C35, 05C69

1 Introduction

Let G be a simple graph having vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, $d(u)$ denotes the degree of u and $N(u)$ the set of vertices adjacent with u. The maximum vertex degree of G is denoted by $\Delta(G)$. $K_{1,n-1}$ and C_n will denote, respectively, the star and the cycle on n vertices. The distance between vertices u and v of a connected graph, denoted by $d(u,v)$, is the length of a shortest path between them. For $x \in V(G)$ and $A \subset V(G)$, the distance $d(x,A)$ between x and A is $\min_{y\in A} d(x,y)$. If $x \in V(G)$, $G-x$ denotes the subgraph of G obtained by deleting x and its incident edges. Similar notations are $G-xy$ and $G+xy$, where $xy \in E(G)$ and $xy \notin E(G)$, respectively. Given a graph G, a subset S of $V(G)$ is said to be an independent set of G if every two vertices of S are not adjacent. The maximum number of vertices in an independent set of G is called the independence number of G and is denoted by $\alpha(G)$. A unicyclic graph G of order n is connected, has n edges and it consists of a cycle C_r, where $3 \leq r \leq n$ and some vertex-disjoint trees having each a vertex common with C_r. It is not difficult to see that if

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G is a unicyclic graph of order $n \geq 3$, then $\lfloor n/2 \rfloor \leq \alpha(G) \leq n-2$. The lower bound can be deduced since a unicyclic graph can be obtained from a tree, which is a bipartite graph, by adding a new edge. The validity of the upper bound follows from the property that if $3 \leq r \leq n$ then $\alpha(C_r) \leq r-2$ (equality holds only for $r=3$ and $r=4$).

For every $n \geq 3$ and $\lfloor n/2 \rfloor \leq s \leq n-2$, the spider graph denoted by $S_\Delta(n,s)$ is a unicyclic graph of order n consisting of $2s-n+1$ edges and $n-s-2$ paths of length 2 having a common endvertex with a triangle K_3; in other words, it is obtained from $K_{1,s+1}+e$ by attaching a pendant edge to $n-s-2$ pendant vertices of $K_{1,s+1}+e$. We have $\alpha(S_\Delta(n,s)) = s$.

The graph, denoted by H_n, is defined as follows: for $n=2k$ it consists of a cycle C_k and k pendant vertices adjacent each to a single vertex of C_k such that each vertex of C_k has degree three. For $n=2k+1$, H_n is composed from C_{k+1} and k pendant vertices adjacent each to a single vertex of C_{k+1} such that k vertices of C_k have degree three and one vertex has degree two.

For other notations in graph theory, we refer [16].

The Randić index $R(G)$ [12], one of the most used molecular descriptors in structure-property and structure-activity relationship studies [5, 6, 7, 11, 13, 14], was defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}.$$

The general Randić connectivity index (or general product-connectivity index) of G, denoted by R_α, was defined by Bollobás and Erdős [1] as

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha,$$

where α is a real number. Then $R_{-1/2}$ is the classical Randić connectivity index and for $\alpha = 1$ it is also known as second Zagreb index and denoted by $M_2(G)$.

This concept was extended to the general sum-connectivity index $\chi_\alpha(G)$ in [20], which is defined by

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u)+d(v))^\alpha,$$

where α is a real number. The sum-connectivity index $\chi_{-1/2}(G)$ was proposed in [19].

The general first Zagreb index (sometimes referred as "zeroth-order general Randić index"), denoted by ${}^0R_\alpha(G)$ was defined as

$${}^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha,$$

where α is a real number. For $\alpha = -1/2$ this index was defined in [9] and [10] and for $\alpha = 2$ it is also known as first Zagreb index and denoted by $M_1(G)$. Notice that $\chi_1(G) = {}^0R_2(G) = M_1(G)$.

Thus, the general Randić connectivity index generalizes both the ordinary Randić connectivity index and the second Zagreb index, while the general sum-connectivity index generalizes both the ordinary sum-connectivity index and the first Zagreb index [20].

Several extremal properties of the sum-connectivity and general sum-connectivity indices for trees, unicyclic graphs and general graphs were given in [3, 4, 19, 20].

Das, Xu and Gutman [2] proved that in the class of trees of order n and independence number s, the spur $S_{n,s}$ maximizes both first and second Zagreb indices and this graph is unique with these properties. Tomescu and Jamil [15] showed that in the same class of trees T, $S_{n,s}$ is the unique graph maximizing general first Zagreb index ${}^0R_\alpha(T)$ for $\alpha > 1$ and general sum-connectivity index $\chi_\alpha(T)$ for $\alpha \geq 1$.

In this paper, we show that the spider graph $S_\Delta(n, s)$ is the unique graph maximizing general first Zagreb index ${}^0R_\alpha(G)$ for $\alpha > 1$ and general sum-connectivity index $\chi_\alpha(G)$ for $\alpha \geq 1$ in the set of unicyclic graphs of order n and independence number s ($\lfloor n/2 \rfloor \leq s \leq n-2$).

2 Preliminary results

The following inequality may be deduced in a straightforward way:

Lemma 2.1. *Let $x > 0$. If $\beta < 0$ then $(1+x)^\beta > 1 + \beta x$.*

The general first Zagreb index and general sum-connectivity index of $S_\Delta(n, s)$ are given by:

$$
\begin{aligned}
{}^0R_\alpha(S_\Delta(n,s)) &= (s+1)^\alpha + s(1-2^\alpha) + 2^\alpha n - 1; \\
\chi_\alpha(S_\Delta(n,s)) &= (n-s)(s+3)^\alpha + (2s-n+1)(s+2)^\alpha + (n-s-2)3^\alpha + 4^\alpha.
\end{aligned}
$$

The cycle C_n has independence number equal to $\lfloor n/2 \rfloor$.

Lemma 2.2. *Let $n \geq 5$. Then (2.1) holds for $\alpha > 1$ and (2.2) holds for $\alpha \geq 1$:*

$$
{}^0R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > {}^0R_\alpha(C_n) \tag{2.1}
$$

$$
\chi_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > \chi_\alpha(C_n). \tag{2.2}
$$

Proof. We get ${}^0R_\alpha(C_n) = n2^\alpha$ and $\chi_\alpha(C_n) = n4^\alpha$. If n is even, $n = 2k$, (2.1) can be written as

$$
(k+1)^\alpha - 2^\alpha k + k - 1 > 0, \tag{2.3}
$$

where $k \geq 3$ and $\alpha > 1$. Consider the function $\varphi(x) = (x+1)^\alpha - 2^\alpha x + x - 1$, where $x \geq 3$. We get $\varphi'(x) = \alpha(x+1)^{\alpha-1} - 2^\alpha + 1 \geq \alpha 4^{\alpha-1} - 2^\alpha + 1$. By letting $\psi(y) = y4^{y-1} - 2^y + 1$, where $y > 1$, we have $\psi'(y) = 4^{y-1}(1 + y \ln 4) - \ln 2 \cdot 2^y$. Since $2^y > 2$ we deduce

$$
\psi'(y) > 2^y \left(\frac{1 + y \ln 4}{2} - \ln 2 \right) > 2^y \left(\frac{1 + \ln 4}{2} - \ln 2 \right) = 2^{y-1} > 0.
$$

Because $\psi(1) = 0$ we have $\psi(y) > 0$ for $y > 1$, thus $\varphi(x)$ is strictly increasing for $x \geq 3$ and $\alpha > 1$. It follows that it is sufficient to prove (2.3) for $k = 3$. For $k = 3$ (2.3) becomes

$$
4^\alpha - 3 \cdot 2^\alpha + 2 > 0, \tag{2.4}
$$

or $(2^\alpha - 1)(2^\alpha - 2) > 0$, which is true for $\alpha > 1$.

If $n = 2k + 1$, where $k \geq 2$, (2.1) becomes (2.3) in which $k \geq 2$. For $k = 2$ (2.3) yields $3^\alpha - 2 \cdot 2^\alpha + 1 > 0$, which holds by Jensen inequality since function x^α is strictly convex for $\alpha > 1$.

In order to prove (2.2) consider first the case n even, $n = 2k$. In this case (2.2) is

$$k(k+3)^\alpha + (k+2)^\alpha + (k-2)3^\alpha - (2k-1)4^\alpha > 0, \tag{2.5}$$

where $k \geq 3$ and $\alpha \geq 1$. For $k = 3$ (2.5) becomes $3 \cdot 6^\alpha + 5^\alpha + 3^\alpha - 5 \cdot 4^\alpha > 0$, which is true since $5^\alpha + 3^\alpha \geq 2 \cdot 4^\alpha$ by Jensen inequality and $3 \cdot 6^\alpha > 3 \cdot 4^\alpha$.

Consider the function $\xi(x) = x(x+3)^\alpha + (x+2)^\alpha + (x-2)3^\alpha - (2x-1)4^\alpha$, where $x \geq 3$. We get $\xi'(x) = (x+3)^\alpha + \alpha x(x+3)^{\alpha-1} + \alpha(x+2)^{\alpha-1} + 3^\alpha - 2 \cdot 4^\alpha$. We have $(x+3)^\alpha + 3^\alpha - 2 \cdot 4^\alpha \geq 6^\alpha + 3^\alpha - 2 \cdot 4^\alpha \geq 2 \cdot 4.5^\alpha - 2 \cdot 4^\alpha > 0$ by Jensen inequality. This implies that $\xi'(x) > 0$, hence $\xi(x)$ is strictly increasing. Thus (2.5) is valid since it holds for $k = 3$. If $n = 2k+1$, where $k \geq 2$, the proof is similar, using in the same way Jensen inequality. □

Lemma 2.3. *If $n \geq 5$ and $\alpha \geq 1$, $\chi_\alpha(S_\Delta(n,s))$ is strictly increasing in s for $\lfloor n/2 \rfloor \leq s \leq n-2$.*

Proof. Let

$$f(x) = (n-x)(x+3)^\alpha + (2x-n+1)(x+2)^\alpha + (n-x)3^\alpha.$$

We have $\chi_\alpha(S_\Delta(n,s)) = f(s) - 2 \cdot 3^\alpha + 4^\alpha$. We will show that $f(x)$ is strictly increasing in x for $n \geq 5$ and $2 \leq (n-1)/2 \leq x \leq n-2$. We have

$$f'(x) = (x+3)^{\alpha-1}(\alpha(n-x) - x - 3) + (x+2)^{\alpha-1}(2x + 4 + 2\alpha x - \alpha n + \alpha) - 3^\alpha.$$

If the coefficient of $(x+3)^{\alpha-1}$ is greater than or equal to zero, then $f'(x) > 0$ since $2\alpha x - \alpha n + \alpha \geq 0$, which implies

$$(x+2)^{\alpha-1}(2x + 4 + 2\alpha x - \alpha n + \alpha) - 3^\alpha \geq 2(x+2)^\alpha - 3^\alpha \geq 2 \cdot 4^\alpha - 3^\alpha > 0.$$

The coefficient of $(x+3)^{\alpha-1}$ is

$$x(-\alpha-1) + \alpha n - 3 \geq (n-2)(-\alpha-1) + \alpha n - 3 = -n + 2\alpha - 1 \geq 0$$

for $\alpha \geq (n+1)/2$.

Suppose that $1 \leq \alpha < (n+1)/2$. We will also prove that $f'(x) > 0$ in this case. We can write $f'(x) = (x+3)^{\alpha-1}E(n,x,\alpha)$, where

$$E(n,x,\alpha) = \alpha(n-x) - x - 3 + \left(1 + \frac{1}{x+2}\right)^{1-\alpha}(2x + 4 + 2\alpha x - \alpha n + \alpha) - \frac{3^\alpha}{(x+3)^{\alpha-1}}.$$

Lemma 2.1 yields

$$\left(1 + \frac{1}{x+2}\right)^{1-\alpha} > 1 + \frac{1-\alpha}{x+2},$$

which implies

$$E(n,x,\alpha) > (x+1)(\alpha+1) + 2 - 2\alpha^2 + \frac{\alpha(\alpha-1)(n+3)}{x+2} - \frac{3^\alpha}{(x+3)^{\alpha-1}}. \tag{2.6}$$

Since $\alpha - 1 < \frac{n-1}{2}$ and $x \geq \frac{n-1}{2}$ it follows that $x > \alpha - 1$, which implies $(x+1)(\alpha+1) > \alpha^2 + \alpha$. Since $x + 2 < n + 3$ we get $\frac{\alpha(\alpha-1)(n+3)}{x+2} \geq \alpha(\alpha - 1)$ and from (2.6) we obtain

$$E(n, x, \alpha) > 2 - \frac{3^\alpha}{(x+3)^{\alpha-1}}.$$

If $\alpha \geq 2$ then $\max_{x \geq 2} \frac{3^\alpha}{(x+3)^{\alpha-1}} = 5(\frac{3}{5})^\alpha \leq \frac{9}{5}$, which implies $E(n, x, \alpha) > 0$. The same conclusion holds if $1 \leq \alpha < 2$ since in this case we have

$$x \geq 2 > \alpha, \quad (x+1)(\alpha+1) > (\alpha+1)^2, \quad \frac{3^\alpha}{(x+3)^{\alpha-1}} = 3\left(\frac{3}{x+3}\right)^{\alpha-1} \leq 3$$

and (2.6) yields $E(n, x, \alpha) > (\alpha+1)^2 + 2 - 2\alpha^2 + \alpha(\alpha-1) - 3 = \alpha \geq 1$. □

The following observation will be useful.

Lemma 2.4. *Let G be a graph and $x \in V(G)$, which is adjacent to pendant vertices $v_1, \ldots, v_r$. If $r \geq 2$ then any maximum independent subset of $V(G)$ contains $v_1, \ldots, v_r$.*

Lemma 2.5. *The function*

$$h(x) = (x-2)((x+a)^\alpha - (x+a-1)^\alpha)$$

is strictly increasing for $x \geq 2$, $a \geq 1$ and $\alpha \geq 1$.

Proof. We get

$$h'(x) = (x+a)^\alpha - (x+a-1)^\alpha + \alpha(x-2)((x+a)^{\alpha-1} - (x+a-1)^{\alpha-1}) > 0$$

for $x \geq 2$, $a \geq 1$ and $\alpha \geq 1$. □

3 Main results

By simple inspection we can see that for $n = 6$ spider graph $S_\Delta(6, s)$ is the unique extremal graph G of order six and independence number s, $3 \leq s \leq 4$, having maximum ${}^0R_\alpha(G)$ unless $s = 3$ and $1 < \alpha < 2$, when ${}^0R_\alpha(S_\Delta(6,3)) < {}^0R_\alpha(H_6)$ (note that H_6 consists of a triangle K_3 and three pendant vertices adjacent to different vertices of K_3). For $n = 6, s = 3$ and $\alpha \in \{1, 2\}$ both graphs H_6 and $S_\Delta(6,3)$ are extremal. The case $n \geq 7$ is settled below.

Theorem 3.1. *Let $n \geq 7$, $\lfloor n/2 \rfloor \leq s \leq n-2$ and G be a unicyclic graph of order n with independence number s. Then for every $\alpha > 1$, ${}^0R_\alpha(G)$ is maximum if and only if $G = S_\Delta(n, s)$.*

Proof. The proof is by induction on n. For $n = 7$ the proof is by inspection, using Jensen inequality or mathematical software [17]; there are 4 graphs with $s = 3$, 15 graphs with $s = 4$ and 5 graphs having $s = 5$.

Let $n \geq 8$ and suppose that the property is true for all unicyclic graphs of order $n-1$. Let G be a unicyclic graph of order n and independence number s having maximum general first Zagreb index. By Lemma 2.2 ${}^0R_\alpha(C_n)$ cannot be maximum; it follows that $\Delta(G) \geq 3$. Its independence number verifies $s \geq 4$. Denote by C the unique cycle of G, whose length is at most $n-1$. G has at least one pendant vertex. Let x_1 be a pendant vertex such that the distance $d(x_1, C)$ is maximum. We shall consider two cases:

- Case 1: $d(x_1, C) \geq 2$ and
- Case 2: $d(x_1, C) = 1$.

Case 1. Let $x_1, x_2, \ldots, x_p$, where $p \geq 3$ and $x_p \in C$ be the unique path from x_1 to C. By letting $d(x_2) = d_2$, since for every vertex u in $N(u)$ at most two vertices are adjacent, we obtain $s \geq \Delta(G) - 1 \geq d_2 - 1$, or $d_2 \leq s + 1$. Other two subcases may hold:

- Subcase 1.1: $\alpha(G - x_1) = \alpha(G) - 1$ and
- Subcase 1.2: $\alpha(G - x_1) = \alpha(G)$.

Subcase 1.1. By the induction hypothesis we can write

$$\begin{aligned} {}^0R_\alpha(G) &= {}^0R_\alpha(G - x_1) + 1 + d_2^\alpha - (d_2 - 1)^\alpha \\ &\leq {}^0R_\alpha(S_\Delta(n - 1, s - 1)) + 1 + d_2^\alpha - (d_2 - 1)^\alpha \\ &= s^\alpha + 2^\alpha(n - s) + s - 2 + 1 + d_2^\alpha - (d_2 - 1)^\alpha. \end{aligned}$$

Since the function $x^\alpha - (x - 1)^\alpha$ is strictly increasing for $x \geq 1$ and $\alpha > 1$, it follows that $d_2^\alpha - (d_2 - 1)^\alpha \leq (s + 1)^\alpha - s^\alpha$, which implies ${}^0R_\alpha(G) \leq {}^0R_\alpha(S_\Delta(n, s))$, equality holding if and only if $d_2 = s + 1$. But this equality is not possible. If $d_2 = s + 1$ holds, then two vertices in $N(x_2)$ are adjacent since otherwise we would have $s \geq d_2$. In this case, since $x_2 \notin C$, G would have at least two cycles, a contradiction.

Consequently, ${}^0R_\alpha(G) < (s + 1)^\alpha + 2^\alpha(n - s) + s - 1 = {}^0R_\alpha(S_\Delta(n, s))$, a contradiction.

Subcase 1.2. Next we assume that $\alpha(G - x_1) = \alpha(G)$. If x_2 would be adjacent to a vertex $w \neq x_1, x_3$, the degree of w cannot be greater than one, since in this case the path $x_1, \ldots, x_p$ would not have maximum length. It follows that $d(w) = 1$ and by Lemma 2.4 every maximum independent set of vertices of G includes both x_1 and w. This implies $\alpha(G - x_1) = \alpha(G) - 1$, which contradicts the hypothesis. It follows that $d_2 = 2$. We can write

$$\begin{aligned} {}^0R_\alpha(G) &= {}^0R_\alpha(G - x_1) + 2^\alpha \\ &\leq {}^0R_\alpha(S_\Delta(n - 1, s)) + 2^\alpha \\ &= (s + 1)^\alpha + 2^\alpha(n - 1 - s) + s - 1 + 2^\alpha \\ &= {}^0R_\alpha(S_\Delta(n, s)). \end{aligned}$$

The equality holds if and only if $G - x_1 = S_\Delta(n - 1, s)$ and pendant vertex x_1 is adjacent to a pendant vertex of $S_\Delta(n - 1, s)$. Let u be the vertex of degree $s + 1$ of $S_\Delta(n - 1, s)$. If x_1 is adjacent to a pendant vertex v_2 of $S_\Delta(n - 1, s)$ such that $d(v_2, u) = 2$, the resulting graph G has $\alpha(G) = s + 1$, which contradicts the hypothesis. We deduce that x_1 is adjacent to a pendant vertex which is adjacent to u in $S_\Delta(n - 1, s)$, which implies that $G = S_\Delta(n, s)$.

Case 2. In this case we shall also consider two subcases:

- Subcase 2.1: There exists a pendant vertex x_1 such that $d(x_1, C) = 1$ and $\alpha(G - x_1) = \alpha(G) - 1$; and
- Subcase 2.2: For all pendant vertices x we have $d(x, C) = 1$ and $\alpha(G - x) = \alpha(G)$.

Subcase 2.1. As for Subcase 1.1 we get $d_2 = d(x_2) \le s + 1$ and by the same arguments ${}^0R_\alpha(G) \le (s+1)^\alpha + 2^\alpha(n-s) + s - 1 = {}^0R_\alpha(S_\Delta(n,s))$ holds, with equality if and only if $d(x_2) = s+1$ and $G - x_1 = S_\Delta(n-1, s-1)$. It follows that x_1 is adjacent to the vertex of degree s in $S_\Delta(n-1, s-1)$, i.e., $G = S_\Delta(n,s)$. Since $d(x_1, C) = \max\{d(x,C) : d(x) = 1\} = 1$, this equality is possible only for $s = n-2$.

Subcase 2.2. In this case a vertex of C may be adjacent to a single pendant vertex x, since otherwise we would have $\alpha(G - x) = \alpha(G) - 1$ by Lemma 2.4. We deduce that G consists of C and some pendant vertices adjacent to vertices of C such that each vertex $y \in C$ has its degree $d(y) \in \{2,3\}$. We shall prove that in this case ${}^0R_\alpha(G) < {}^0R_\alpha(S_\Delta(n,s))$, a contradiction.

Suppose that on C there exist four consecutive vertices x, u, v, y such that $d(u) = d(v) = 2$. In this case we shall define a new unicyclic graph G_1 of order n by $G_1 = G - vy + uy$. We deduce ${}^0R_\alpha(G_1) - {}^0R_\alpha(G) = 3^\alpha + 1^\alpha - 2 \cdot 2^\alpha > 0$ by Jensen inequality since $\alpha > 1$. If on C there exist six vertices x, r, y, p, s, q (y may coincide with p) such that $d(x) = d(y) = d(p) = d(q) = 3$ and $d(r) = d(s) = 2$, we define a new unicyclic graph G_2 with the same vertex set as follows: $G_2 = G - \{xr, ry\} + \{xy, rs\}$. By the same argument we obtain ${}^0R_\alpha(G_2) > {}^0R_\alpha(G)$. If $G \ne H_n$, by applying step by step this type of transformations we get H_n, such that ${}^0R_\alpha(H_n) > {}^0R_\alpha(G)$.

We have ${}^0R_\alpha(H_n) = k \cdot 3^\alpha + k$ for $n = 2k$ and $k \cdot 3^\alpha + 2^\alpha + k$ for $n = 2k+1$ and

$$ {}^0R_\alpha(S_\Delta(2k,k)) = (k+1)^\alpha + k2^\alpha + k - 1 \text{ and} $$
$$ {}^0R_\alpha(S_\Delta(2k+1,k) = (k+1)^\alpha + (k+1)2^\alpha + k - 1. $$

In both cases, $n = 2k$ or $n = 2k+1$ the inequalities ${}^0R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > {}^0R_\alpha(H_n)$ coincide with

$$ (k+1)^\alpha - k(3^\alpha - 2^\alpha) - 1 > 0 \tag{3.1} $$

for every $k \ge 4$ and $\alpha > 1$. Let $g(x) = (x+1)^\alpha - x(3^\alpha - 2^\alpha) - 1$. We have

$$ g(4) = 5^\alpha - 4 \cdot 3^\alpha + 4 \cdot 2^\alpha - 1 > 0 \text{ for } \alpha > 1 \text{ [17] and} $$
$$ g'(x) = \alpha(x+1)^{\alpha-1} - 3^\alpha + 2^\alpha. $$

$g'(x)$ is strictly increasing and $g'(4) = \alpha 5^{\alpha-1} - 3^\alpha + 2^\alpha > 0$ for $\alpha > 1$ [17]. It follows that $g'(x) > 0$, hence $g(x)$ is strictly increasing for $x \ge 4$ and $\alpha > 1$ and (3.1) is proved. Consequently, we can write ${}^0R_\alpha(G) \le {}^0R_\alpha(H_n) < {}^0R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) \le {}^0R_\alpha(S_\Delta(n,s))$ since the last term is strictly increasing in s, a contradiction. □

Since the function ${}^0R_\alpha(S_\Delta(n,s))$ is strictly increasing in s, $\lfloor n/2 \rfloor \le s \le n-2$, we deduce:

Corollary 3.2 ([8, 18]). *Let G be a unicyclic graph of order $n \ge 7$. Then for every $\alpha > 1$, ${}^0R_\alpha(G)$ is maximum if and only if $G = S_\Delta(n, n-2) = K_{1,n-1} + e$.*

A similar result holds for general sum-connectivity index.

Theorem 3.3. *Let $n \ge 3$, $\lfloor n/2 \rfloor \le s \le n-2$ and G be a unicyclic graph of order n with independence number s. Then for every $\alpha \ge 1$, $\chi_\alpha(G)$ is maximum if and only if $G = S_\Delta(n,s)$. For $n = 6$ and $\alpha = 1$ there exists another extremal graph, H_6.*

Proof. We shall use induction on n in the same way as in the proof of Theorem 3.1. For $n = 3$ there is a unique unicyclic graph on three vertices, $S_\Delta(3,1) = K_3$. For $n = 4$ there are two unicyclic graphs, C_4 and $K_{1,3} + e = S_\Delta(4,2)$ and the theorem is verified.

Let $n \geq 5$ and suppose that the theorem is true for all unicyclic graphs of order $n-1$. Let G be a unicyclic graph of order n and independence number s having maximum general sum-connectivity index. By Lemma 2.2 $\chi_\alpha(C_n)$ cannot be maximum; it follows that $\Delta(G) \geq 3$. Denote by C the unique cycle of G, whose length is at most $n-1$. Let x_1 be a pendant vertex such that the distance $d(x_1, C)$ is maximum. We shall consider four cases:

- Case 1.1: $d(x_1, C) \geq 2$ and $\alpha(G - x_1) = \alpha(G) - 1$;
- Case 1.2: $d(x_1, C) \geq 2$ and $\alpha(G - x_1) = \alpha(G)$;
- Case 2.1: $\max\{d(x, C) \mid d(x) = 1\} = 1$ and there exists a pendant vertex x_1 such that $\alpha(G - x_1) = \alpha(G) - 1$;
- Case 2.2: $\max\{d(x, C) \mid d(x) = 1\} = 1$ and for all pendant vertices x we have $\alpha(G - x) = \alpha(G)$.

Case 1.1. Let $x_1, x_2, x_3, \ldots$ be the path between x_1 and C. Since this path has maximum length, it follows that x_3 is the unique vertex in $N(x_2)$ such that $d_3 = d(x_3) \geq 2$. As in the proof of Theorem 3.1 we deduce $d_2 = d(x_2) \leq s + 1$.

We have

$$\begin{aligned}\chi_\alpha(G) = \chi_\alpha(G - x_1) + (d_2 + 1)^\alpha + (d_2 - 2)((d_2 + 1)^\alpha - d_2^\alpha) + (d_2 + d_3)^\alpha \\ - (d_2 + d_3 - 1)^\alpha.\end{aligned}$$

x_2 being adjacent to $d_2 - 1$ pendant vertices and in $G - x_2x_3$ the degree of x_3 being $d_3 - 1$, it follows that $d_2 - 1 + d_3 - 2 \leq s$, or $d_2 + d_3 \leq s + 3$. We get $(d_2 + 1)^\alpha \leq (s + 2)^\alpha$ with equality if and only if $d_2 = s+1$ and $(d_2+d_3)^\alpha - (d_2+d_3-1)^\alpha \leq (s+3)^\alpha - (s+2)^\alpha$ with equality only if $d_2 + d_3 = s + 3$. Since by Lemma 2.5 the function $(x - 2)((x + 1)^\alpha - x^\alpha)$ is strictly increasing in x for $x \geq 2$ and $\alpha \geq 1$, by the induction hypothesis we obtain

$$\begin{aligned}\chi_\alpha(G) &\leq \chi_\alpha(S_\Delta(n - 1, s - 1)) + (s + 2)^\alpha + (s - 1)((s + 2)^\alpha - (s + 1)^\alpha) \\ &\quad + (s + 3)^\alpha - (s + 2)^\alpha \\ &= (n - s)(s + 2)^\alpha + (2s - n)(s + 1)^\alpha + (n - s - 2)3^\alpha + 4^\alpha \\ &\quad + (s - 1)((s + 2)^\alpha - (s + 1)^\alpha) + (s + 3)^\alpha.\end{aligned}$$

By denoting the last expression by $F(n, s, \alpha)$, we have $F(n, s, \alpha) \leq \chi_\alpha(S_\Delta(n, s))$ if and only if

$$(n - s - 1)(s + 3)^\alpha + (n - s - 1)(s + 1)^\alpha \geq 2(n - s - 1)(s + 2)^\alpha. \tag{3.2}$$

Since $n - s - 1 \geq 1$, (3.2) is equivalent to $(s + 3)^\alpha + (s + 1)^\alpha \geq 2(s + 2)^\alpha$, which is true by Jensen inequality, with equality only for $\alpha = 1$. If the inequality is strict, G cannot be extremal, a contradiction. For $\alpha = 1$ we have equality only for $d_2 = s + 1$ and $d_2 + d_3 = s + 3$, which implies $d_3 = 2$ and $G - x_1 = S_\Delta(n - 1, s - 1)$, x_2 being the vertex of degree s in $S_\Delta(n - 1, s - 1)$. In this case we have $d(x_1, C) = 1$, which contradicts the hypothesis.

Case 1.2. As in the proof of Theorem 3.1 we obtain $x_2 = d(x_2) = 2$ and $d_3 = d(x_3) \leq \Delta(G) \leq s+1$. By the induction hypothesis we get

$$\begin{aligned}\chi_\alpha(G) &= \chi_\alpha(G - x_1) + 3^\alpha + (d_3+2)^\alpha - (d_3+1)^\alpha \\ &\leq \chi_\alpha(S_\Delta(n-1,s)) + 3^\alpha + (s+3)^\alpha - (s+2)^\alpha \\ &= \chi_\alpha(S_\Delta(n,s)),\end{aligned}$$

with equality if and only if $G - x_1 = S_\Delta(n-1,s)$, $d_2 = 2$ and $d_3 = s+1$, i.e., $G = S_\Delta(n,s)$.

Case 2.1. In this case x_1 is adjacent to $x_2 \in C$. Let x_3 and x_4 be the vertices adjacent to x_2 on C and denote $d(x_2) = d_2 \geq 3$, $d(x_3) = d_3$ and $d(x_4) = d_4$. We deduce

$$\begin{aligned}\chi_\alpha(G) = \chi_\alpha(G - x_1) + (d_2+1)^\alpha + (d_2-3)((d_2+1)^\alpha - d_2^\alpha) + (d_2+d_3)^\alpha \\ - (d_2+d_3-1)^\alpha + (d_2+d_4)^\alpha - (d_2+d_4-1)^\alpha.\end{aligned}$$

x_2 is adjacent with $d_2 - 2$ pendant vertices and in $G - x_2x_3$ the degree of x_3 is $d_3 - 1$. It follows that $d_2 - 2 + d_3 - 1 \leq s$, or $d_2 + d_3 \leq s+3$. Similarly, $d_2 + d_4 \leq s+3$. One obtains

$$\begin{aligned}(d_2+d_3)^\alpha - (d_2+d_3-1)^\alpha \leq (s+3)^\alpha - (s+2)^\alpha; \\ (d_2+d_4)^\alpha - (d_2+d_4-1)^\alpha \leq (s+3)^\alpha - (s+2)^\alpha.\end{aligned}$$

Since $d_2 \leq s+1$, by Lemma 2.5 we deduce

$$(d_2-3)((d_2+1)^\alpha - d_2^\alpha) \leq (s-2)((s+2)^\alpha - (s+1)^\alpha).$$

By the induction hypothesis we get

$$\begin{aligned}\chi_\alpha(G) &\leq \chi_\alpha(S_\Delta(n-1,s-1)) + (s+2)^\alpha + (s-2)((s+2)^\alpha - (s+1)^\alpha) \\ &\quad + 2(s+3)^\alpha - 2(s+2)^\alpha \\ &= (n-s)(s+2)^\alpha + (2s-n)(s+1)^\alpha + (n-s-2)3^\alpha + 4^\alpha \\ &\quad - (s+2)^\alpha + (s-2)((s+2)^\alpha - (s+1)^\alpha) + 2(s+3)^\alpha.\end{aligned}$$

This upper bound is less than or equal to $\chi_\alpha(S_\Delta(n,s))$ if and only if

$$(n-s-2)(s+3)^\alpha + (n-s-2)(s+1)^\alpha \geq 2(n-s-2)(s+2)^\alpha. \tag{3.3}$$

If $s = n-2$ then (3.3) is an equality, $S_\Delta(n-1,s-1)$ has no pendant path of length 2, it coincides with $K_{1,n-2}+e$, $d_2 = s+1$, $d_3 = d_4 = 2$ and all inequalities become equalities. In this case $G = S_\Delta(n,s)$. If $s < n-2$ then $\chi_\alpha(G - x_1) < \chi_\alpha(S_\Delta(n-1,s-1))$ since $S_\Delta(n-1,s-1)$ has pendant paths of length 2 and $G - x_1$ does not have by hypothesis. If $s < n-2$ then (3.3) is valid by Jensen inequality (for $\alpha = 1$ (3.3) is an equality), but in this case we have $\chi_\alpha(G) < \chi_\alpha(S_\Delta(n,s))$, a contradiction.

Case 2.2. As in the proof of Theorem 3.1 we deduce that G consists of C and some pendant vertices adjacent to vertices of C such that each vertex $y \in C$ has its degree $d(y) \in \{2,3\}$. We shall prove that in this case $\chi_\alpha(G) < \chi_\alpha(S_\Delta(n,s))$ unless $\alpha = 1$ and $G = H_6$, a contradiction.

Suppose that on C there exist four consecutive vertices x, u, v, y such that $d(u) = d(v) = 2$. In this case we shall define a new unicyclic graph G_1 of order n by $G_1 = G - vy + uy$. We deduce

$$\chi_\alpha(G_1) - \chi_\alpha(G) = (d(x)+3)^\alpha + (d(y)+3)^\alpha - (d(x)+2)^\alpha - (d(y)+2)^\alpha > 0.$$

If on C there exist six vertices x, r, y, p, s, q (y may coincide with p) such that $d(x) = d(y) = d(p) = d(q) = 3$ and $d(r) = d(s) = 2$, we define a new unicyclic graph G_2 with the same vertex set as follows: $G_2 = G - \{xr, ry\} + \{xy, rs\}$. We obtain

$$\chi_\alpha(G_2) - \chi_\alpha(G) = 3 \cdot 6^\alpha + 4^\alpha - 4 \cdot 5^\alpha > 0$$

since $6^\alpha + 4^\alpha \geq 2 \cdot 5^\alpha$ and $2 \cdot 6^\alpha > 2 \cdot 5^\alpha$. If $G \neq H_n$, by applying step by step this type of transformations we get H_n, such that $\chi_\alpha(H_n) > \chi_\alpha(G)$.

We have $\chi_\alpha(H_n) = k\,6^\alpha + k\,4^\alpha$ for $n = 2k$ and $(k-1)6^\alpha + k\,4^\alpha + 2 \cdot 5^\alpha$ for $n = 2k+1$. We get

$$\chi_\alpha(S_\Delta(2k,k)) = k(k+3)^\alpha + (k+2)^\alpha + (k-2)3^\alpha + 4^\alpha \text{ and}$$
$$\chi_\alpha(S_\Delta(2k+1,k)) = (k+1)(k+3)^\alpha + (k-1)3^\alpha + 4^\alpha.$$

We shall prove that $\chi_\alpha(S_\Delta(2k,k)) \geq \chi_\alpha(H_n)$ for $n = 2k$ and $k \geq 3$ (equality holds only for $k = 3$ and $\alpha = 1$) and $\chi_\alpha(S_\Delta(2k+1,k)) > \chi_\alpha(H_n)$ for $n = 2k+1$ and $k \geq 2$. Since for $n = 5$ and $n = 7$ it can be easily verified that there is no unicyclic graph of order n in Case 2.2, it follows that for $n = 2k+1$ we may consider that $k \geq 4$. It follows that it is necessary to show that (3.4) holds for $k \geq 3$ (with equality only for $k = 3$ and $\alpha = 1$) and (3.5) is true for $k \geq 4$.

$$k(k+3)^\alpha + (k+2)^\alpha + (k-2)3^\alpha + 4^\alpha \geq k\,6^\alpha + k\,4^\alpha \tag{3.4}$$
$$(k+1)(k+3)^\alpha + (k-1)3^\alpha + 4^\alpha > (k-1)6^\alpha + k\,4^\alpha + 2 \cdot 5^\alpha \tag{3.5}$$

For $\alpha = 1$ (3.4) is equivalent to $k^2 - 3k \geq 0$ with equality only for $k = 3$. Suppose that $\alpha > 1$ and let

$$\rho(x) = x(x+3)^\alpha + (x+2)^\alpha + (x-2)3^\alpha - (x-1)4^\alpha - x6^\alpha.$$

Since $\rho'(x)$ is strictly increasing for $x \geq 3$, we get

$$\rho'(x) \geq \rho'(3) = 3\alpha\,6^{\alpha-1} + \alpha\,5^{\alpha-1} + 3^\alpha - 4^\alpha > 0$$

for $\alpha > 1$ [17], which implies $\rho(x) \geq \rho(3) = 5^\alpha + 3^\alpha - 2 \cdot 4^\alpha > 0$ for $\alpha > 1$ by Jensen inequality. This proves (3.4).

Similarly, let

$$\varphi(x) = (x+1)(x+3)^\alpha + (x-1)3^\alpha - (x-1)6^\alpha - (x-1)4^\alpha - 2 \cdot 5^\alpha.$$

Since $\varphi'(x)$ is strictly increasing in $x \geq 4$ for $\alpha \geq 1$ and

$$\varphi'(4) = 7^\alpha + 5\alpha 7^{\alpha-1} - 6^\alpha - 4^\alpha + 3^\alpha > 0$$

for $\alpha \geq 1$ [17], it follows that for $x \geq 4$ we have

$$\varphi(x) \geq \varphi(4) = 5 \cdot 7^\alpha + 3 \cdot 3^\alpha - 3 \cdot 6^\alpha - 3 \cdot 4^\alpha - 2 \cdot 5^\alpha > 0$$

for $\alpha \geq 1$ [17] and (3.5) is justified.

Consequently, if $G \neq H_6$ we can write

$$\chi_\alpha(G) \leq \chi_\alpha(H_n) < \chi_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) \leq \chi_\alpha(S_\Delta(n, s))$$

since by Lemma 2.3 the last term is strictly increasing in s, a contradiction. □

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Optimal orientations of strong products of paths

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Abstract

Let $\mathrm{diam}_{\min}(G)$ denote the minimum diameter of a strong orientation of G and let $G \boxtimes H$ denote the strong product of graphs G and H. In this paper we prove that $\mathrm{diam}_{\min}(P_m \boxtimes P_n) = \mathrm{diam}(P_m \boxtimes P_n)$ for $m, n \geq 5$, $m \neq n$, and $\mathrm{diam}_{\min}(P_m \boxtimes P_n) = \mathrm{diam}(P_m \boxtimes P_n) + 1$ for $m, n \geq 5$, $m = n$. We also prove that $\mathrm{diam}_{\min}(G \boxtimes H) \leq \max\{\mathrm{diam}_{\min}(G), \mathrm{diam}_{\min}(H)\}$ for any connected bridgeless graphs G and H.

Keywords: Diameter, strong orientation, strong product.

Math. Subj. Class.: 05C12, 05C76

1 Introduction

Let $D = (V(D), A(D))$ be a directed graph. If $(u, v) \in A(D)$, we write $u \to v$. A *uv-path* is a directed path $u = u_1u_2 \ldots u_n = v$ from a vertex u to a vertex v. The *length* of the path $u = u_1u_2 \ldots u_n = v$ is $n - 1$. If every vertex in D is reachable from every other vertex in D, we say that directed graph D is *strong* (there is a directed uv-path in D for every $u, v \in V(D)$). The *distance* from u to v is the length of a shortest directed uv-path in D, denoted by $\mathrm{dist}_D(u, v)$. The greatest distance among all pairs of vertices in D is the diameter of D, so

$$\mathrm{diam}(D) = \max\{\mathrm{dist}_D(u, v) \mid u, v \in V(D)\}.$$

Note that the distance of two vertices u, v in undirected graph G, $\mathrm{dist}_G(u, v)$, is the length of a shortest undirected uv-path in G and the greatest distance between any two vertices in G is the diameter of G, denoted by $\mathrm{diam}(G)$.

Let G be an undirected graph. An *orientation* of G is a digraph D obtained from G by assigning to each edge in G a direction. Let $\mathcal{D}(G)$ denote the family of all strong orientations of G. In [9] it is proved that every connected bridgeless graph admits a strong orientation. We define the minimum diameter of a strong orientation of G as

$$\mathrm{diam}_{\min}(G) = \min\{\mathrm{diam}(D) \mid D \in \mathcal{D}(G)\}.$$

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The parameter $\operatorname{diam}_{\min}(G)$ was studied by many authors, because it is important from theoretical and practical points of view, as an application in traffic control problems. Orientations of graphs can be viewed as arrangements of one-way streets, if G is thought of as the system of two-way streets in a city, and we want to make every street in the city one-way and still get from every point to every other point (see [9, 10]).

For every bridgeless connected graph G of radius r it was shown, see [1], that $\operatorname{diam}_{\min}(G) \leq 2r^2 + 2r$. There were also some determined values of the minimum diameter of a strong orientation of the Cartesian product of graphs. For Cartesian product of two paths it was proved that $\operatorname{diam}_{\min}(P_m \,\Box\, P_n) = \operatorname{diam}(P_m \,\Box\, P_n)$, for $m \geq 3$ and $n \geq 6$, see [5]. In [8] it was proved that $\operatorname{diam}_{\min}(C_m \,\Box\, C_n) = \operatorname{diam}(C_m \,\Box\, C_n)$ for $m, n \geq 6$. In [7] Koh and Tay proved that $\operatorname{diam}_{\min}(T_1 \,\Box\, T_2) = \operatorname{diam}(T_1 \,\Box\, T_2)$ for trees T_1 and T_2 with diameters at least 4. They also studied the diameter of orientations of $K_m \,\Box\, K_n$, $K_m \,\Box\, P_n$, $P_m \,\Box\, C_n$ and $K_m \,\Box\, C_n$ (see [4, 5, 6]).

In [3], the upper bound for the strong radius and the strong diameter of Cartesian product of graphs are determined.

In this article we consider the minimum diameter of strong orientations of strong products of graphs. The *strong product* of graphs G and H is the graph, denoted by $G \boxtimes H$, with the vertex set $V(G \boxtimes H) = V(G) \times V(H)$ where two distinct vertices (u, v) and (u', v') are adjacent in $G \boxtimes H$ if and only if $uu' \in E(G)$ and $v = v'$, or $u = u'$ and $vv' \in E(H)$, or $uu' \in E(G)$ and $vv' \in E(H)$. For $v \in V(H)$ we define the G-layer G_v:

$$G_v = \{(u, v) \mid u \in V(G)\}.$$

Analogously we define H-layers.

In the next section we prove that $\operatorname{diam}_{\min}(P_m \boxtimes P_n) = \operatorname{diam}(P_m \boxtimes P_n)$, for $m, n \geq 5$, $m \neq n$ and that $\operatorname{diam}_{\min}(P_m \boxtimes P_n) = \operatorname{diam}(P_m \boxtimes P_n) + 1$, for $m, n \geq 5$, $m = n$.

2 Orientations of $P_m \boxtimes P_n$

In [7] Koh and Tay proved that $\operatorname{diam}_{\min}(P_m \,\Box\, P_n) = \operatorname{diam}(P_m \,\Box\, P_n)$, for $m \geq 5$ and $n \geq 5$. We use some of their notations. So we will define four sections of $V(P_m \boxtimes P_n)$ and two basic orientations of $P_s \boxtimes P_t$, where $s, t \geq 3$, similarly as it was introduced in [7]. For $m, n \geq 5$ we define

(i) Southwest Section SW $= \left\{(i, j) \mid 1 \leq i \leq \left\lceil \frac{m}{2} \right\rceil, 1 \leq j \leq \left\lceil \frac{n}{2} \right\rceil\right\}$;

(ii) Northwest Section NW $= \left\{(i, j) \mid 1 \leq i \leq \left\lceil \frac{m}{2} \right\rceil, \left\lceil \frac{n+1}{2} \right\rceil \leq j \leq n\right\}$;

(iii) Southeast Section SE $= \left\{(i, j) \mid \left\lceil \frac{m+1}{2} \right\rceil \leq i \leq m, 1 \leq j \leq \left\lceil \frac{n}{2} \right\rceil\right\}$;

(iv) Northeast Section NE $= \left\{(i, j) \mid \left\lceil \frac{m+1}{2} \right\rceil \leq i \leq m, \left\lceil \frac{n+1}{2} \right\rceil \leq j \leq n\right\}$.

We define two basic orientations of $P_s \boxtimes P_t$, where $s, t \geq 3$: if $s \leq t$, we define the orientation F_1 of $P_s \boxtimes P_t$ as:

(i) For $1 \leq i \leq s-1$ and $2 \leq j \leq t$, $(i, j) \to (i+1, j-1)$;

(ii) For $1 \leq i \leq s-1$ and $1 \leq j \leq t-1$, $(i+1, j+1) \to (i, j)$ if $j - i \geq t - s$ and $(i, j) \to (i+1, j+1)$ if $j - i < t - s$;

(iii) For $1 \leq i \leq s-1$ and $2 \leq j \leq t$, $(i, j) \to (i, j-1)$;

(iv) For $1 \leq j \leq t-1$, $(s, j) \to (s, j+1)$;

(v) For $1 \leq i \leq s-1$ and $1 \leq j \leq t-1$, $(i,j) \to (i+1,j)$;

(vi) For $2 \leq i \leq s$, $(i,t) \to (i-1,t)$;

and if $s > t$, we define the orientation F_2 of $P_s \boxtimes P_t$ as:

(i) For $2 \leq i \leq s$ and $1 \leq j \leq t-1$, $(i,j) \to (i-1,j+1)$;

(ii) For $1 \leq i \leq s$ and $1 \leq j \leq t$, $(i+1,j+1) \to (i,j)$ if $i-j \geq s-t$ and $(i,j) \to (i+1,j+1)$ if $i-j < s-t$;

(iii) For $1 \leq i \leq s-1$ and $1 \leq j \leq t-1$, $(i,j) \to (i,j+1)$;

(iv) For $2 \leq j \leq t$, $(s,j) \to (s,j-1)$;

(v) For $2 \leq i \leq s$ and $1 \leq j \leq t-1$, $(i,j) \to (i-1,j)$;

(vi) For $1 \leq i \leq s-1$, $(i,t) \to (i+1,t)$.

The orientation F_1 of $P_3 \boxtimes P_4$ and the orientation F_2 of $P_4 \boxtimes P_3$ is shown in Figure 1.

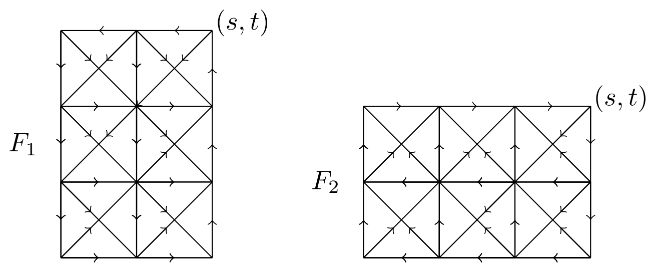

Figure 1: Orientations F_1 and F_2.

Observation 2.1. *If $s < t$, for any $(i,j) \in V(F_1)$,* $\mathrm{dist}_{F_1}((i,j),(s,t-1)) \leq t-2$.

Proof. Let $(i,j) \in V(F_1)$. We shall consider four cases.

(i) If $j \neq t$ and $j \geq i+t-s-1$, then $(i,j) \to (i+1,j) \to \cdots \to (j-(t-s)+1,j) \to (j-(t-s)+2,j+1) \to \cdots \to (s,t-1)$ is a path of length at most $s-1 \leq t-2$.

(ii) If $j \neq t$ and $j < i+t-s-1$, then $(i,j) \to (i+1,j+1) \to \cdots \to (s,j+s-i) \to (s,j+s-i+1) \to \cdots \to (s,t-1)$ is a path of length at most $t-2$.

(iii) If $j = t$ and $i \neq s$, then $(i,t) \to (i+1,t-1) \to (i+2,t-1) \to \cdots \to (s,t-1)$ is a path of length at most $s-1 \leq t-2$.

(iv) If $j = t$ and $i = s$, then $(s,t) \to (s-1,t-1) \to (s,t-1)$ is a path of length two. $\square$

Observation 2.2. *If $s < t$, for any $(i,j) \in V(F_1)$,* $\mathrm{dist}_{F_1}((i,j),(s,t)) \leq t-1$.

Proof. Since $(s,t-1) \to (s,t)$, the claim follows by Observation 2.1:

$$\mathrm{dist}_{F_1}((i,j),(s,t)) = \mathrm{dist}_{F_1}((i,j),(s,t-1)) + 1 \leq s-1+1 \leq t-1. \qquad \square$$

Observation 2.3. *If $s < t$, for any $(i,j) \in V(F_1)$,* $\mathrm{dist}_{F_1}((s-1,t),(i,j)) \leq t-1$.

Proof. Let $(i,j) \in V(F_1)$. We shall consider four cases.

(i) If $i \neq s$ and $j > i+t-s$, then $(s-1,t) \to (s-2,t) \to \cdots \to (i+(t-j),t) \to (i+(t-j)-1,t-1) \to \cdots \to (i,j)$ is a path of length at most $s-2 \leq t-2$.

(ii) If $i \neq s$ and $j \leq i+t-s$, then $(s-1,t) \to (s-1,t-1) \to (s-2,t-2) \to \cdots \to (i,i+t-s) \to (i,i+t-s-1) \to \cdots \to (i,j)$ is a path of length at most $t-1$.

(iii) If $i = s$ and $j \neq t$, $(s-1,t) \to (s-1,t-1) \to (s-1,t-2) \to \cdots \to (s-1,j+1) \to (s,j)$ is a path of length at most $t-1$.

(iv) If $i = s$ and $j = t$, then $(s-1,t) \to (s,t-1) \to (s,t)$ is a path of length two. □

Observation 2.4. *If $s < t$, for any $(i,j) \in V(F_1)$, $\text{dist}_{F_1}((s,t),(i,j)) \leq t-1$.*

Proof. Since $(s,t) \to (s-1,t)$ and $(s,t) \to (s-1,t-1)$, the proof is similar as the proof of Observation 2.3. □

Observation 2.5. *If $s = t$, for any $(i,j) \in V(F_1)$, $\text{dist}_{F_1}((i,j),(s,s)) \leq s$.*

Proof. Let $(i,j) \in V(F_1)$. We shall consider three cases.

(i) If $j \neq t$ and $j \geq i-1$, then $(i,j) \to (i+1,j) \to \cdots \to (j+1,j) \to (j+2,j+1) \to \cdots \to (s,s-1) \to (s,s)$ is a path of length at most s.

(ii) If $j \neq t$ and $j < i-1$, then $(i,j) \to (i+1,j+1) \to \cdots \to (s,j+s-i) \to (s,j+s-i+1) \to \cdots \to (s,s)$ is a path of length at most $s-1$.

(iii) If $j = s$ and $i \neq s$, then $(i,s) \to (i+1,s-1) \to (i+2,s-1) \to \cdots \to (s,s-1) \to (s,s)$ is a path of length at most s. □

Observation 2.6. *If $s = t$, for any $(i,j) \in V(F_1)$, $\text{dist}_{F_1}((s,s),(i,j)) \leq s-1$.*

Proof. Let $(i,j) \in V(F_1)$. We shall consider three cases.

(i) If $i \neq s$ and $j > i$, then $(s,s) \to (s-1,s) \to \cdots \to (i+(s-j),s) \to (i+(s-j)-1,t-1) \to \ldots \to (i,j)$ is a path of length at most $s-1$.

(ii) If $i \neq s$ and $j \leq i$, then $(s,s) \to (s-1,s-1) \to \cdots \to (i,i) \to (i,i-1) \to \ldots \to (i,j)$ is a path of length at most $s-1$.

(iii) If $i = s$ and $j \neq s-1$, $(s,s) \to (s-1,s-1) \to (s-1,s-2) \to \cdots \to (s-1,j+1) \to (s,j)$ is a path of length at most $s-1$.

(iv) If $i = s$ and $j = s-1$, then $(s,s) \to (s-1,s-1) \to (s,s-1)$ is a path of length two. □

Similarly as above, we can prove next Observations 2.7–2.10.

Observation 2.7. *If $s > t$, for any $(i,j) \in V(F_2)$, $\text{dist}_{F_2}((s,t-1),(i,j)) \leq s-1$.*

Observation 2.8. *If $s > t$, for any $(i,j) \in V(F_2)$, $\text{dist}_{F_2}((s,t),(i,j)) \leq s-1$.*

Observation 2.9. *If $s > t$, for any $(i,j) \in V(F_2)$, $\text{dist}_{F_2}((i,j),(s-1,t)) \leq s-2$.*

Observation 2.10. *If $s > t$, for any $(i,j) \in V(F_2)$, $\text{dist}_{F_2}((i,j),(s,t)) \leq s-1$.*

In [7], Koh and Tay also introduced a key-vertex $v \in V(F)$ of digraph F. Let $F \in \mathcal{D}(P_s \boxtimes P_t)$. We say that a vertex $v \in V(F)$ is a *key-vertex* of F if

$$\mathrm{dist}_F(u,v) \leq \max\{t,s\} \quad \text{and} \quad \mathrm{dist}_F(v,u) \leq \max\{t,s\}$$

for all $u \in V(F)$. Note that (s,t) is a key-vertex of F_1 and of F_2.

Analogously as F_1 and F_2, we define 6 other isomorphic orientations F_i, $3 \leq i \leq 8$ of $P_s \boxtimes P_t$ as shown in Figures 2 and 3.

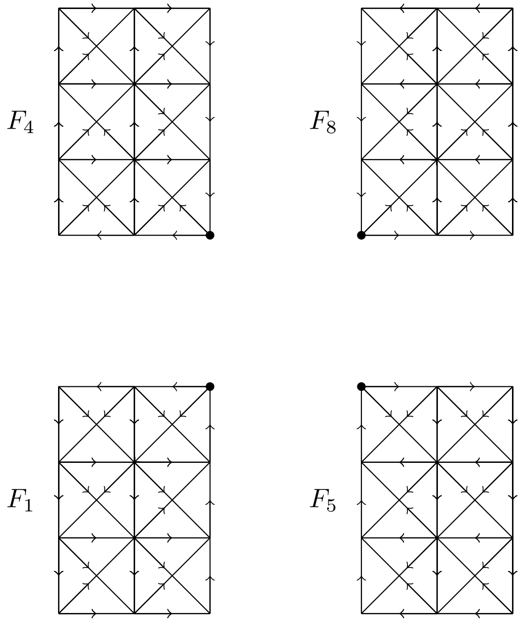

Figure 2: Orientations F_1, F_4, F_5 and F_8.

Obviously vertices denoted by black dots in Figures 2 and 3 are key-vertices of F_i for $i = 1, \ldots, 8$ (similar arguments as in Observations 2.1–2.6).

Lemma 2.11. *Let* $m, n \geq 5$, $m \neq n$ *and* $m, n \equiv 1 \pmod 2$. *Then*

$$\mathrm{diam}_{\min}(P_m \boxtimes P_n) \leq \max\{m-1, n-1\}.$$

Proof. Let $m < n$. We define the orientation D of $P_m \boxtimes P_n$ by F_1, F_4, F_5 and F_8:

(a) orient the section NW as F_4;

(b) orient the section NE as F_8;

(c) orient the section SW as F_1;

(d) orient the section SE as F_5.

As an illustration, the orientation of $P_5 \boxtimes P_7$ is shown in Figure 4. The vertex $z = (\frac{m+1}{2}, \frac{n+1}{2})$ is the key-vertex of each F_i, for $i = 1, 4, 5, 8$. For any $u, v \in V(D)$,

$$\mathrm{dist}_D(u,v) \leq \mathrm{dist}_D(u,z) + \mathrm{dist}_D(z,v).$$

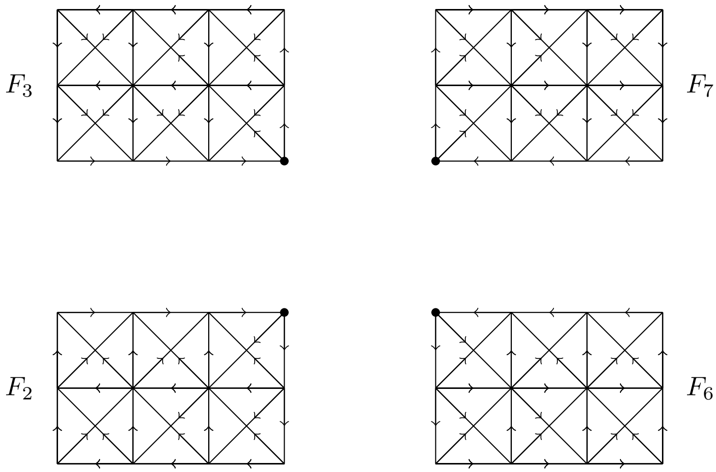

Figure 3: Orientations F_2, F_3, F_6 and F_7.

Since $\mathrm{dist}_D(u,z) \le \frac{n-1}{2}$ and $\mathrm{dist}_D(z,v) \le \frac{n-1}{2}$ (similarly as in Observation 2.2 and Observation 2.4), we have

$$\mathrm{dist}_D(u,v) \le \frac{n-1}{2} + \frac{n-1}{2} = n-1.$$

If $m > n$ we define the orientation D of $P_m \boxtimes P_n$ by F_2, F_3, F_6 and F_7. Similarly as above, we have

$$\mathrm{dist}_D(u,v) \le \mathrm{dist}_D(u,z) + \mathrm{dist}_D(z,v) \le \frac{m-1}{2} + \frac{m-1}{2} = m-1$$

(see Observation 2.10 and Observation 2.8). □

Lemma 2.12. *Let $m,n \ge 6$, $m \ne n$ and $m,n \equiv 0 \pmod 2$. Then*

$$\mathrm{diam}_{\min}(P_m \boxtimes P_n) \le \max\{m-1, n-1\}.$$

Proof. Let $m < n$. Denote $z_1 = (\frac{m}{2}, \frac{n}{2})$, $z_4 = (\frac{m}{2}, \frac{n}{2}+1)$, $z_5 = (\frac{m}{2}+1, \frac{n}{2})$ and $z_8 = (\frac{m}{2}+1, \frac{n}{2}+1)$. We define the orientation D of $P_m \boxtimes P_n$ by F_1, F_4, F_5 and F_8 as follows:

(a) orient the section NW as F_4;

(b) orient the section NE as F_8;

(c) orient the section SW as F_1;

(d) orient the section SE as F_5;

(e) Orient $z_1 \to (\frac{m}{2}-1, \frac{n}{2}+1)$, $(\frac{m}{2}+1, \frac{n}{2}-1) \to z_1$, $z_4 \to (\frac{m}{2}-1, \frac{n}{2})$, $(\frac{m}{2}+1, \frac{n}{2}+2) \to z_4$, $z_5 \to (\frac{m}{2}+2, \frac{n}{2}+1)$, $(\frac{m}{2}, \frac{n}{2}-1) \to z_5$, $z_8 \to (\frac{m}{2}+2, \frac{n}{2})$, $(\frac{m}{2}, \frac{n}{2}+2) \to z_8$, and orient all other edges arbitrarily.

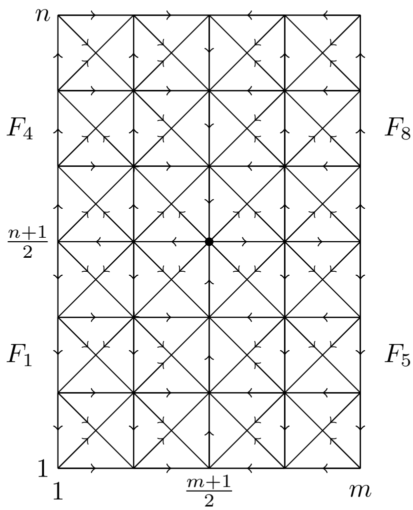

Figure 4: The orientation D of $P_5 \boxtimes P_7$.

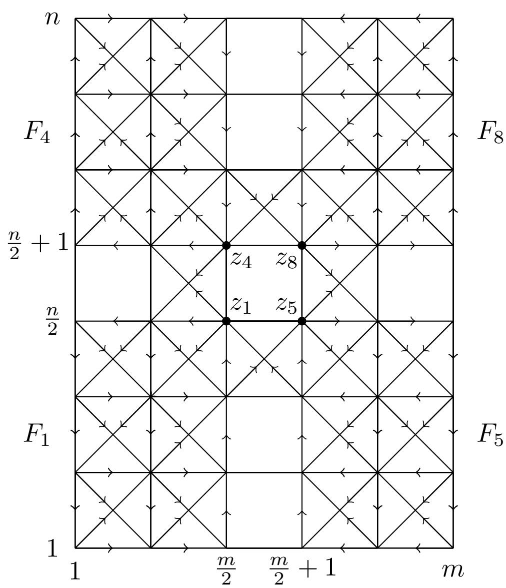

Figure 5: The orientation D of $P_6 \boxtimes P_8$.

The orientation D is shown in Figure 5. Note that vertices z_1, z_4, z_5 and z_8 are key-vertices of F_i, for $i = 1, 4, 5, 8$.

Let $u, v \in V(D)$. We claim that $\mathrm{dist}_D(u, v) \leq n - 1$. There are four cases.

(i) If u and v are in the same section, then we have

$$\mathrm{dist}_D(u, v) \leq \mathrm{dist}_D(u, z_i) + \mathrm{dist}_D(z_i, v) \leq \frac{n}{2} - 1 + \frac{n}{2} - 1 = n - 2$$

as in Observation 2.2 and Observation 2.4.

(ii) If $u \in \mathrm{NW}$ and $v \in \mathrm{SW}$, then (see Observation 2.2 and Observation 2.3):

$$\begin{aligned}\mathrm{dist}_D(u, v) &\leq \mathrm{dist}_D(u, z_4) + \mathrm{dist}_D\left(z_4, (\tfrac{m}{2} - 1, \tfrac{n}{2})\right) + \mathrm{dist}_D\left((\tfrac{m}{2} - 1, \tfrac{n}{2}), v\right)\\ &\leq \frac{n}{2} - 1 + 1 + \frac{n}{2} - 1 = n - 1.\end{aligned}$$

The argument is similar if $u \in \mathrm{SW}$ and $v \in \mathrm{NW}$, or $u \in \mathrm{NE}$ and $v \in \mathrm{SE}$, or $u \in \mathrm{SE}$ and $v \in \mathrm{NE}$.

(iii) If $u \in \mathrm{SW}$ and $v \in \mathrm{SE}$, then the claim follows from Observation 2.1 and Observation 2.4, similarly as above. Also, if $u \in \mathrm{SE}$ and $v \in \mathrm{SW}$, or $u \in \mathrm{NW}$ and $v \in \mathrm{NE}$, or $u \in \mathrm{NE}$ and $v \in \mathrm{NW}$, then the argument is analogous.

(iv) If $u \in \mathrm{SW}$ and $v \in \mathrm{NE}$, then (see Observation 2.1 and Observation 2.3) we have

$$\begin{aligned}\mathrm{dist}_D(u, v) &\leq \mathrm{dist}_D\left(u, (\tfrac{m}{2}, \tfrac{n}{2} - 1)\right) + \mathrm{dist}_D\left((\tfrac{m}{2}, \tfrac{n}{2} - 1), z_5\right) +\\ &\qquad + \mathrm{dist}_D\left(z_5, (\tfrac{m}{2} + 2, \tfrac{n}{2} + 1)\right) + \mathrm{dist}_D\left((\tfrac{m}{2} + 2, \tfrac{n}{2} + 1), v\right)\\ &\leq \frac{n}{2} - 2 + 1 + 1 + \frac{n}{2} - 1 = n - 1.\end{aligned}$$

The argument is similar for $u \in \mathrm{NE}$ and $v \in \mathrm{SW}$, or $u \in \mathrm{NW}$ and $v \in \mathrm{SE}$, or $u \in \mathrm{SE}$ and $v \in \mathrm{NW}$.

Analogously if $m > n$, we have $\mathrm{dist}_D(u, v) \leq m - 1$ for any $u, v \in V(D)$. $\square$

Lemma 2.13. *Let $m \geq 5$, $n \geq 6$, $m \equiv 1 \pmod 2$ and $n \equiv 0 \pmod 2$. Then*

$$\mathrm{diam}_{\min}(P_m \boxtimes P_n) \leq \max\{m - 1, n - 1\}. \tag{2.1}$$

Proof. Let $m < n$. Denote $z_1 = (\frac{m+1}{2}, \frac{n}{2})$ and $z_4 = (\frac{m+1}{2}, \frac{n}{2} + 1)$. We define the orientation D of $P_m \boxtimes P_n$ by F_1, F_4, F_5 and F_8 as follows:

(a) orient the section NW as F_4;

(b) orient the section NE as F_8;

(c) orient the section SW as F_1;

(d) orient the section SE as F_5;

(e) orient $z_4 \to (\frac{m+1}{2} - 1, \frac{n}{2})$, $z_1 \to z_4$, $z_4 \to (\frac{m+1}{2} + 1, \frac{n}{2})$, and orient all other edges arbitrarily.

The orientation D is shown in Figure 6. Note that vertex z_1 is a key-vertex of F_1 and F_5 and that vertex z_4 is a key-vertex of F_4 and F_8.

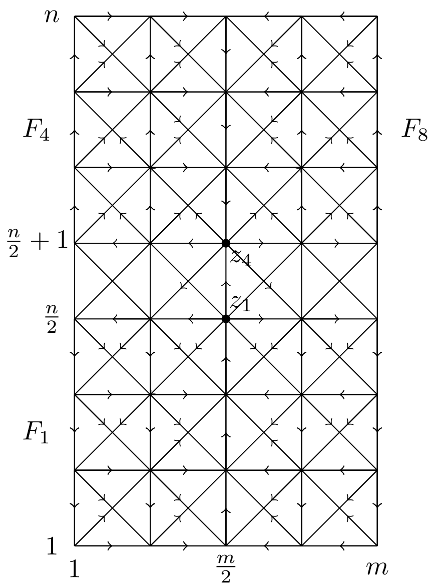

Figure 6: The orientation D of $P_5 \boxtimes P_8$.

Let $u, v \in V(D)$. There are three cases.

(i) If $u \in \text{NW} \cup \text{NE}$ and $v \in \text{NW} \cup \text{NE}$, then we have

$$\text{dist}_D(u,v) \leq \text{dist}_D(u,z_4) + \text{dist}_D(z_4,v) \leq \frac{n}{2} - 1 + \frac{n}{2} - 1 = n-2$$

(see Observation 2.2 and Observation 2.4). The case that $\{u,v\} \subseteq \text{SW} \cup \text{SE}$ is similar.

(ii) If $u \in \text{SW} \cup \text{SE}$ and $v \in \text{NW} \cup \text{NE}$, then (see Observation 2.2 and Observation 2.4):

$$\begin{aligned}\text{dist}_D(u,v) &\leq \text{dist}_D(u,z_1) + \text{dist}_D(z_1,z_4) + \text{dist}_D(z_4,v) \\ &\leq \frac{n}{2} - 1 + 1 + \frac{n}{2} - 1 = n-1.\end{aligned}$$

(iii) If $u \in \text{NW} \cup \text{NE}$ and $v \in \text{SW}$, then from Observation 2.2 and Observation 2.3:

$$\begin{aligned}\text{dist}_D(u,v) &\leq \text{dist}_D(u,z_4) + \text{dist}_D\left(z_4, \left(\tfrac{m+1}{2}-1, \tfrac{n}{2}\right)\right) + \\ &\quad + \text{dist}_D\left(\left(\tfrac{m+1}{2}-1, \tfrac{n}{2}\right), v\right) \\ &\leq \frac{n}{2} - 1 + 1 + \frac{n}{2} - 1 = n-1.\end{aligned}$$

The case that $u \in \text{NW} \cup \text{NE}$ and $v \in \text{SE}$ is similar.

Let $m > n$. Denote $z_2 = (\frac{m+1}{2}, \frac{n}{2})$ and $z_3 = (\frac{m+1}{2}, \frac{n}{2}+1)$. We define the orientation D of $P_m \boxtimes P_n$ by F_2, F_3, F_6 and F_7 as follows:

(a) orient the section NW as F_3;

(b) orient the section NE as F_7;

(c) orient the section SW as F_2;

(d) orient the section SE as F_6;

(e) orient $(\frac{m+1}{2}-1, \frac{n}{2}) \to z_3$, $z_3 \to z_2$, $(\frac{m+1}{2}+1, \frac{n}{2}) \to z_3$ and all other edges oriented arbitrarily.

The rest of the proof is analogously as above. □

Note that if $m \geq 5$ and $n \geq 6$, $m \equiv 0 \pmod 2$ and $n \equiv 1 \pmod 2$, we also have (2.1).

Lemma 2.14. *Let $m \geq 5$, $m \equiv 1 \pmod 2$. Then*

$$\operatorname{diam}_{\min}(P_m \boxtimes P_m) \leq m.$$

Proof. Denote $z = (\frac{m+1}{2}, \frac{m+1}{2})$. We define the orientation D of $P_m \boxtimes P_m$ by F_1, F_4, F_5 and F_8 as follows:

(a) orient the section NW as F_4;

(b) orient the section NE as F_8;

(c) orient the section SW as F_1;

(d) orient the section SE as F_5.

Note that z is a key-vertex of F_i, for $i = 1, 4, 5, 8$. For any $u, v \in D$ we have

$$\operatorname{dist}_D(u, v) \leq \operatorname{dist}_D(u, z) + \operatorname{dist}_D(z, v) \leq \frac{m+1}{2} + \frac{m-1}{2} = m$$

as in Observation 2.5 and Observation 2.6. □

Lemma 2.15. *Let $m \geq 6$, $m \equiv 0 \pmod 2$. Then*

$$\operatorname{diam}_{\min}(P_m \boxtimes P_m) \leq m.$$

Proof. The proof is similarly as the proof of Lemma 2.12 (it follows from Observations 2.1, 2.3, 2.5 and 2.6). □

In [2], it is proved that if (u, v) and (u', v') are vertices of a strong product $G \boxtimes H$, then

$$\operatorname{dist}_{G \boxtimes H}((u, v), (u', v')) = \max\{\operatorname{dist}_G(u, u'), \operatorname{dist}_H(v, v')\}.$$

Since $\operatorname{diam}(P_m) = m - 1$, we get $\operatorname{diam}(P_m \boxtimes P_n) = \max\{m-1, n-1\}$. Since $\operatorname{diam}(P_m \boxtimes P_n) = \operatorname{dist}_{P_m \boxtimes P_m}((1,1), (m,m)) = m - 1$ and there is only one path from $(1, 1)$ to (m, m) in $P_m \boxtimes P_m$ possessing the length $m - 1$, it follows that

$$\operatorname{dist}_D((1,1), (m,m)) > m - 1 \quad \text{or} \quad \operatorname{dist}_D((m,m), (1,1)) > m - 1$$

for any $D \in \mathcal{D}(P_m \boxtimes P_n)$. To combine these two observations with Lemmas 2.11–2.15, we obtain the following theorem:

Theorem 2.16. *If* $m, n \geq 5$, *then*

$$\operatorname{diam}_{\min}(P_m \boxtimes P_n) = \begin{cases} \operatorname{diam}(P_m \boxtimes P_n), & \text{if } m \neq n; \\ \operatorname{diam}(P_m \boxtimes P_n) + 1, & \text{if } m = n. \end{cases}$$

At the end of this section, we give the bounds of $\operatorname{diam}_{\min}(P_n \boxtimes P_m)$ for $m < 5$. From Figure 7, we see that $n - 1 \leq \operatorname{diam}_{\min}(P_n \boxtimes P_2) = n$ for $n > 2$, $n - 1 \leq \operatorname{diam}_{\min}(P_n \boxtimes P_3) = n$ for $n > 3$ and $n - 1 \leq \operatorname{diam}_{\min}(P_n \boxtimes P_4) = n + 1$ for $n > 4$.

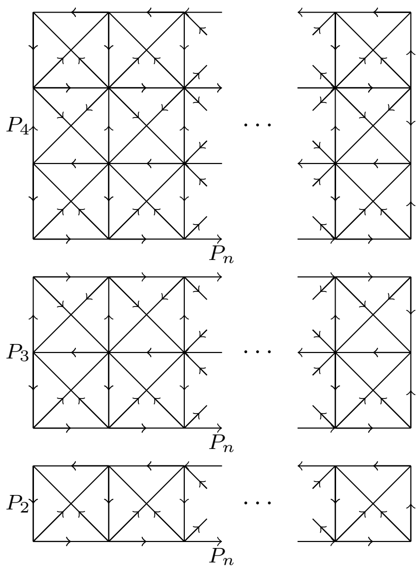

Figure 7: Orientations of $P_n \boxtimes P_2$, $P_n \boxtimes P_3$ and $P_n \boxtimes P_4$.

3 Strong orientation of graphs

In this section we shall prove the next theorem.

Theorem 3.1. *Let G and H be connected bridgeless graphs. Then*

$$\operatorname{diam}_{\min}(G \boxtimes H) \leq \max\{\operatorname{diam}_{\min}(G), \operatorname{diam}_{\min}(H)\}.$$

Proof. Let D_G be a strong orientation of G such that $\operatorname{diam}(D_G) = \operatorname{diam}_{\min}(G) = d_1$ and let D_H be a strong orientation of H such that $\operatorname{diam}(D_H) = \operatorname{diam}_{\min}(H) = d_2$. We define the orientation $D_{G \boxtimes H}$ of $G \boxtimes H$ as:

(a) Every edge with endvertices in layers G_v, $v \in V(H)$ gets the orientation D_G.

(b) Every edge with endvertices in layers H_u, $u \in V(G)$ gets the orientation D_H.

(c) If $u \to u'$ in G and $v \to v'$ in H, then $(u, v) \to (u', v')$, all other edges are oriented arbitrarily.

We have to prove that for every pair of vertices (u, v), (u', v') in $G \boxtimes H$ there is a directed path P from (u, v) to (u', v') in $D_{G \boxtimes H}$, such that the length of P is at most $\max\{d_1, d_2\}$.

If (u, v) and (u', v) are vertices in the same G-layer or if (u, v) and (u, v') are vertices in the same H-layer, then there is a directed path from (u, v) to (u', v) in $D_{G \boxtimes H}$ of length at most d_1 or a directed path from (u, v) to (u, v') of length at most d_2.

Now let (u, v) and (u', v') be arbitrary vertices in $D_{G \boxtimes H}$. There is a directed path $u = u_1 u_2 \ldots u_m = u'$ in G of length at most d_1 and there is a directed path $v = v_1 v_2 \ldots v_n = v'$ in H of length at most d_2. Without loss of generality we can assume $m \geq n$. We have

$$(u, v) \to (u_2, v_2) \to (u_3, v_3) \to \cdots \to (u_n, v_n) \to \\ (u_{n+1}, v_n) \to \cdots \to (u_m, v_n) = (u', v')$$

is a path of length at most d_1. □

Since $\operatorname{diam}_{\min}(C_3) = 2$ and $\operatorname{diam}_{\min}(C_3 \boxtimes C_3) = 2$, the bound is tight.

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On the anti-Kekulé problem of cubic graphs*

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Abstract

An edge set S of a connected graph G is called an anti-Kekulé set if $G - S$ is connected and has no perfect matchings, where $G - S$ denotes the subgraph obtained by deleting all edges in S from G. The anti-Kekulé number of a graph G, denoted by $ak(G)$, is the cardinality of a smallest anti-Kekulé set of G. It is NP-complete to determine the anti-Kekulé number of a graph. In this paper, we show that the anti-Kekulé number of a 2-connected cubic graph is either 3 or 4, and the anti-Kekulé number of a connected cubic bipartite graph is always equal to 4. Furthermore, a polynomial time algorithm is given to find all smallest anti-Kekulé sets of a connected cubic graph.

Keywords: Anti-Kekulé set, anti-Kekulé number, cubic graphs.

Math. Subj. Class.: 05C10, 05C70, 05C90

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1 Introduction

Let G be a graph. A *perfect matching* of a graph G is a set of non-adjacent edges that covers all vertices of G. A perfect matching of a graph is also called a *Kekulé structure* in mathematical chemistry and statistical physics. An edge set S of a connected graph G is called an *anti-Kekulé set* if $G - S$ is connected and has no perfect matchings, where $G - S$ denotes the subgraph obtained by deleting all edges in S from G. The *anti-Kekulé number* of a graph G, denoted by $ak(G)$, is the cardinality of a smallest anti-Kekulé set of G. The anti-Kekulé number of a graph is hard to be determined in general. It has been proved recently that it is an NP-complete problem to determine the anti-Kekulé number of a connected bipartite graph by Lü, Li and Zhang [17].

In chemistry and physics, graphs are used to represent the skeletons of molecules, and Kekulé structures (or perfect matchings) are used to model special structures of bonds between atoms. For example, for a benzenoid hydrocarbons, graphens or fullerenes, a Kekulé structure of these molecules stands for double bonds between atoms. An anti-Kekulé set is a set of double bonds whose removal significantly affects the whole molecule structure by the valence bond (VB) theory (cf. [15]).

A fullerene is a 3-connected plane cubic graph such that every face is either a hexagon or a pentagon. For example, C_{60} is a fullerene with 60 vertices such that all pentagons are disjoint. The anti-Kekulé number of C_{60} is proved to be 4 by Vukičević [26]. A leapfrog fullerene is a fullerene obtained by the leapfrog operation (see [16]). Kutnar et al. [16] obtained a bound for the anti-Kekulé number of leapfrog fullerenes as follows.

Theorem 1.1 ([16])**.** *Let G be a leapfrog fullerene. Then $3 \leq ak(G) \leq 4$.*

The above result was improved by Yang et al. [28] by proving that all fullerenes have anti-Kekulé number 4. The anti-Kekulé numbers of other interesting graphs, such as benzenoid hydrocarbons [2, 27], fence graphs [22], infinite triangular, rectangular and hexagonal grids [25] as well as cata-condensed phenylenes [35], have been investigated.

The result on fullerenes has been generalized to general cubic graphs with high cyclic edge-connectivity in [30]. A graph G is cyclically k-edge-connected if G cannot be separated into two components, each containing a cycle, by deletion of fewer than k edges. The *cyclic edge-connectivity* $c\lambda(G)$ of a graph G is the maximum k such that G is cyclically k-edge-connected. An edge set S is called an *odd cycle edge-transversal* of a graph G if $G - S$ is bipartite. The size of a smallest odd cycle edge-transversal of G is denoted by $\tau_{\text{odd}}(G)$.

Theorem 1.2 ([30])**.** *Let G be a cyclically 4-edge-connected cubic graph. Then either $ak(G) = 4$ or $1 \leq \tau_{odd}(G) \leq 3$.*

The result above can be used to determine the anti-Kekulé number of fullerenes. Since a smallest odd cycle-transversal of a fullerene graph contains at least 6 edges and the cyclic edge-connectivity of a fullerene graph is 5 (see [5, 20]), Theorem 1.2 implies that every fullerene has anti-Kekulé number 4. However, Theorem 1.2 is not applicable to determine the anti-Kekulé numbers of some interesting graphs, such as, some boron-nitrogen fullerenes with low cyclic edge-connectivity, $(3, 6)$-fullerenes etc.

A $(k, 6)$-cage ($k \geq 3$) is a 3-connected cubic plane graph whose faces are either k-gons or hexagons. Došlić [5] shows that $(k, 6)$-cages only exist for $k = 3$, 4 and 5. A fullerene is a $(5, 6)$-cage and the $(4, 6)$-cages and $(3, 6)$-cages are usually called $(4, 6)$-fullerenes (or boron-nitrogen fullerens) and $(3,6)$-fullerenes, respectively. Many researches have investigated the properties of these graphs in both mathematics and chemistry, such as hamiltonicity [9, 10], resonance [29, 31, 33], the forcing matching number [13, 34], and energy spectra of $(3,6)$-fullerenes [4, 14] which determines their electronic and magnetic properties [3, 21].

The cyclic edge-connectivity of $(k,6)$-cages has been obtained by Došlić in [5]. Let $\mathcal{T}$ be a family of $(4,6)$-fullerenes, which consists of a tube with n layers of hexagons (i.e. each layer is a cyclic chain of three hexagons) capped on both ends by a cap formed by three quadrangles.

Theorem 1.3 ([5])**.** *Let G be a $(k,6)$-cage. Then $c\lambda(G) = 3$ if $G \in \mathcal{T}$, and $c\lambda(G) = k$ otherwise.*

In this paper, we consider the anti-Kekulé number of connected cubic graphs including those with low cyclic edge-connectivity. The following is our first major result.

Theorem 1.4. *If G is a 2-connected cubic graph, then $3 \leq ak(G) \leq 4$.*

Since a leapfrog fullerene is 3-connected, Theorem 1.1 is a direct corollary of Theorem 1.4. For bipartite cubic graphs, the result can be strengthened as follows.

Theorem 1.5. *If G is a connected cubic bipartite graph, then $ak(G) = 4$.*

Theorems 1.4 and 1.5 can be applied to determine the anti-Kekulé numbers of boron-nitrogen fullerenes, $(3,6)$-fullerenes, toroidal and bipartite Klein-bottle fullerenes (see Section 3 for details). Based on Theorems 1.4 and 1.5, a polynomial time algorithm is given to find all smallest anti-Kekulé sets of a connected cubic graph G in Section 4.

2 Proofs of main results

The well-known theorem of Tutte is essential to our proof of the main results.

Theorem 2.1 (Tutte's Theorem [23])**.** *A graph G has a perfect matching if and only if $c_o(G-U) \leq |U|$ for any $U \subseteq V(G)$, where $c_o(G-U)$ is the number of odd components of $G-U$.*

A *bridge* is an edge of a connected graph whose deletion disconnects the graph. By Petersen's Theorem [19], every cubic graph without bridges has a perfect matching. Therefore, the anti-Kekulé number of a 2-connected cubic graph G (note that a cubic graph possesses the same connectivity and edge-connectivity) is at least one, that is, $ak(G) \geq 1$. Indeed, this lower bound can be improved and we present the proof by using Tutte's Theorem. For $X \subseteq V(G)$, let $\partial(X)$ denote the set of edges with one end in X and the other end in $V(G)-X$. We also denote $d(X) = |\partial(X)|$.

Proof of Theorem 1.4. Let A be an anti-Kekulé set of size $ak(G)$. According to the definition, $G' := G - A$ has no perfect matchings. Hence, Theorem 2.1 implies that there exists $S \subseteq V(G')$ such that $c_o(G'-S) > |S|$. Choose such an S with the maximum size.

Claim 1. *$G'-S$ has no even components and it has exactly $|S|+2$ odd components.*

Suppose by the contrary, $G'-S$ has an even component H. Thus, for any given vertex $v \in V(H)$, $H - \{v\}$ has at least one odd component. Let $S' = S \cup \{v\}$. Then $G'-S'$ has at least $c_o(G'-S)+1$ odd components. That is,

$$c_o(G'-S') \geq c_o(G'-S) + 1 > |S| + 1 = |S'|,$$

contradicting the choice of S. Therefore $G' - S$ has no even component.

Since G is a cubic graph, it has an even number of vertices. This implies that $c_o(G'-S)$ and $|S|$ are of the same parity, thus $c_o(G'-S) \geq |S|+2$. For any edge $e \in A$, since A is an anti-Kekulé set with the smallest cardinality, $G'+e$ has a perfect matching (note that $G'+e$ is the graph with vertex set $V(G')$ and edge set $E(G') \cup \{e\}$). Hence $c_o(G'+e-S) \leq |S|$ by Theorem 2.1. Moreover, adding any edge e to $G' - S$ will connect at most two odd components. Therefore, $|S| \geq c_o(G'+e-S) \geq c_o(G'-S) - 2 \geq |S|$ and thus, $c_o(G'-S) - 2 = |S|$.

Claim 2. *Let G_i, with $1 \leq i \leq |S|+2$, be the odd components of $G' - S$. We have*

$$\sum_{i=1}^{|S|+2} d(G_i) - 2ak(G) \leq 3|S|. \tag{2.1}$$

We count the number of edges between S and the odd components, which is denoted by N, in two different ways. On one hand, S contributes at most $3|S|$ to N. On the other hand, all the odd components send out $\sum_{i=1}^{|S|+2} d(G_i) - 2ak(G)$ edges to N. Thus $\sum_{i=1}^{|S|+2} d(G_i) - 2ak(G) = N \leq 3|S|$ and the claim holds.

Since G is 2-edge-connected, $d(G_i) \geq 2$ for every i. By a simple computation $d(G_i) = 3|V(G_i)| - 2|E(G_i)|$, which implies that $d(G_i)$ and $|V(G_i)|$ are of the same parity. Since every G_i is an odd component, $|V(G_i)|$ is odd and hence $d(G_i)$ is odd, therefore $d(G_i) \geq 3$.

Substituting this inequality into Equation (2.1), we have

$$3(|S|+2) - 2ak(G) \leq \sum_{i=1}^{|S|+2} d(G_i) - 2ak(G) \leq 3|S|,$$

and so $ak(G) \geq 3$.

Now we are going to establish an upper bound on $ak(G)$ and it is sufficient to find an anti-Kekulé set of size 4. Let $a \in V(G)$ and let b as well as c be its two distinct neighbors. Denote the two edges incident with b other than ab by e_1 and e_2, similarly, denote the two edges incident with c other than ac by e_3 and e_4. Hence, removing $E_a = \{e_1, e_2, e_3, e_4\}$ from G will obtain a subgraph without perfect matchings. Therefore, E_a is an anti-Kekulé set if $G - E_a$ is connected (there exists some vertex a such that $G - E_a$ is not connected, see Figure 1). Consider the following two cases according to the different connectivities.

Case 1. *G is 3-connected.*

We are going to prove that for any vertex a in G, $G - E_a$ is connected. Suppose by the contrary that $G - E_a$ is not connected. Then the vertices of G are divided into two parts X and $\overline{X}$ with a subset $E' \subseteq E_a$ connecting them. Since G is 3-connected, E' consists of three or four edges in E_a. If it contains three edges, by symmetry, we assume $E' = \{e_1, e_2, e_3\}$. Since there are exactly three edges between X and $\overline{X}$, the edge ab lies in the same part. We may assume that both a and b belong to X. Since $\{ab, e_3\}$ divides G into two parts $\overline{X} \cup \{b\}$ and $X \setminus \{b\}$, $\{ab, e_3\}$ is a 2-edge-cut of G which is a contradiction (note that a 2-edge-cut is an edge-cut of size 2). If E' contains four edges, that is $E' = E_a = \{e_1, e_2, e_3, e_4\}$, then by a similar argument as above, we know that a, b and c lie in the same part, and moreover $\{ab, ac\}$ forms a 2-edge-cut of G which is a contradiction.

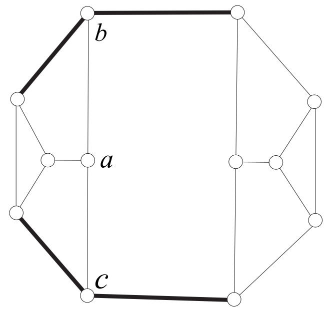

Figure 1: E_a are the bold edges.

Note that $G - E_a$ is connected and $G - E_a$ has no perfect matchings. Therefore, E_a is an anti-Kekulé set of size 4 and we have $ak(G) \leq 4$.

Case 2. *G has connectivity* 2.

Since G is 2-connected but not 3-connected, there exist 2-edge-cuts. Moreover, each 2-edge-cut is an independent set, otherwise the third edge incident to their common end vertex is a bridge, which contradicts that G is 2-connected. Every 2-edge-cut will split G into exactly two subgraphs. Among those subgraphs, denote the subgraph with smallest cardinality by G' and the corresponding 2-edge-cut by $E = \{e_4, e_5\}$. Also, denote the end-vertices of e_4 and e_5 in G' by v and u, respectively. Moreover, let G'' be the other subgraph obtained by deleting E.

Claim 3. $uv \notin E(G)$.

Assume $uv \in E(G)$. Then the edges incident with u or v other than uv, e_4 and e_5 form a 2-edge-cut. The deletion of this 2-edge-cut creates a subgraph with cardinality smaller than G', contradicting the choice of E.

Claim 4. *No* 2*-edge-cut of G contains an edge $e \in E(G')$.*

Suppose the claim is false and there exists $e \in E(G')$ that lies in some 2-edge-cut $E' = \{e, e'\}$. No matter where e' lies in, the subgraph induced by $V(G'') \cup \{u\}$ or $V(G'') \cup \{v\}$ belongs to a component created by the deletion of E'. Thus the cardinality of the other component is smaller than G', which contradicts the choice of E and the claim holds.

Let s be a neighbor of v in G'. Since s is of degree 3, there exists a neighbor t $(\neq u)$ of it in G'. Let e_1 and e_2 be two incident edges of t other than st, and let e_3 be the edge incident with v other than sv and e_2. We claim that $\{e_1, e_2, e_3, e_4\}$ is an anti-Kekulé set. It is obvious that $G - \{e_1, e_2, e_3, e_4\}$ has no perfect matchings. If $G - \{e_1, e_2, e_3, e_4\}$ is not connected, then, similar to Case 1, we obtain a 2-edge-cut containing at least one edge in G'. This is a contradiction and completes the proof. □

The condition "2-edge-connected" in Theorem 1.4 is necessary because there exist cubic graphs with bridges and their anti-Kekulé number is less than 3 (see Figure 2). More precisely, we have the following result.

Theorem 2.2. *If G is a connected cubic graph with bridges, then $ak(G) \leq 2$.*

Proof. Choose a bridge such that the deletion of it will give a subgraph with the smallest cardinality, we denote this subgraph by G' and the corresponding bridge by e. Let the end vertex of e in G' be u and let v be a neighbor of u in G'. Moreover, let the two other edges incident with v other than uv be e_1 and e_2. Similar to the proof of Case 2 in Theorem 1.4, we have $G - \{e_1, e_2\}$ is connected. Since any bridge separates G into two odd components, any perfect matching M of G should contain e. Also, M contains one edge in $\{e_1, e_2\}$ and thus, $G - \{e_1, e_2\}$ has no perfect matchings. As a result, $\{e_1, e_2\}$ is an anti-Kekulé set and so $ak(G) \leq 2$. □

Figure 2 presents three cubic graphs with anti-Kekulé numbers 0, 1 and 2, and the sets of bold edges denote their smallest anti-Kekulé sets respectively.

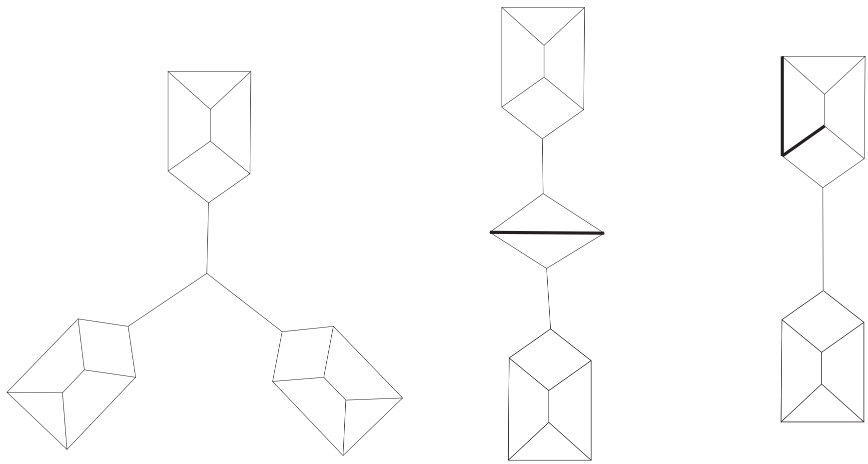

Figure 2: Three cubic graphs with anti-Kekulé numbers 0, 1 and 2 respectively.

If the graphs being considered are bipartite, then a stronger result can be obtained by using Hall's Theorem.

Theorem 2.3 (Hall's Theorem [11])**.** *Let G be a bipartite graph with bipartition W and B. Then G has a perfect matching if and only if $|W| = |B|$ and for any $U \subseteq W$, $|N(U)| \geq |U|$ holds.*

Proof of Theorem 1.5. First we show that a connected cubic bipartite graph is essentially 2-connected. By Theorem 2.3, a k-regular bipartite graph contains a perfect matching. Removing that perfect matching will result in a $(k-1)$-regular bipartite graph, and the same argument can be applied repeatedly. Finally, we deduce that a k-regular bipartite graph can be decomposed into k disjoint perfect matchings. Since G is a cubic bipartite graph, it can be decomposed into three disjoint perfect matchings M_1, M_2 and M_3, that is, $E(G) = M_1 \cup M_2 \cup M_3$. For any $e \in E(G)$, without loss of generality, let $e \in M_1$. Since M_1 and M_2 are disjoint perfect matchings of G, $M_1 \cup M_2$ consists of disjoint even cycles and e lies in one of them. Hence e is not a bridge and G is 2-edge-connected. Furthermore, a 2-edge-connected cubic graph is 2-connected, thus G is 2-connected.

According to Theorem 1.4, we have $3 \leq ak(G) \leq 4$. Suppose by the contrary that $ak(G) \neq 4$, that is, $ak(G) = 3$. Let $A = \{e_1, e_2, e_3\}$ be an anti-Kekulé set. Then $G - A$

has no perfect matchings. Assume W and B are the bipartition of G. According to Hall's theorem, there exists $S \subseteq W$ such that

$$|N_{G-A}(S)| \leq |S| - 1. \tag{2.2}$$

On the other hand, since A is an anti-Kekulé set with the smallest cardinality, we have

$$|S| \leq |N_{G-A+e_i}(S)| \tag{2.3}$$

for $i = 1, 2$ and 3. Adding an edge e_i to $G - A$ will increase the neighbors of S by one (at most). Hence

$$|N_{G-A+e_i}(S)| \leq |N_{G-A}(S)| + 1. \tag{2.4}$$

Combining inequalities (2.2), (2.3) and (2.4), we obtain $|S| = |N_{G-A}(S)| + 1$. Let $S' = N_{G-A}(S)$. The edges going out from S are divided into two parts: either goes into A or goes into S'. Thus the number of edges between S and S' is $3|S| - 3$. Since $|S'| = |S| - 1$, there is no edge between S' and $W - S$. Therefore, A is an edge-cut, which contradicts the definition of anti-Kekulé set and the proof is complete. □

3 Applications

In this section, we apply Theorems 1.4 and 1.5 to obtain the anti-Kekulé numbers of several families of interesting graphs, such as boron-nitrogen fullerenes and $(3, 6)$-fullerenes.

Theorem 3.1. *If G is a $(4, 6)$-fullerene, then $ak(G) = 4$.*

Proof. Since G is bipartite, the result follows immediately by Theorem 1.5. □

Note that there are two classes of boron-nitrogen fullerenes, one with cyclic edge-connectivity 3 and the other with cyclic edge-connectivity 4. The anti-Kekulé number of the latter can be obtained by Theorem 1.2. Now we are going to determine the anti-Kekulé number of $(3, 6)$-fullerenes and the following lemma is required. A cyclic 3-edge-cut of a $(3, 6)$-fullerene is called *trivial* if it is formed by the edges incident to a triangle in common. A 3-edge-cut is called *trivial* if they are incident to a common vertex. Let T_n $(n \geq 1)$ be the graph consisting of n concentric layers of hexagons in which each layer is a cyclic chain of two hexagons, capped on each end by a cap formed by two adjacent triangles (see Figure 3).

Lemma 3.2 ([29]).

(i) Every cyclic 3-edge-cut of a $(3, 6)$-fullerene with connectivity 3 is trivial.

(ii) The connectivity of a $(3, 6)$-fullerene is 2 if and only if it is isomorphic to T_n for some $n \geq 1$.

Theorem 3.3. *If G is a $(3, 6)$-fullerene, then $ak(G) = 3$.*

Proof. Let G be a $(3, 6)$-fullerene. Note that a $(3, 6)$-fullerene has connectivity either 2 or 3. Thus, Theorem 1.4 implies that $3 \leq ak(G) \leq 4$. To show that $ak(G) = 3$, it suffices to give an anti-Kekulé set of size 3.

First, assume that the connectivity of G is 2. By Lemma 3.2, G has two triangles sharing a common edge. Let S be the edge set of such a triangle (see Figure 3). Then

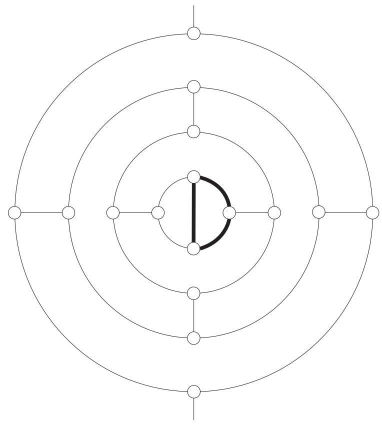

Figure 3: A $(3, 6)$-fullerene T_3 and the set of bold edges form an anti-Kekulé set of it.

$G - S$ has two vertices of degree 1 adjacent to a common vertex. Hence $G - S$ has no perfect matching. Clearly, $G - S$ is connected. So S is an anti-Kekulé set of size 3.

In the following, assume that G is 3-connected. Let S be a 3-edge-cut and let G_1 as well as G_2 be the two components of $G - S$. If S is not trivial, then $d(G_i) = 3$ and $|V(G_i)| \geq 2$ for $i = 1, 2$. Since $|V(G_i)|$ and $d(G_i)$ are of the same parity, it follows that $|V(G_i)| \geq 3$. Hence

$$|E(G_i)| - |V(G_i)| = \frac{3|V(G_i)| - 3}{2} - |V(G_i)| = \frac{|V(G_i)| - 3}{2} \geq 0.$$

Therefore both G_1 and G_2 contain cycles. So S is a cyclic 3-edge-cut. By Lemma 3.2, S is a trivial cyclic 3-edge-cut. Hence, a 3-edge-cut of G is either a trivial 3-edge-cut or a trivial cyclic 3-edge-cut.

Let abc be a triangle of G. Let e_1 be the edge incident with a but not inside of the triangle, and e_2 be the edge incident with c but not contained in the triangle. The edge set $S = \{e_1, e_2, ac\}$ does not isolate a vertex or a triangle. So S is not an edge-cut. In the subgraph $G - S$, both a and c have degree 1 and both of them are adjacent to b. So $G - S$ has no perfect matching. Therefore, S is an anti-Kekulé set. This completes the proof. □

Furthermore, since a toroidal fullerene or a bipartite Klein-bottle fullerene, whose definitions can be found in [32], is a cubic bipartite graph, the following result is a direct consequence of Theorem 1.5. Note that this result can also be deduced from Theorem 1.2.

Corollary 3.4. *If G is either a toroidal fullerene or a bipartite Klein-bottle fullerene, then $ak(G) = 4$.*

4 Finding all the smallest anti-Kekulé sets

The anti-Kekulé problem of graphs can be stated as follows.

Instance: *A nonempty graph $G = (V, E)$ having a perfect matching and a positive k.*
Question: *Is there a subset $B \subseteq E$ with $|B| \leq k$ such that $G' = (V, E \setminus B)$ is connected and G' has no Kekulé structure?*

In [17], the authors showed that anti-Kekulé problem on bipartite graphs is NP-complete. So it is hard to find a smallest anti-Kekulé set of a given graph. However, for cubic graphs, the problem becomes much easier by Theorems 1.4 and 1.5: all the smallest anti-Kekulé sets of a cubic graph can be found in polynomial time. The algorithm finding all smallest anti-Kekulé sets S of a cubic graph G depends on how to find a maximum matching in the graph $G - S$. If the maximum matching of $G - S$ has size exactly $n/2$ where n is the number of vertices of G, then it is a perfect matching of $G - S$.

For a given graph G with n vertices, Edmonds [6] found an algorithm to find a maximum matching of G in $O(n^4)$ steps, which is the blossom algorithm. An efficient implementation of Edmonds' algorithm takes $O(n^3)$ steps to find a maximum matching [7]. For bipartite graphs, Hopcroft and Karp [12] gave an algorithm taking $O(n^{5/2})$ steps to find a maximum matching. Later, Micali and Vazirani [18, 24], Gabow and Tarjan [8], and Blum [1] have given algorithms to find a maximum matching of G in $O(\sqrt{n}m)$ steps, where m is the number of edges of G.

Theorem 4.1 ([1, 8, 18]). *Let G be a graph with n vertices and m edges. It takes $O(\sqrt{n}m)$ steps to find a maximum matching of G.*

The connectedness of a graph G with n vertices can be determined by the breadth-first search (BFS) algorithm, which takes $O(n)$ steps. Based on Theorems 1.4 and 1.5, by applying the BFS algorithm and the maximum matching algorithm to $G - S$, we can find all smallest anti-Kekulé sets S of a cubic graph G.

Algorithm (Finding all smallest anti-Kekulé sets)

Input: *A cubic graph G with n vertices.*
Output: *All the smallest anti-kekulé sets of G.*

Step 1. Let $k = 0$. Use the maximum matching algorithm on G. If G has a maximum matching of size $n/2$, go to Step 2. Otherwise, $ak(G) = 0$ and stop. Then $\varnothing$ is the only smallest anti-Kekulé set of G.

Step 2. Set $k \leftarrow k + 1$. Screen all edge subsets S of size k and let $\mathcal{F}_k := \{S \mid |S| = k \text{ and } S \subset E(G)\}$. Go to Step 3.

Step 3. Choose an S from $\mathcal{F}_k$, apply the BFS algorithm to find a spanning tree of $G-S$. If $G-S$ has no spanning tree, go to Step 4. Otherwise, apply the maximum matching algorithm to $G - S$. If $G - S$ has a maximum matching of size $n/2$, go to Step 4. Otherwise, label S as a smallest anti-Kekulé set and go to Step 4.

Step 4. Set $\mathcal{F}_k \leftarrow \mathcal{F}_k \setminus \{S\}$. If $\mathcal{F}_k \neq \varnothing$, return to Step 3. Otherwise, go to Step 5.

Step 5. If there is no labeled edge set, go to Step 2. Otherwise, output all labeled sets and stop.

The screening process in Step 2 takes at most $\binom{m}{k}$ steps. By Theorem 1.4, $k \leq 4$. So the worst case takes $\binom{m}{4}$ steps, which is $O(m^4)$ steps. It takes $O(n)$ steps to run BFS algorithm for $G - S$ and $O(\sqrt{n}m)$ steps to find a maximum matching of $G - S$. So for a given S, it takes at most $O(\sqrt{n}m)$ steps to determine whether it is an anti-Kekulé set or not. Therefore, the worst case takes $O(\sqrt{n}m^5)$ steps to find all smallest anti-Kekulé sets of G. Since G is a cubic graph, $m = 3n/2$. So we have the following result.

Theorem 4.2. *Let G be a connected cubic graph with n vertices. Then it takes $O(n^{11/2})$ steps to find out all the smallest anti-Kekulé sets of G.*

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Automorphism groups of Walecki tournaments with zero and odd signatures

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Abstract

Walecki tournaments were defined by Alspach in 1966. They form a class of regular tournaments that posses a natural Hamilton directed cycle decomposition. It has been conjectured by Kelly in 1964 that every regular tournament possesses such a decomposition. Therefore Walecki tournaments speak in favor of the conjecture. A second interest in Walecki tournaments arises from the mapping between cycles of the complementing circular shift register and isomorphism classes of Walecki tournaments. The problem of enumerating non-isomorphic Walecki tournaments has not been solved to date. We characterize the arc structure of Walecki tournaments whose corresponding binary sequences have zero and odd signature. Automorphism groups are determined for zero signature Walecki tournaments and for odd signature Walecki tournaments with the zero signature Walecki subtournaments.

Walecki tournaments possess a broad range of subtournaments isomorphic to some Walecki tournament. Subtournaments of odd signature Walecki tournaments induced by the outsets of the central vertex are proven to be either regular or almost regular.

Keywords: Tournaments, Hamilton directed cycles, automorphism groups.

Math. Subj. Class.: 05C20, 05C45, 05E18, 20B25

1 Introduction

Walecki tournaments were defined by Alspach in 1966. They form a class of regular tournaments that posses a natural Hamilton directed cycle decomposition. It has been conjectured by Kelly in 1964 that every regular tournament possesses such a decomposition. An approximate version of Kelly's conjecture has been proven by Kühn et al. [9]. Kelly's conjecture has been verified for regular tournaments on n vertices, whenever n is sufficiently

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large in [8]. Counting Walecki-type Hamiltonian cycle systems up to isomorphism has been solved by Brugnoli [6]. The problem of enumerating non-isomorphic Walecki tournaments has not been solved to date. It was published as an open problem by Alspach [2]. Research of this paper continues the work of Aleš [1].

We first define cycles for the complementing circular shift register on binary sequences of length n (see Subsection 1.1). Walecki tournaments are defined in Subsection 1.2. Section 2 determines the arc structure of Walecki tournaments, while Section 3 focuses on Walecki tournaments with zero signature. A specific permutation is proven to be an automorphism for Walecki tournaments. For n odd, transitive subtournaments induced by outsets and insets of specific vertices are discussed in Subsection 3.1.1 and, for n even, almost-regular and transitive subtournaments are studied in Subsection 3.1.2. Section 3.2 contains characterization of automorphism groups of Walecki tournaments with zero signature. Section 4 contains results on odd signature Walecki tournaments and Subsection 4.2 contains characterization of automorphism groups of Walecki tournaments with odd signature with a zero subsignature.

For theoretical background on tournaments we refer the reader to Beineke and Reid [5], Moon [12], and for topics on permutation groups to Burnside [7] and Wielandt [13].

Automorphism groups of Walecki tournaments were computed with algorithm NAUTY (No AUTomorphisms, Yes?). Dr. Brendan McKay has made the graph isomorphism program NAUTY available to the academic community and it proved to be an indispensible tool in this research (see McKay [10, 11]).

1.1 Cycles of the complementing circular shift register

Let E_n denote the set of all binary sequences $e = (e_1, e_2, \ldots, e_n)$ with $e_i = 0$ or 1 for all i. When considering particular binary sequences we will use $e_1e_2 \cdots e_n$ to denote $(e_1, e_2, \ldots, e_n)$. We use standard notation $\overline{e_i}$ to denote $(e_i + 1)$ modulo 2 and $\overline{e}$ to denote $(\overline{e_1}, \overline{e_2}, \ldots, \overline{e_n})$.

Let $R\colon E_n \to E_n$, a *complementing circular shift register* operator, be defined by $(R(e))_i = e_{i+1}$, if $1 \le i \le n-1$ and $(R(e))_n = \overline{e_1}$. For an integer $k \ge 2$, we have $(R^k(e))_i = (R(R^{k-1}(e)))_i$. It is clear that $R^k(e) \in E_n$ for all $k \ge 1$. If $e \in E_n$, the *period* of e is defined to be the smallest positive integer k such that $R^k(e) = e$. That is, $R^k(e) = e$, and $R^j(e) \ne e$ for $2 \le j \le k-1$.

A subset $\{e, R(e), \ldots, R^{m-1}(e)\}$ of E_n is called an *m-cycle* of operator R if e has period m. Define $e \sim_R f$ if and only if $f = R^k(e)$ for $e, f \in E_n$ and some integer k. It is easy to verify that $\sim_R$ is an *equivalence relation* on E_n. Let $[e]_R$, or $[e]$ if no confusion will arise, denote the equivalence class containing $e \in E_n$ under the relation $\sim_R$. If not otherwise stated, we will consider the lexicographically smallest element of $[e]_R$ to be the canonical equivalence class representative. This representation is canonical since no two distinct binary sequences have the same lexicographic order.

Let f and h be sequences in E_{n_1} and E_{n_2}, respectively, and let $e = fh$ denote the sequence of length $n_1 + n_2$ in $E_{n_1+n_2}$.

For completness reasons we state results obtained by Alspach [4] which have direct implications on the structure of Walecki tournaments with non-trivial automorphism groups.

Lemma 1.1 (Alspach, 1966). *Let $e \in E_n$. If a positive integer k divides n such that n/k is odd and if*

$$e = f\overline{f}f\overline{f}\ldots\overline{f}f, \text{ for } f \in E_k,$$

then $R^{2k}(e) = e$. Moreover, e and f have the same period.

Lemma 1.2 (Alspach, 1966)**.** *If $e \in E_n$ has period m, where $m < 2n$, then $m = 2r$ where r divides $n, n/r$ is odd, $r < n$, and $e = f\overline{f}f\overline{f}\ldots\overline{f}f$ such that $f \in E_r$ and the period of f is $2r = m$.*

1.2 Definition of Walecki tournaments

Let $[v(0), v(1), \ldots, v(2n)]$ be a given undirected Hamilton cycle of order $2n+1$ on the vertex set $\{v(0), v(1), \ldots, v(2n)\}$. Let $\tau \in \mathbb{S}_{2n+1}$ be the permutation of $\{v(0), v(1), \ldots, v(2n)\}$ defined by $\tau = (v(0))(v(1)v(2)v(4)v(6)\cdots v(2n-2)v(2n)v(2n-1)v(2n-3)\cdots v(5)v(3))$. We define the *$v$-labeling* of the vertices of Walecki tournaments as follows: $2n$ vertices on the circumference of a circle are labeled as $v(1), v(2), v(4), \ldots, v(2n-2), v(2n), v(2n-1), \ldots, v(5)$, $v(3)$ with the central vertex labeled $v(0)$.

The permutation τ corresponds to the clockwise rotation of the vertices on the circumference of the circle with $v(0)$ as a fixed point in the center. Figure 1 shows the action of the permutation $\tau \in \mathbb{S}_{2n+1}$ on vertices of the given Hamilton cycle. A Walecki tournament on $2n+1$ vertices is then defined by assigning to each of the n *undirected* Hamilton cycles $H_1 = [v(0), v(1), \ldots, v(2n)]$, $H_2 = [\tau(v(0)), \tau(v(1)), \ldots, \tau(v(2n))]$, $\ldots, H_n = [\tau^{n-1}(v(0)), \tau^{n-1}(v(1)), \ldots, \tau^{n-1}(v(2n))]$ one of the two possible orientations. For example, Figure 2 shows the directed Hamilton cycle $\overrightarrow{H_1} = [v(0), v(1), \ldots, v(2n)]$. Directed Hamilton cycle $\overleftarrow{H_1}$ has all the arcs of $\overrightarrow{H_1}$ reversed, that is, $\overleftarrow{H_1} = [v(0), v(2n), \ldots, v(1)]$. It is easy to see that the union of n Hamilton directed cycles indeed forms a regular tournament.

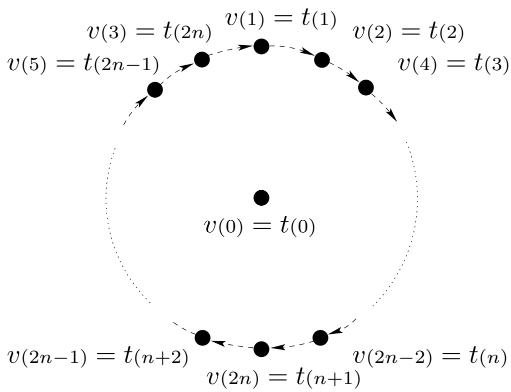

Figure 1: The diagram shows the action of the permutation $\tau \in \mathbb{S}_{2n+1}$ on vertices of the Walecki tournament $W(e)$. Vertex $v(0)$ is fixed by τ.

Let $e \in E_n$ be a binary sequence of length n. Define components of e as follows, $e_i = 0$, if $v(0) \to \tau^{i-1}(v(1))$, and $e_i = 1$, if $v(0) \leftarrow \tau^{i-1}(v(1))$, for $1 \le i \le n$, where arrows $\to$ and $\leftarrow$ denote arcs in a tournament. This establishes a one-to-one correspondence between all 2^n possible orientations of n Hamilton cycles and the elements of E_n. For example, Figure 3 shows Walecki tournaments $W(0)$ and $W(00)$ on 3 and 5 vertices, respectively, Figure 4 shows Walecki tournament $W(000)$ on 7 vertices, and Figure 5 shows Walecki tournament $W(0000)$ on 9 vertices, where $W(e)$ denotes a Walecki tournament with Hamilton cycles directed according to elements of the sequence e.

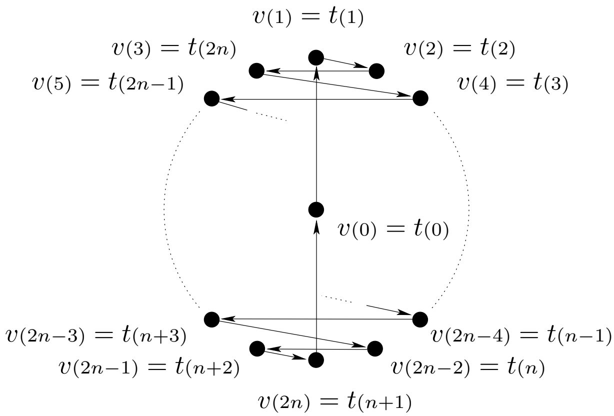

Figure 2: The directed Hamilton cycle $\overrightarrow{H_1} = [v(0), v(1), \ldots, v(2n)]$.

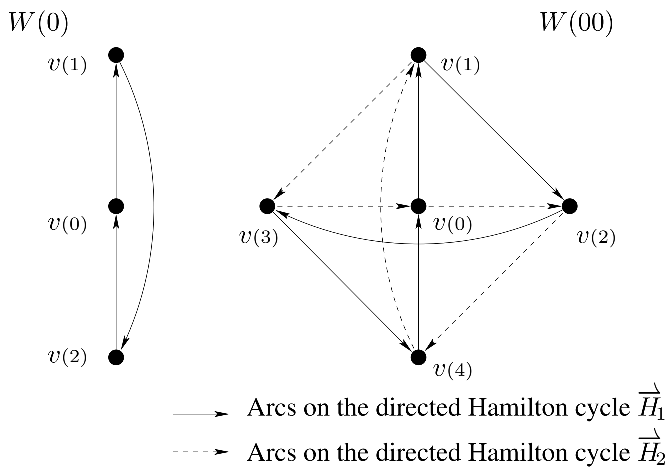

Figure 3: Walecki tournaments $W(0)$ and $W(00)$.

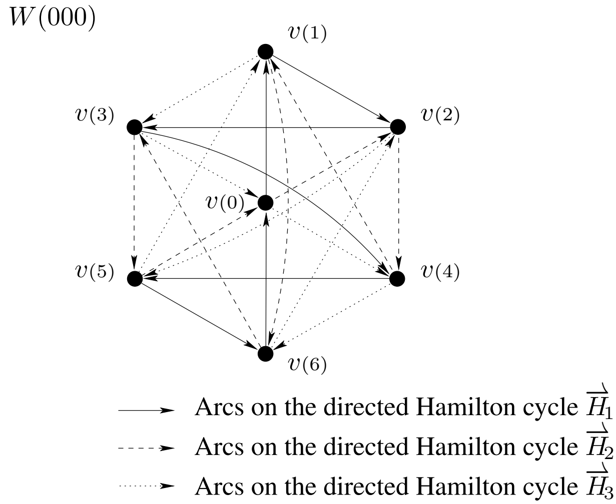

Figure 4: Walecki tournament $W(000)$.

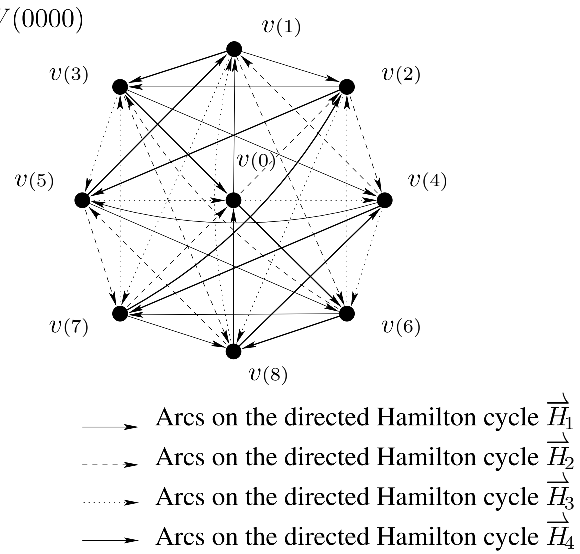

Figure 5: Walecki tournament $W(0000)$.

We state a necessary condition for isomorphism of two Walecki tournaments which can be easily proven using isomorphism τ^k for $1 \leq k \leq 2n$.

Proposition 1.3 (Alspach, 1966)**.** *Let n be a positive integer and let $e \in E_n$. If k is an integer such that $1 \leq k \leq 2n$, then*

$$W(e) \cong W(R^k(e)).$$

Let η denote the permutation $\tau^n \in \mathbb{S}_{2n+1}$. That is,

$$\eta = (v(0))(v(1)\ v(2n))(v(2)\ v(2n-1)) \dots (v(n)\ v(n+1)).$$

Notice that $\tau(v(0)) = \eta(v(0)) = v(0)$. The n *directed* cycles of $W(e)$ are

$$H_k = [\tau^{k-1}(\eta^{e_k}(v(0))), \tau^{k-1}(\eta^{e_k}(v(1))), \dots, \tau^{k-1}(\eta^{e_k}(v(2n)))],$$

for $1 \leq k \leq n$.

In order to simplify notation we introduce the t-labeling $\{t(0), t(1), \dots, t(2n)\}$ of the vertices of Walecki tournaments, where $t(0) = v(0)$ and $t(i) = \tau^{i-1}(v(1))$, $1 \leq i \leq 2n$ (see Figure 2). The action of τ on $\{t(0), t(1), \dots, t(2n)\}$ is given by $\tau = (t(0))(t(1)\ t(2) \cdots t(2n))$.

2 Arc structure of Walecki tournaments

In 1964 Kelly conjectured that every regular tournament admits a decomposition into Hamilton directed cycles (see Moon [12]). Walecki tournaments are regular and possess a natural Hamilton directed cycle decomposition (see Alspach [3]). The class of Walecki tournaments speaks in favor of the above conjecture. Therefore knowledge of their structure would be of importance. They posses a rich collection of induced subtournaments ranging from transitive to regular as we shall see later. In some instances outsets of $v(0)$ induce regular or almost regular subtournaments. In other cases outsets of $v(0)$ induce subtournaments whose scores differ for at most 2.

We will first state various results which give insight into the arc structure of an arbitrary Walecki tournament. The reader can find the proofs in [1].

Proposition 2.1. *Walecki tournaments are self-complementary and*

$$\operatorname{AntiAut}(W(e)) = \operatorname{Aut}(W(e))\eta,$$

where $\operatorname{AntiAut}$ *denotes the antiautomorphism group of a tournament.*

Proposition 2.2. *Let T be a tournament and let $V(T)$ denote the vertex set of T. For $v \in V(T)$ and $g \in \operatorname{Aut}(T)_v$,*

$$g(N^+(v)) = N^+(v) \quad \textit{and} \quad g(N^-(v)) = N^-(v),$$

where $\operatorname{Aut}(T)_v$ denotes the subgroup of $\operatorname{Aut}(T)$ which fixes v.

Proposition 2.3. *Let $W(e)$ be a Walecki tournament of order $2n+1$ and let k be an integer such that $1 \leq k \leq 2n$. If $t(0) \to t(k) \in \overrightarrow{H_k}$, then $t(n+k) \to t(0) \in \overrightarrow{H_k}$.*

Proposition 2.4. *Let $W(e)$ be a Walecki tournament of order $2n+1$ and let i and j be integers such that $0 \leq i, j \leq 2n-1$. If $t(i) \to t(j)$, then $t(n+i) \leftarrow t(n+j)$.*

The following result is used in many proofs about the structure of Walecki tournaments. It uses the binary sequence $e \in E_n$ to determine the direction of a particular arc in $W(e)$. The arcs are grouped according to the Hamilton directed cycle they belong to.

Lemma 2.5. *Let $e \in E_n$ and let $W(e)$ be the corresponding Walecki tournament. Let i and j be integers such that $1 \le i < j \le 2n$. In the case when $j - i$ is even, let $k = i + 1 + (j - i)/2$.*

- *If $1 \le k \le n$, then $t(j+e_k) \to t(i) \to t(j+\bar{e}_k)$ and $t(j+n+e_k) \leftarrow t(i+n) \leftarrow t(j+n+\bar{e}_k)$.*
- *If $n+1 \le k \le 2n$, then $t(j-n+e_{k-n}) \to t(i-n) \to t(j-n+\bar{e}_{k-n})$ and $t(j+e_{k-n}) \leftarrow t(i) \leftarrow t(j+\bar{e}_{k-n})$.*

In the case when $j - i$ is odd, let $\ell = i + 1 + (j - i - 1)/2$.

- *If $1 \le \ell \le n$, then $t_{(j-e_\ell)} \leftarrow t(i) \leftarrow t(j-\bar{e}_\ell)$ and $t_{(j+n-e_\ell)} \to t(i+n) \to t(j+n-\bar{e}_l)$.*
- *If $n+1 \le \ell \le 2n$, then $t(j-n-e_{\ell-n}) \leftarrow t(i-n) \leftarrow t(j-n-\bar{e}_{\ell-n})$ and $t(j-e_{\ell-n}) \to t(i) \to t(j-\bar{e}_{l-n})$.*

Proof. Let i and j be as in the conditions of the Proposition 2.4. We first consider the case when $j-i$ is even. Let $k = i+1+(j-i)/2$. The structure of the Hamilton directed cycle $\overrightarrow{H_k}$ implies that if $e_k = 0$, then $t(j) \to t(i)$ and $t(i) \to t(j+1)$ (see Figure 6). On the other

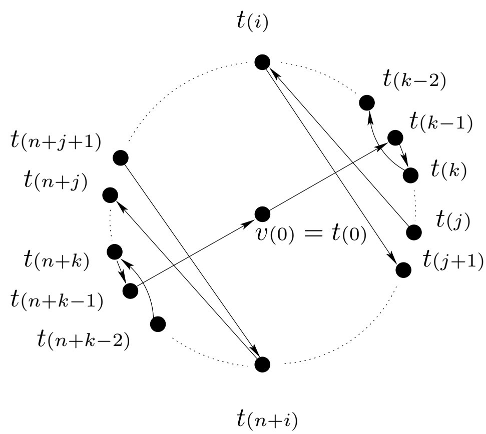

Figure 6: The diagram shows the case when $j - i$ is even and $e_k = 0$ from the proof of Lemma 2.5.

hand, if $e_k = 1$, then $t(j+1) \to t(i)$ and $t(i) \to t(j)$, implying $t(j+e_k) \to t(i) \to t(j+\bar{e}_k)$. Proposition 2.4 implies $t(j+n+e_k) \leftarrow t(i+n) \leftarrow t(j+n+\bar{e}_k)$. To prove the next two statements substitute above $j-n$ for j and $i-n$ for i. The remaining cases are proven similarly. $\square$

3 Zero signature Walecki tournaments

Let $[e]_R$ be an equivalence class of binary n-sequences under the relation $\sim_R$ defined in Subsection 1.1. We say that $[e]_R$ has *zero signature* if the lexicographically smallest sequence of $[e]_R$ is $(0, 0, \ldots, 0)$. Tournaments corresponding to the zero signature sequences, as we shall see, have a surprisingly simple automorphism group. In the case of odd n,

$$\sigma = (t(0))(t(1)t(2)\cdots t(n))\ (t(2n)t(2n-1)\cdots t(n+1)) \in \mathbb{S}_{2n+1}$$

is in fact an automorphism of $W((0,0,\dots,0))$ as proven in Theorem 3.3. We will prove in Theorem 3.4 and Theorem 3.6 that Walecki tournaments of order $2n+1$ with *zero signature* possess transitive subtournaments of order n that are induced by the outset of vertex $v_{(1)}$. When n is odd they also contain circulant subtournaments of order n induced by the outset of vertex $v_{(0)}$. This furthermore implies that these subtournaments are regular. For example see Figure 4 which shows Walecki tournament $W(000)$.

The next couple results are needed for characterizing the arc structure of Walecki tournaments for the case when n is odd, $n \geq 3$, and $e = (0,0,\dots,0) \in E_n$. We omit straightforward proofs.

Proposition 3.1. *Let $e \in E_n$ and $n \geq 3$. Consider the Walecki tournament $W(e)$. If $e_i = e_{i+1}$ and $1 \leq i \leq n-1$, then τ is dominance-preserving on $\overrightarrow{H_i}$ and τ^{-1} is dominance-preserving on $\overrightarrow{H}_{i+1}$.*

Notice that permutation τ is not an automorphism of $W(e)$.

Lemma 3.2. *Let $e \in E_n$ and $n \geq 3$. Consider the Hamilton directed cycle $\overrightarrow{H_i}$, $1 \leq i \leq n$, in the Walecki tournament $W(e)$. Let $u \to w$ be any arc of $\overrightarrow{H_i}$ of the form $u = \tau^{i-1}(v_{(2j)})$ and $w = \tau^{i-1}(v_{(2j+1)})$ or $u = \tau^{i-1}(v_{(2j+1)})$ and $w = \tau^{i-1}(v_{(2j+2)})$, $1 \leq j \leq n-2$. If $\rho \in \mathbb{S}_{2n+1}$ is a permutation of $\{v_{(0)}, v_{(1)}, \dots, v_{(2n)}\}$ such that $\rho = \tau$ on $\tau^{i-1}(v_{(2j)})$, $1 \leq j \leq n-2$, and $\rho = \tau^{-1}$ on $\tau^{i-1}(v_{(2j+1)})$, $1 \leq j \leq n-2$. Then ρ is dominance-preserving on the arc $u \to w$.*

Let n be odd and let the permutation $\sigma \in \mathbb{S}_{2n+1}$ be defined by

$$\sigma = (t_{(0)})(t_{(1)}\, t_{(2)} \cdots t_{(n)})(t_{(2n)}\, t_{(2n-1)} \cdots t_{(n+1)}),$$

(see Figure 7). That is,

$$\sigma = (v_{(0)})(v_{(1)}\, v_{(2)}\, v_{(4)} \cdots v_{(2n-4)}\, v_{(2n-2)})(v_{(3)}\, v_{(5)} \cdots v_{(2n-3)}\, v_{(2n-1)}\, v_{(2n)}).$$

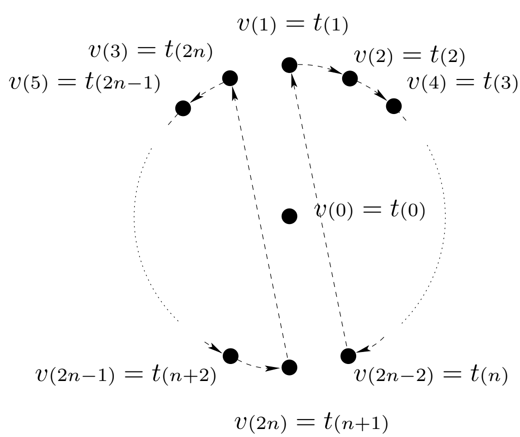

Figure 7: The action of the permutation $\sigma \in \mathbb{S}_{2n+1}$.

Theorem 3.3. *Let $e = (0,0,\dots,0)$, be the binary n-sequence of all 0s. If n is odd, and $n \geq 3$, then σ is an automorphism of $W(e)$.*

Proof. We want to show that σ is dominance-preserving on all of $W(e)$. By definition, σ fixes $t(0)$, cyclically permutes the vertices of the outset of $t(0)$, and cyclically permutes the vertices of the inset of $t(0)$. Thus, σ is dominance-preserving on the arcs incident with $t(0)$. Figure 7 shows the action of $\sigma \in \mathbb{S}_{2n+1}$ on vertices of the Walecki tournament $W(e)$, for $e = (0, 0, \ldots, 0) \in E_n, n$ odd and $n \geq 3$.

Note that σ restricted to $V^+ = N^+(t(0)) - \{t(n)\} = \{t(1), t(2), \ldots , t(n-1)\}$ has the same action as τ. It then follows from Proposition 3.1 that σ is dominance-preserving on any arc both of whose vertices lie in V^+ because such an arc is not in $\overrightarrow{H_n}$. Similarly, σ restricted to $V^- = N^-(t(0)) - \{t(n+1)\} = \{t(n+2), t(n+3), \ldots, t(2n)\}$ has the same action as τ^{-1}. Again it follows from Proposition 3.1 that σ is dominance-preserving on any arc both of whose vertices lie in V^- because such an arc is not in $\overrightarrow{H_1}$. (Figure 1 shows the action of the permutation τ on vertices of the Walecki tournament $W(e)$.)

By Lemma 3.2, σ is dominance-preserving on any arc with one end vertex in V^+ and the other end vertex in V^- because σ acts like τ on V^+ and τ^{-1} on V^-. It remains to show that σ is dominance-preserving on any arc incident with $t(n) = v(2n-2)$ or $t(n+1) = v(2n)$. Since $e_n = 0$ we have $v(2n-2) \to v(2n) \in \overrightarrow{H_n}$. Furthermore, $\sigma(v(2n-2)) = v(1) = \tau^0(v(1)) = \tau^{n-1}(v(2n-1))$ and $\sigma(v(2n)) = v(3) = \tau^{-1}(v(1)) = \tau^{n-1}(v(2n))$ imply $\sigma(v(2n-2)) \to \sigma(v(2n)) \in \overrightarrow{H_n}$.

We divide the proof for the arcs incident with either $v(2n-2)$ or $v(2n)$ into two cases. Let $u \in V^- \cup V^+$. First we consider arcs $u \to v(2n-2)$ and $u \to v(2n)$. We use Lemma 2.5 extensively. We remind the reader that arcs $\tau^{k-1}(v(i)) \to \tau^{k-1}(v(i+1)), 1 \leq i \leq 2n-1$, belong to the Hamilton directed cycle H_k. In the figures accompanying this proof we use arrows $\dashrightarrow$ to denote the action of σ and arrows $\longrightarrow$ to denote arcs of the tournament.

Case 1.1. Let $u \in V^-$. If k is an integer such that $1 \leq k \leq (n-1)/2$, then vertices $t(n+2k+1)$ and $t(n+2k)$ belong to V^-, and arcs $t(n+2k+1) = \tau^{k-1}(v(2(n-k)-1)) \to t(n) = \tau^{k-1}(v(2(n-k)))$ and $t(n+2k) = \tau^{k-1}(v(2(n-k)+1)) \to t(n+1) = \tau^{k-1}(v(2(n-k+1)))$ belong to the Hamilton directed cycle $\overrightarrow{H_k}$ (see Figure 8). Now, σ is dominance-preserving on these

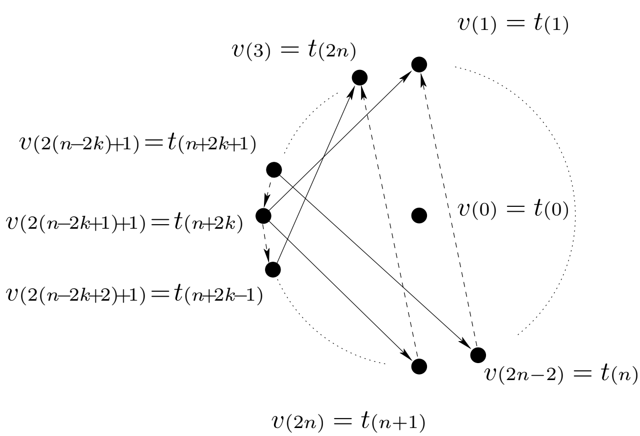

Figure 8: The diagram shows the action of the permutation $\sigma \in \mathbb{S}_{2n+1}$ on arcs from Case 1.1 for the proof of Theorem 3.3.

two arcs since $\sigma(t(n+2k+1)) = t(n+2k) = \tau^{k+(n-1)/2}(v(n+2k-1))$ and $\sigma(t(n)) = t(1) = \tau^{k+(n-1)/2}(v(n+2k))$ imply

$$\sigma(v(2(n-2k)+1)) \to \sigma(v(2n-2)) \in \overrightarrow{H}_{k+(n+1)/2}.$$

Also $\sigma(t(n+2k)) = t(n+2k-1) = \tau^{k+(n-3)/2}(v(n+2k-1))$ and $\sigma(t(n+1)) = t(2n) = \tau^{k+(n-3)/2}(v(n+2k))$ imply

$$\sigma(v(2(n-2k+1)+1)) \to \sigma(v(2n)) \in \overrightarrow{H}_{k+(n-1)/2}.$$

Case 1.2. Let $u \in V^+$. If k is an integer such that $(n+1)/2 \leq k \leq n-1$, then vertices $t(2k-n+1)$ and $t(2k-n+2)$ belong to V^+, and arcs $t(2k-n+1) \to t(n)$ and $t(2k-n+2) \to t(n+1)$ belong to the Hamilton directed cycle $\overrightarrow{H}_k$ (see Figure 9). Similarly as before we have

$$\sigma(v(2(2k-n))) \to \sigma(v(2n-2)) \in \overrightarrow{H}_{k-(n-3)/2}$$

and

$$\sigma(v(2(2k-n-1))) \to \sigma(v(2n)) \in \overrightarrow{H}_{k-(n-1)/2}.$$

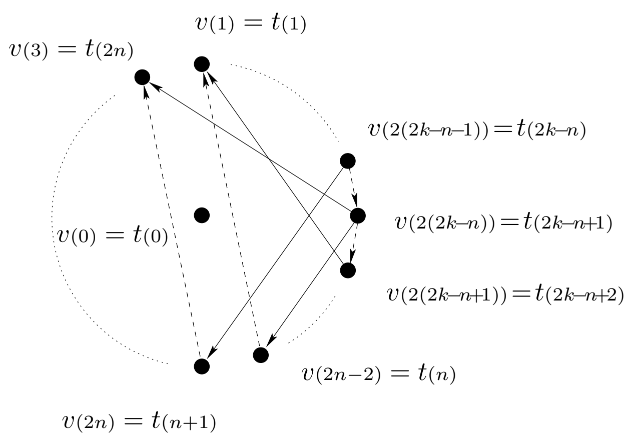

Figure 9: The action of the permutation $\sigma \in \mathbb{S}_{2n+1}$ on arcs from Case 1.2 for the proof of Theorem 3.3.

Next we consider arcs $v(2n-2) \to u$ and $v(2n) \to u$ for $u \in V^- \cup V^+$. We state all cases but leave the proofs to the reader.

Case 2.1. Let $u \in V^-$. If k is an integer such that $2 \leq k \leq (n-1)/2$, then vertices $v(2(n-2k+1)+1)$ and $v(2(n-2k+2)+1)$ belong to V^-. We have to consider vertices $v(3)$ and $v(2n-1) \in V^-$ as a special case.

Case 2.2. Let $u \in V^+$. If k is an integer such that $(n+3)/2 \leq k \leq n-1$, then vertices $v(2(2k-n-1))$ and $v(2(2k-n+2))$ belong to V^+. We consider vertex $v(1) \in V^+$ as a special case.

Therefore $u \to w$ implies $\sigma(u) \to \sigma(w)$ for every arc $u \to w$ in $W(e)$ and so $\sigma \in \mathrm{Aut}(W(e))$. □

The importance of σ in the theory of automorphism groups of Walecki tournaments was previously unknown. However, once zero signature sequences were determined as a potential source of Walecki tournaments with non-trivial automorphism groups, permutation σ became a natural candidate for a generator.

3.1 Subtournaments of zero signature Walecki tournaments

Next we characterize specific subtournaments of zero signature Walecki tournaments, which prove to be transitive for n odd and almost regular or transitive for n even.

3.1.1 Transitive subtournaments for n odd

In the following result we prove transitivity of subtournaments of Walecki tournament with zero signature for n odd. The linear orderings of subsets of vertices that induce transitive subtournaments are given in the proof.

Theorem 3.4. *Let $T = W(e)$ for $e = (0,0,\ldots,0) \in E_n$, n odd, and $n \geq 3$. For $t_{(i)} \in N^+(t_{(0)})$ and $t_{(j)} \in N^-(t_{(0)})$ the tournaments*

$$\langle N^+(t_{(i)})\rangle, \quad T\langle N^-(t_{(j)})\rangle, \quad T\langle N^-(t_{(i)}) - \{t_{(0)}\}\rangle, \quad \textit{and} \quad T\langle N^+(t_{(j)}) - \{t_{(0)}\}\rangle$$

are transitive subtournaments of T.

Proof. Proposition 2.1 tells us that $W(e) \cong \overline{W(e)}$. Since $\sigma \in \mathrm{Aut}(T)$, it suffices to prove the theorem for the vertex $t_{(1)} \in N^+(t_{(0)})$. Let us consider the outset of vertex $t_{(1)}$. The arcs $v_{(2i+1)} \to v_{(2i+2)}$ lie in $\overrightarrow{H_1}$ for $0 \leq i \leq n-1$ so that $t_{(1)} = \tau^i(v_{(2i+1)}) \to \tau^i(v_{(2i+2)}) = \tau^{2i+1}(v_{(1)}) \in \overrightarrow{H}_{i+1}$. Hence

$$N^+(t_{(1)}) = \{t_{(2i+2)} \mid 0 \leq i \leq n-1\}. \tag{3.1}$$

We prove that the vertices of $N^+(t_{(1)})$ in the order $t_{(2n)}, t_{(2)}, t_{(2n-2)}, t_{(4)}, \ldots, t_{(2n-2i)}$, $t_{(2i+2)}, \ldots, t_{(n+3)}, t_{(n-1)}, t_{(n+1)}$ determine the score sequence $(s_j)_{j=0}^{n-1}$, where $s_j = j$ for $0 \leq j \leq n-1$. That is, $s_{2i} = s(t_{(2n-2i)}) = 2i$ for $0 \leq i \leq (n-3)/2$, $s_{2i+1} = s(t_{(2i+2)}) = 2i+1$ for $0 \leq i \leq (n-3)/2$, and $s_{n-1} = s(t_{(n+1)}) = n-1$. We prove this by showing that all arcs in the subtournament $T\langle N^+(t_{(1)})\rangle$ point from right to left in the ordering of the vertices given above. Figure 10 shows seven different types of arcs considered. We divide the proof into several cases and show details for some of them. In all of them the index i is an integer such that $0 \leq i \leq (n-3)/2$.

Case 1.1. Since $t_{(n+1)} = \tau^{(n+1)/2+i}(v_{(n-2i-1)})$ and $t_{(2i+2)} = \tau^{(n+1)/2+i}(v_{(n-2i)})$, the arcs of type $t_{(n+1)} \to t_{(2i+2)}$ belong to cycles $\overrightarrow{H}_{(n+3)/2+i}$.

We omit proofs of $t_{(n+1)} \to t_{(2n-2i)} \in H_{(n+1)/2-i}$ and $t_{(2i)} \to t_{(2n-2i)} \in \overrightarrow{H_1}$. In the remaining cases the index j is in the range $i \leq j \leq (n-3)/2$.

Case 1.2. Since $t_{(2j+2)} = \tau^{i+j+1}(v_{(2(j-i))})$ and $t_{(2i+2)} = \tau^{i+j+1}(v_{(2(j-i)+1)})$, it is $t_{(2j+2)} \to t_{(2i+2)} \in \overrightarrow{H}_{i+j+2}$.

We omit proofs of $t_{(2j+2)} \to t_{(2n-2i)} \in \overrightarrow{H}_{j-i+1}$, $t_{(2n-2j)} \to t_{(2i+2)} \in \overrightarrow{H}_{n+i-j+1}$, and $t_{(2n-2j)} \to t_{(2n-2i)} \in \overrightarrow{H}_{n-i-j}$.

It follows that the scores of vertices in the subtournament $T\langle N^+(t_{(1)})\rangle$ are $s_j = j$ for $0 \leq j \leq n-1$. Thus, the subtournament $T\langle N^+(t_{(1)})\rangle$ is transitive.

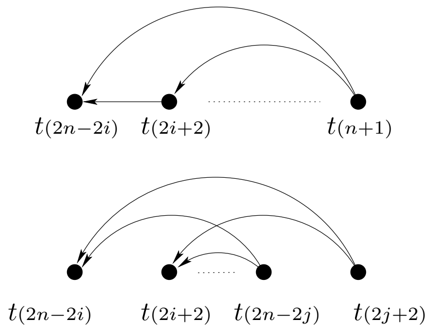

Figure 10: Seven different types of arcs from Case 1.1 and Case 1.2 of the proof of transitivity of the tournament $T\langle N^+(v_{(1)})\rangle$ from Theorem 3.4.

Next we consider the set of vertices $N^-(t_{(1)}) - \{t_{(0)}\}$. Since $N^+(t_{(1)}) = \{t_{(2i+2)} \mid 1 \le i \le n-1\}$, it follows that $N^-(t_{(1)}) - \{t_{(0)}\} = \{t_{(2i+1)} \mid 1 \le i \le n-1\}$. We will prove that the labeling of the vertices of $N^-(t_{(1)}) - \{t_{(0)}\}$ in the order $t_{(2n-1)}, t_{(3)}, t_{(2n-3)}, t_{(5)}, \ldots, t_{(2n-2i+1)}, t_{(2i+1)}, \ldots, t_{(n+2)}, t_{(n)}$ determines the score sequence $(s_j)_{j=0}^{n-1}$, where $s_j = j$ for $0 \le j \le n-2$. That is, $s_{2i-2} = s(t_{(2n-2i+1)}) = 2i-2$, for $1 \le i \le \frac{n-1}{2}$, and $s_{2i-1} = s(t_{(2i+1)}) = 2i-1$, for $1 \le i \le \frac{n-1}{2}$. Similarly as in the previous case one can prove that all arcs in the subtournament $T\langle N^-(t_{(1)}) - \{t_{(0)}\}\rangle$ point from right to left in the ordering of the vertices given above. Thus, the subtournament $T\langle N^-(t_{(1)}) - \{t_{(0)}\}\rangle$ is transitive. $\square$

3.1.2 Almost-regular and transitive subtournaments for n even

When n is even σ is not an automorphism because an automorphism group of a tournament has to have an odd order.

Theorem 3.5. *Let $T = W(e)$ for $e = (0, 0, \ldots, 0) \in E_n$, n even, and $n \ge 4$. The subtournaments $T\langle N^+(t_{(0)})\rangle$ and $T\langle N^-(t_{(0)})\rangle$ are almost regular.*

Proof. It follows from the definition of Walecki tournaments that $N^+(t_{(0)}) = \{t_{(i)} \mid 1 \le i \le n\}$. Equation (3.1) also holds for n even. Hence, $N^+(t_{(1)}) = \{t_{(2i)} \mid 1 \le i \le n\}$, implying $N^+(t_{(0)}) \cap N^+(t_{(1)}) = \{t_{(2i)} \mid 1 \le i \le n/2\}$. Therefore, $|N^+(t_{(0)}) \cap N^+(t_{(1)})| = n/2$. It is easy to verify that $N^+(t_{(2)}) = \{t_{(2i+1)} \mid 1 \le i \le n-1\} \cup \{t_{(2n)}\}$, which implies $N^+(t_{(0)}) \cap N^+(t_{(2)}) = \{t_{(2i+1)} \mid 1 \le i \le n/2 - 1\}$. Furthermore, $|N^+(t_{(0)}) \cap N^+(t_{(2)})| = n/2 - 1$.

The scores of the remaining vertices in $N^+(t_{(0)})$ can be obtained similarly, then we omit the proofs. They alternate between $n/2$ and $n/2 - 1$ which proves that $T\langle N^+(t_{(0)})\rangle$ is almost regular. Since T is self-complementary, this completes the proof. $\square$

Theorem 3.6. *Let $T = W(e)$ for $e = (0, 0, \ldots, 0) \in E_n$, n even, and $n \ge 4$. For $t^+ \in N^+(t_{(0)})$ and $t^- \in N^-(t_{(0)})$ the tournaments*

$$T\langle N^+(t^+)\rangle, \quad T\langle N^-(t^+) - \{t_{(0)}\}\rangle, \quad T\langle N^+(t^-) - \{t_{(0)}\}\rangle, \quad \textit{and} \quad T\langle N^-(t^-)\rangle$$

are transitive subtournaments of T.

Proof. Proposition 2.1 tells us that $T \cong \overline{T}$. Hence, it suffices to prove the theorem for vertices in $N^+(t(0))$. The proof of transitivity of $T\langle N^+(t(1))\rangle$ and $T\langle N^-(t(1)) - \{t(0)\}\rangle$ is similar to the proof of Theorem 3.4, the difference being that n is even. This changes the proof in two ways. First, the vertices of $N^+(t(1))$ in the order $t(2n), t(2), t(2n-2), t(4), \ldots, t(2n-2i), t(2i+2), \ldots, t(n+2), t(n)$ determine the score sequence $(0, 1, 2, \ldots, n-1)$.

Furthermore, since n is even we have $\sigma \notin \mathrm{Aut}(T)$. Therefore, one has to prove that the subtournaments $T\langle N^+(t^+)\rangle$ and $T\langle N^-(t^+) - \{t(0)\}\rangle$ are transitive for all $t^+ \in N^+(t(0))$. The proofs are similar to the initial case and we omit them. □

3.2 Automorphism groups of Walecki tournaments with zero signature

The arc structure of Walecki tournaments with zero signature plays a major role in determining their automorphism groups.

Theorem 3.7. *Automorphism groups of Walecki tournaments with zero signature are cyclic:*

$$\mathrm{Aut}(W(0)) = \mathbb{Z}_3, \quad \mathrm{Aut}(W(00)) = \mathbb{Z}_5, \quad \mathrm{Aut}(W(e)) = \mathbb{Z}_n, \quad \textit{for } n \textit{ odd, } n \geq 3,$$

and

$$\mathrm{Aut}(W(e)) = \mathbb{Z}_1, \quad \textit{for } n \textit{ even, } n \geq 4,$$

where $\mathbb{Z}_n$ denotes the cyclic group of order n and $e = (0, 0, \ldots, 0) \in E_n$.

Proof. We leave the proof of initial cases as an exercise for the reader. Let T denote the Walecki tournament $W(e)$ and let G denote its automorphism group $\mathrm{Aut}(T)$. We use Orbit Stabilizer Theorem two times to get

$$|G| = |\mathcal{O}(v(0))||G_{v(0)}| = |\mathcal{O}(v(0))||\mathcal{O}(v(1))||G_{v(0),v(1)}|, \tag{3.2}$$

where $\mathcal{O}(v(1))$ denotes the orbit of vertex $v(1)$ for the subgroup $G_{v(0)}$ of G.

Case 1. Let us assume that n is odd, $n \geq 3$, and $e = (0, 0, \ldots, 0) \in E_n$. We first consider the cardinality of $\mathcal{O}(v(0))$. $T\langle N^+(v(0))\rangle$ is an almost regular tournament. Therefore, it is not transitive. On the other hand, $T\langle N^+(v(i))\rangle$ is transitive for $v(i) \in N^+(v(0))$ (see Theorem 3.4). Thus, $v(0)$ cannot be mapped to a vertex from $N^+(v(0))$ by elements of G. Proposition 2.1 implies $T \cong \overline{T}$ with the graph anti-automorphism τ^n. Therefore, $v(0)$ cannot be mapped to a vertex from $N^-(v(0))$ by elements of G. We have proven that $v(0)$ must be fixed under the action of G, and thus

$$|\mathcal{O}(v(0))| = 1. \tag{3.3}$$

The fact that $v(0)$ cannot be mapped to any vertex in $N^-(v(0))$ can also be proven directly for $n \geq 5$. Let us consider $T\langle N^+(v(0)) - v(i)\rangle$ for $v(i) \in N^+(v(0))$. $T\langle N^+(v(0))\rangle$ is regular of degree $(n-1)/2$. Thus, $T\langle N^+(v(0)) - v(i)\rangle$ has $(n-1)/2$ vertices of degree $(n-1)/2$ and $(n-1)/2$ vertices of degree $(n-3)/2$. Therefore, if $n \geq 5$, the subtournament $T\langle N^+(v(0)) - \{v(i)\}\rangle$ is not transitive. However, $T\langle N^+(v(j)) - \{v(0)\}\rangle$ is transitive for $v(j) \in N^-(v(0))$. Therefore, $v(0)$ cannot be mapped to $v(j) \in N^-(v(0))$ by elements of G if $n \geq 5$. We cannot use the same argument for $n = 3$ since the subtournament $T\langle N^+(v(0)) - v(i)\rangle$, for $v(i) \in N^+(v(0))$, is a tournament on two vertices and is therefore transitive.

Next we determine $|\mathcal{O}(v(1))|$. Since $v(0)$ is a fixed point for any element ρ in G, $\rho(N^+(v(0))) = N^+(v(0))$. Hence, $\rho(v(1)) \in N^+(v(0))$ and $|\mathcal{O}(v(1))| \leq |N^+(v(0))| = n$. We proved that the permutation $\sigma \in \mathbb{S}_{2n+1}$ of $V(T)$ defined by

$$\sigma = \big(v(1)\ v(2)\ v(4) \cdots v(2n-4)\ v(2n-2)\big)\big(v(3)\ v(5) \cdots v(2n-3)\ v(2n-1)\ v(2n)\big),$$

is an element in G. Since $\sigma(v(0)) = v(0)$, $\sigma \in G_{v(0)}$. Hence, $\langle\sigma\rangle \subseteq G_{v(0)}$. The orbit of $v(1)$ for σ is $N^+(v(0))$ implying

$$|\mathcal{O}(v(1))| = n. \tag{3.4}$$

Last we prove that $G_{v(0),v(1)} = id$. The subtournaments $T\langle N^+(v(1))\rangle$ and $T\langle N^-(v(1)) - \{v(0)\}\rangle$ are transitive, implying that any automorphism $\rho \in G_{v(0),v(1)}$ fixes all other vertices. Figure 11 shows the partition of the vertices of T with respect to the outsets and insets of vertices $v(0)$ and $v(1)$. Therefore, $G_{v(0),v(1)} = id$, that is,

$$|G_{v(0),v(1)}| = 1. \tag{3.5}$$

Equations (3.2), (3.3), (3.4), and (3.5) imply that $|G| = n$. Now, $\langle\sigma\rangle \subseteq G_{v(0)} \subseteq G$ and since $\langle\sigma\rangle \cong \mathrm{Z}_n$ we have $G \cong \mathrm{Z}_n$.

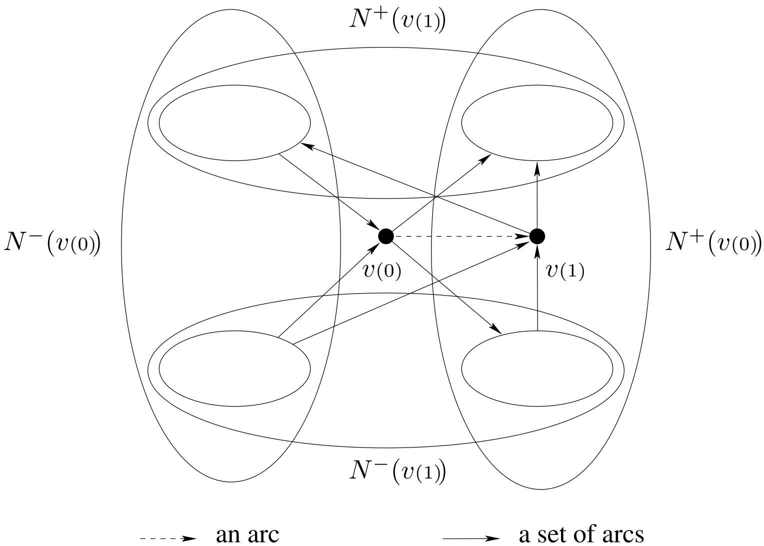

Figure 11: The partition of the vertices of the Walecki tournament $W(e)$, for $e = (0, 0, \ldots, 0) \in E_n$, n odd, and $n \geq 3$, with respect to the outsets and insets of vertices $v(0)$ and $v(1)$. Only the arcs essential for the proof of Theorem 3.7 are drawn.

Case 2. Let us assume n is even, $n \geq 4$, and $e = (0, 0, \ldots, 0) \in E_n$. We first consider the cardinality of $\mathcal{O}(v(0))$. The subtournament $T\langle N^+(v(0))\rangle$ is almost regular (see Theorem 3.5). Therefore, it is not transitive. On the other hand, $T\langle N^+(v(i))\rangle$ is transitive for $v(i) \in N^+(v(0))$ (see Theorem 3.6). Thus, $v(0)$ cannot be mapped to a vertex from $N^+(v(0))$ by elements of G.

Proposition 2.1 implies implies $T \cong \overline{T}$ via the graph anti-automorphism τ^n. Therefore, $v(0)$ cannot be mapped to a vertex from $N^-(v(0))$ by elements of G. We have proven that

$v(0)$ must be fixed under the action of G, and thus

$$|\mathcal{O}(v(0))| = 1. \tag{3.6}$$

Next we determine $|\mathcal{O}(v(1))|$. Since $v(0)$ is a fixed point for any element ρ in G, $\rho(N^+(v(0))) = N^+(v(0))$. Hence, $\rho(v(1)) \in N^+(v(0))$. As seen in the proof of Theorem 3.5, $|N^+(v(0)) \cap N^+(v(1))| = n/2$ and $|N^+(v(0)) \cap N^-(v(1))| = n/2 - 1$. Furthermore, $T\langle N^+(v(1))\rangle$ and $T\langle N^-(v(1))\rangle$ are both transitive which implies that $T\langle N^+(v(0)) \cap N^+(v(1))\rangle$ and $T\langle N^+(v(0)) \cap N^-(v(1))\rangle$ are transitive. Moreover, $v(1)$ is dominated by $N^+(v(0)) \cap N^-(v(1))$ implying that $T\langle (N^+(v(0)) \cap N^-(v(1))) \cup \{v(1)\}\rangle$ is transitive. Let $X = N^+(v(0)) \cap N^+(v(1))$ and $Y = (N^+(v(0)) \cap N^-(v(1))) \cup \{v(1)\}$. Now, vertices of X have score $n/2 - 1$ in $T\langle N^+(v(0))\rangle$. Similarly, vertices of Y have score $n/2$ in $T\langle N^+(v(0))\rangle$. Therefore, X and Y have to be fixed setwise. Hence,

$$|\mathcal{O}(v(1))| = 1. \tag{3.7}$$

Last we prove that $G_{v(0),v(1)} = id$. Subtournaments $T\langle N^+(v(1))\rangle$ and $T\langle N^-(v(1)) - \{v(0)\}\rangle$ are transitive and thus any automorphism fixing both $v(0)$ and $v(1)$ fixes all other vertices. Therefore, $G_{v(0),v(1)} = id$ which implies

$$|G_{v(0),v(1)}| = 1. \tag{3.8}$$

Equations (3.2), (3.6), (3.7), and (3.8) imply that $|G| = 1$ and $G \cong \mathrm{Z}_1$. This completes the proof. □

4 Odd signature Walecki tournaments

A sequence $f\overline{f}\ldots\overline{f}f \in E_n$, for $f \in E_r$ and $n/r > 1$ has an *odd signature*. Notice, that n/r is odd. If there exists an element in the equivalence class $[e]_R$ of odd signature, then all elements in $[e]_R$ have odd signature. We say that such an equivalence class has odd signature.

Furthermore, a sequence $f\overline{f}\ldots f\overline{f}$, for $f \in E_r$ and $n/2r > 1$ has an *even signature*. Let e be such a sequence. Not all sequences of the equivalence class $[e]_R$ have an even signature. For example, sequences $(0,0,1,0)$ and $(0,1,0,1)$ both belong to the same equivalence class. However, only the latter has an even signature. We say that an equivalence class $[e]_R$ has even signature if there exists a sequence in $[e]_R$ with even signature.

To simplify terminology we will refer to an equivalence class with a given signature as a "sequence" with that signature. We call a sequence *periodic* if it has either zero, odd, or even signature. All other sequences are called *aperiodic*. We will furthermore simplify terminology by referring to a Walecki tournament whose corresponding binary sequence has odd signature, for example, as a Walecki tournament with odd signature.

Let $e \in E_n$, let n be divisible by r, and $m = 2r$. We introduce a partition of $V(W(e)) - \{t(0)\}$ into m-sets $M_1, M_2, \ldots, M_{n/r}$, where $M_i = \{t((i-1)m+j) \mid 1 \leq j \leq m\}$, for $1 \leq i \leq n/r$, and $|M_i| = m$. First we prove the following result that relates the structure of Walecki tournament $W(e)$ and Walecki tournament $W(f)$, where e has either odd signature $e = f\overline{f}\ldots\overline{f}f \in E_n$ or even signature $e = f\overline{f}\ldots f\overline{f} \in E_n$, and $f \in E_r$ has either a zero signature or is aperiodic.

Theorem 4.1. *Let $n \geq 1, f \in E_r$, and let r divide n. If $e = f\overline{f}\ldots\overline{f}f \in E_n$ or $e = f\overline{f}\ldots f\overline{f} \in E_n$, then $W(e)\langle\{t(0)\} \cup M_1\rangle \cong W(f)$.*

Proof. Let $1 \leq k \leq r$. Let $t_{(i)}$ denote a vertex of $W(e)$ and let $\overline{t}_{(i)}$ denote a vertex of $W(f)$, likewise for $v_{(i)}$ and $\overline{v}_{(i)}$. We define a function $\psi\colon \{t_{(0)}\} \cup M_1 \to V(W(f))$ by $\psi(t_{(0)}) = \overline{t}_{(0)}$ and $\psi(t_{(i)}) = \overline{t}(i)$, for $1 \leq i \leq 2r$. Clearly, ψ is a bijection. We will show that the Hamilton directed cycle $\overrightarrow{H_k}$ in $W(f)$ is a union of ψ-images of directed paths belonging to Hamilton directed cycles $\overrightarrow{H_k}$ and $\overrightarrow{H}_{r+k}$ in $W(e)$.

Let $\overrightarrow{P_k}$ denote the directed path $[t_{(0)}, t_{(k)}, \ldots, t_{(2k)}]$ on $\overrightarrow{H_k}$ and let $\overrightarrow{P}_{r+k}$ denote the directed path $[t_{(0)}, t_{(r+k)}, \ldots, t_{(2k)}]$ on $\overrightarrow{H}_{r+k}$ (see Figure 12). A ψ-image of a directed path $\overrightarrow{P}$ is a directed path comprised of the ψ-images of vertices of $\overrightarrow{P}$. The ψ-image of $\overrightarrow{P_k}$ is $\overrightarrow{P'_k}$. Similarly, the ψ-image of $\overrightarrow{P}_{r+k}$ is $\overrightarrow{P'}_{r+k}$.

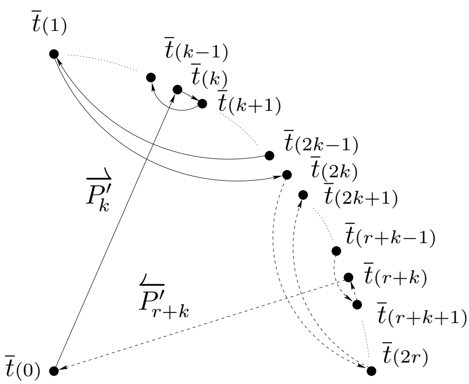

Figure 12: Hamilton directed cycle from the proof of Theorem 4.1.

The definition of Walecki tournaments implies that ψ is dominance-preserving on paths $\overrightarrow{P_k}$ and $\overrightarrow{P}_{r+k}$. The signature of $e = f\overline{f}\ldots\overline{f}f$ implies that if $e_k = 0$, then $e_{r+k} = 1$ and $\overrightarrow{H'_k} = \overrightarrow{P'_k} \cup \overleftarrow{P'}_{r+k}$, where $\overleftarrow{P'}_{r+k}$ denotes the path $\overrightarrow{P'}_{r+k}$ with all of its arcs reversed (see Figure 12). If $e_k = 1$, then $e_{r+k} = 0$ and $\overleftarrow{H'_k} = \overleftarrow{P'}_{r+k} \cup \overrightarrow{P'_k}$. Therefore, $W(e)\langle\{t_{(0)}\} \cup M_1\rangle \cong W(f)$. □

Figure 13 shows Walecki tournament $W(000111000)\langle\{t_{(0)} \cup M_1\}\rangle \cong W(000)$, an example of a Walecki tournament from Theorem 4.1.

If we consider the case when $e \in E_n$ has period $m < 2n$, then Lemma 1.2 implies that $m = 2r$, n/r is odd, $e = f\overline{f}\ldots\overline{f}f \in E_n$, and $f \in E_r$. The special form of e implies various symmetries in the corresponding Walecki tournament.

Lemma 4.2. *Let $n \geq 5$ and let $e \in E_n$ with period $m = 2r < 2n$. If k is an integer such that $1 \leq k \leq r$, then $t_{(2ri+rf_k+k)} \in N^+(t_{(0)})$ and $t_{(2ri+r\overline{f}_k+k)} \in N^-(t_{(0)})$, for $0 \leq i \leq n/r - 1$.*

Proof. Let k be an integer such that $1 \leq k \leq r$. Since $e = f\overline{f}\ldots\overline{f}f$ it follows that $e_{2ri+k} = f_k$ for $0 \leq i \leq (n/r-1)/2$. Therefore, if $f_k = 0$, then $t_{(2ri+k)} \in N^+(t_{(0)})$ and if $f_k = 1$, then $t_{(2ri+k)} \in N^-(t_{(0)})$ for $0 \leq i \leq (n/r-1)/2$.

On the other hand, $e_{2ri+r+k} = \overline{f}_k$ for $0 \leq i \leq (n/r-1)/2 - 1$. Now, if $f_k = 0$, then $t_{(2ri+r+k)} \in N^-(t_{(0)})$ and if $f_k = 1$, then $t_{(2ri+r+k)} \in N^+(t_{(0)})$. If $t_{(0)} \to t_{(k)} \in \overrightarrow{H_k}$, then $t_{(n+k)} \to t_{(0)} \in \overrightarrow{H_k}$, which proves the remaining cases. □

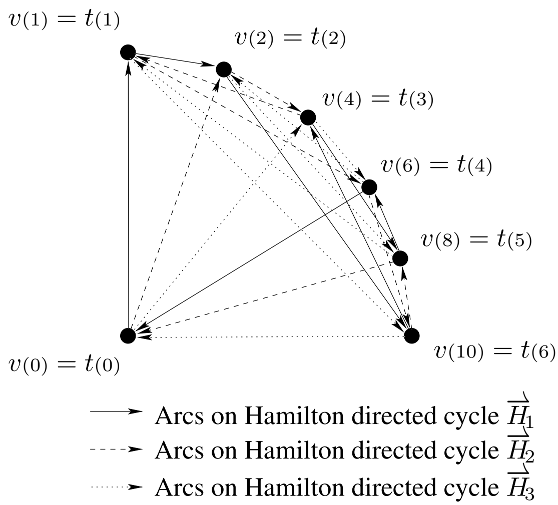

Figure 13: Walecki tournament $W(000)$ as an induced subtournament of $W(000111000)$.

Lemma 4.3. *Let $n \geq 5$ and let $e \in E_n$ with period $m = 2r < 2n$. If k is an integer such that $1 \leq k \leq r$, then $t(\overline{f}_k+2(2ri+k)-1) \in N^+(t(1))$ and $t(f_k+2(2ri+k)-1) \in N^-(t(1))$, for $0 \leq i \leq (n/r-1)/2$.*

Moreover, $t(f_k+2(2ri+r+k)-1) \in N^+(t(1))$ and $t(\overline{f}_k+2(2ri+r+k)-1) \in N^-(t(1))$, for $0 \leq i \leq (n/r-1)/2-1$.

Proof. Let $e \in E_n$ have period $m < 2n$. Lemma 1.2 implies that $m = 2r$, n/r is odd, $e = f\overline{f}\ldots\overline{f}f \in E_n$, and $f \in E_r$. The special form of e tells us that $e_{2ri+k} = f_k$ for $0 \leq i \leq (n/r-1)/2$. The structure of the Hamilton directed cycle $\overrightarrow{H_k}$ implies that if $f_k = 0$, then $t(2(2ri+k)-1) \in N^-(t(1))$ and $t(2(2ri+k)) \in N^+(t(1))$. Furthermore, if $f_k = 1$, then $t(2(2ri+k)-1) \in N^+(t(1))$ and $t(2(2ri+k)) \in N^-(t(1))$. Therefore, $t(2(2ri+k)+\overline{f}_k-1) \in N^+(t(1))$ and $t(2(2ri+k)+f_k-1) \in N^-(t(1))$.

The special form of e also implies $e_{2ri+r+k} = \overline{f}_k$ for $0 \leq i \leq (n/r-1)/2-1$, then the remaining cases can be proven similarly as above. $\square$

Now, let $e \in E_n$ have odd signature. Theorem 4.1 implies the existence of n/r Walecki subtournaments $T\langle\{t(0)\} \cup M_i\rangle$, for $1 < i < n/r$, of tournament $T = W(e)$. We determine subtournaments of $W(e)$ which are isomorphic to some Walecki tournament with odd signature. This is a generalization of Theorem 4.1 for odd signature Walecki tournaments. The vertices that induce the subtournament are chosen on the circumference in clockwise order starting at the vertex $t(1)$.

Theorem 4.4. *Let $n \geq 5$ and let $e = f\overline{f}\ldots\overline{f}f \in E_n$ with period $m = 2r < 2n$, and $f \in E_r$. If ℓ is an odd integer such that $1 \leq \ell \leq n/r-2$ then, $W(e)\big\langle\{t(0)\} \cup \{M_1 \cup M_2 \cup \cdots \cup M_\ell\}\big\rangle \cong W(e')$, where $e' = f\overline{f}\ldots\overline{f}f \in E_{\ell r}$.*

Proof. If $\ell = 1$, the conclusion is just Theorem 4.1. Let ℓ be an odd integer such that $3 \leq \ell \leq n/r-2$ and let $e' = f\overline{f}\ldots\overline{f}f \in E_{\ell r}$. Let $t(i)$ denote a vertex of $W(e)$ and $\overline{t}(i)$ denote a vertex of $W(e')$, likewise for $v(i)$ and $\overline{v}(i)$. We define a function $\psi\colon \{t(0)\} \cup M_1 \cup M_2 \cup \cdots \cup M_\ell \to V(W(e'))$ by $\psi(t(0)) = \overline{t}(0)$ and $\psi(t(i)) = \overline{t}(i)$, for $0 \leq i \leq 2\ell r-1$.

Clearly, ψ is a bijection. We will show that the Hamilton directed cycle $\overrightarrow{H_k}$ in $W(e')$ is a union of ψ-images of directed paths belonging to Hamilton directed cycles $\overrightarrow{H_k}$ and $\overrightarrow{H}_{\ell r+k}$ in $W(e)$ when $\ell r + k \leq n$, otherwise, $\overrightarrow{H'_k}$ is a union of ψ-images of directed paths belonging to Hamilton cycles $\overrightarrow{H_k}$ and $\overrightarrow{H}_{n-\ell r+k}$.

Case 1. Let us first consider the case when $\ell r + k \leq n$. The ψ-image of $\overrightarrow{P_k}$ is the path $\overrightarrow{P'_k}$ as in the proof of the Theorem 4.1, $\psi(\overrightarrow{P_k}) = \overrightarrow{P'_k}$. The ψ-image of $\overrightarrow{P}_{\ell r+k}$ is $\overrightarrow{P'}_{\ell r+k}$. The definition of Walecki tournaments implies that ψ is dominance-preserving on paths $\overrightarrow{P_k}$ and $\overrightarrow{P}_{\ell r+k}$. By assumption, the difference between $\ell r + k$ and k ia an *odd* multiple of r. Furthermore, odd signature of e implies that if $e_k = 0$ then $e_{\ell r+k} = 1$ and $\overrightarrow{H'_k} = \overrightarrow{P'_k} \cup \overleftarrow{P'}_{\ell r+k}$ (see Figure 14). If $e_k = 1$ then $e_{\ell r+k} = 0$ and $\overrightarrow{H'_k} = \overleftarrow{P'}_{\ell r+k} \cup \overleftarrow{P'_k}$.

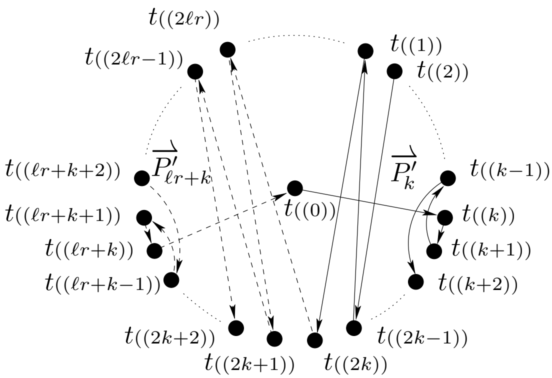

Figure 14: Hamilton directed cycle constructed from directed paths from Case 1 of the proof of Theorem 4.4.

Case 2. Let $\ell r + k > n$. Note that $n - \ell r < k \leq \ell r$. Define $\overrightarrow{P_k}$ as in the previous case and let $\overrightarrow{P}_{\ell r+k-n}$ denote the directed path $[t(2k), t(2\ell r), t(2k+1), t(2\ell r-1), t(2k+1), \ldots, t(\ell r+k+2), t(\ell r+k-1), t(\ell r+k+1), t(\ell r+k), t(0)]$ on $\overrightarrow{H}_{\ell r+k-n}$. The ψ-image of $\overrightarrow{P}_{\ell r+k-n}$ is $\overrightarrow{P'}_{\ell r+k-n}$. By the definition of Walecki tournaments ψ is dominance-preserving on the path $\overrightarrow{P}_{\ell r+k}$. Now, n/r is odd and, by assumption, ℓ is also odd which implies that the difference $\ell r - n = (\ell - n/r)r$ is an even multiple of r. Furthermore, the odd signature of e implies that if $e_k = 0$ then $e_{\ell r+k-n} = 0$ and $\overrightarrow{H'_k} = \overrightarrow{P'_k} \cup \overrightarrow{P'}_{\ell r+k-n}$ (see Figure 15). If $e_k = 1$ then $e_{\ell r+k-n} = 1$ and $\overrightarrow{H'_k} = \overleftarrow{P'}_{\ell r+k-n} \cup \overleftarrow{P'_k}$. This completes the proof. □

The importance of τ^m for the automorphism groups of Walecki tournaments with odd signature was previously unknown. The subtournaments $T\langle\{t(0)\} \cup M_i\rangle$, for $1 \leq i \leq n/r$, are isomorphic to $W(f)$. This suggests that the permutation τ^m, which is a product of $m = 2r$ disjoint cycles of length n/r, might be an automorphism of $W(e)$.

Proposition 4.5. *Let $n \geq 5$. If $e \in E_n$ has period $m < 2n$, then $\tau^m \in \mathrm{Aut}(W(e))$.*

Proof. We have $m = 2r$, n/r is odd, $e = f\overline{f}\ldots\overline{f}f \in E_n$, $f \in E_r$, and e and f have the same period $2r$, and $R^m(e) = R^{2r}(e) = e$. The statement follows by Theorem 1.3. □

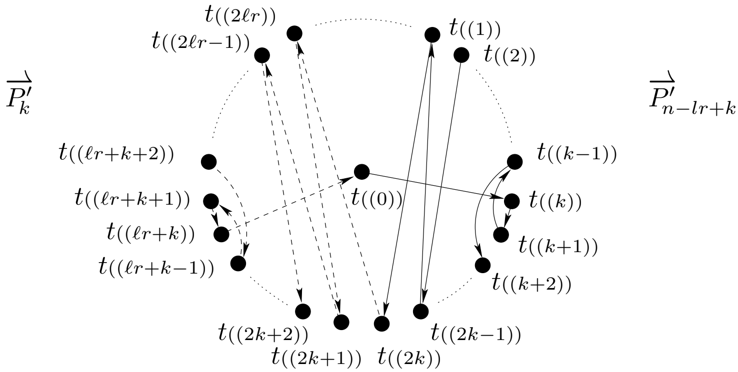

Figure 15: Hamilton directed cycle constructed from directed paths from Case 2 of the proof of Theorem 4.4.

4.1 Subtournaments of odd signature Walecki tournaments

A second partition of $V(W(e)) - \{t_{(0)}\}$ is now introduced. The partition is defined by the orbits $O_1, O_2, \ldots, O_m$, for the permutation τ^m acting on $V(W(e)) - \{t_{(0)}\}$. The orbits have length n/r and can be expressed as follows:

$$O_\ell = \{t_{(im+\ell)} \mid 0 \leq i \leq n/r - 1\}, \tag{4.1}$$

for $1 \leq \ell \leq m$ and $m = 2r$.

Let $1 \leq k \leq m$. One can easily prove that if $f_k = 0$, then $O_k \subseteq N^+(t_{(0)})$ and $O_{r+k} \subseteq N^-(t_{(0)})$. Moreover, if $f_k = 1$, then $O_k \subseteq N^-(t_{(0)})$ and $O_{r+k} \subseteq N^+(t_{(0)})$. In order to simplify the notation we introduce the permutation $\zeta \in \mathbb{S}_{2r}$ acting on the set $\{1, 2, \ldots, 2r\}$ defined by $\zeta = (1\ r+1)(2\ r+2)\cdots(r\ 2r)$. That is, $\zeta(i) = i + r$ for $1 \leq i \leq r$, and $\zeta(i) = i - r$ for $r + 1 \leq i \leq 2r$. Note that for $1 \leq k \leq r$,

$$O_{\zeta^{f_k}(k)} = \{t_{(im+\zeta^{f_k}(k))} \mid 0 \leq i \leq n/r - 1\}. \tag{4.2}$$

It follows from the observations above that $O_{\zeta^{f_k}(k)} \subseteq N^+(t_{(0)})$ and $O_{\zeta^{\overline{f}_k}(k)} \subseteq N^-(t_{(0)})$. Therefore,

$$N^+(t_{(0)}) = \bigcup_{k=1}^{r} O_{\zeta^{f_k}(k)} \tag{4.3}$$

and

$$N^-(t_{(0)}) = \bigcup_{k=1}^{r} O_{\zeta^{\overline{f}_k}(k)}. \tag{4.4}$$

Orbits and m-sets are *orthogonal* in the sense that each orbit contains exactly one vertex of each m-set, and vice-versa.

The arc structure of subtournaments induced by the orbits O_ℓ, for the permutation τ^m, is determined by the value of e_ℓ, for $1 \leq \ell \leq m$.

Theorem 4.6. *Let T denote the Walecki tournament $W(e)$ for $e \in E_n$ and $n \geq 5$. If e has period $m < 2n$, then the orbits $O_1, O_2, \ldots, O_m$ for the permutation τ^m acting on*

$V(W(e)) - \{t(0)\}$ induce regular tournaments $T\langle O_1\rangle, T\langle O_2\rangle, \ldots, T\langle O_m\rangle$. If ℓ is an integer such that $1 \le \ell \le m$, the subtournaments $T\langle O_\ell \cap N^+(t(1))\rangle$ and $T\langle O_\ell \cap N^-(t(1))\rangle$ are transitive and the directions of all their arcs are determined by e_ℓ.

Proof. Under the conditions for the sequence $e \in E_n$, Proposition 4.5 implies that $O_1, O_2, \ldots, O_m$ are orbits for the permutation $\tau^m \in \mathrm{Aut}(T)$ which proves that the subtournaments $T\langle O_1\rangle, T\langle O_2\rangle, \ldots, T\langle O_m\rangle$ are regular. To prove the rest of the theorem we first consider the subtournaments $T\langle O_1 \cap N^+(t(1))\rangle$ and $T\langle O_1 \cap N^-(t(1))\rangle$. We make use of Lemma 4.2 and Lemma 4.3.

Let $m = 2r$. Lemma 1.1 implies that $e = f\overline{f}\ldots\overline{f}f$ where $f \in E_r$. Vertices of an arbitrary orbit were determined in (4.1) and (4.2).

We may assume $f_1 = 0$ for if not we may work with $\overline{W(e)}$ instead. We first consider the orbit containing vertex $t(1)$. Since $f_1 = 0$ we have $O_{\varsigma^{f_1}(1)} = O_1 \subseteq N^+(t(0))$ and $O_1 = \{t(2ri+1) \mid 0 \le i \le n/r - 1\}$. Let $Y^+ = O_1 \cap N^+(t(1))$ and $Y^- = O_1 \cap N^-(t(1))$. Since $e_{r+1} = \overline{f}_1 = 1$, we have $t(2r+1) \in Y^+$. Similarly, $e_{2r+1} = f_1 = 0$ implies $t(4r+1) \in Y^-$. Furthermore, $\tau^m \in \mathrm{Aut}(T)$ implies $Y^+ = \{t(4ri+2r+1) \mid 0 \le i \le (n/r-3)/2\}$ and $Y^- = \{t(4ri+1) \mid 1 \le i \le (n/r-1)/2\}$.

Let us consider Y^+. We will prove that considering the vertices of Y^+ in the order $t(2r+1), t(6r+1), \ldots, t(2n-4r+1)$, all arcs point from right to left in the subtournament $T\langle Y^+\rangle$. Let $0 \le i \le (n/r-3)/2$. The equalities

$$\tau^{4rj+2r}(1) = \tau^{2r(j+i+1)}(\tau^{2r(j-i)}(1)) = \tau^{2r(j+i+1)}(4r(j-i))$$

and

$$\tau^{4ri+2r}(1) = \tau^{2r(j+i+1)}(\tau^{2r(i-j)}(1)) = \tau^{2r(j+i+1)}(4r(j-i)+1)$$

imply that the arc $t(4rj+2r+1) \to t(4ri+2r+1)$ belongs to the Hamilton directed cycle $\overrightarrow{H}_{2r(j+i+1)+1}$. This proves the subtournament $T\langle Y^+\rangle$ transitive. Moreover, $\tau^m(Y^+) = Y^-$ implies that the subtournament $T\langle Y^-\rangle$ is also transitive.

Next we consider orbits in $N^+(t(0))$ that do not contain vertex $t(1)$. Equation (4.3) implies that $O_{\varsigma^{f_k}(k)} \subseteq N^+(t(0))$, for $2 \le k \le r$. Let us first assume that $f_k = 0$. Using Equation (4.2) we have $O_{\varsigma^{f_k}(k)} = O_k = \{t(2ri+k) \mid 0 \le i \le n/r - 1\}$. We further divide the proof depending on the parity of k.

Case 1. Let k be odd. Clearly, $k+1$ is even so $e_{(k+1)/2} = f_{(k+1)/2}$ and $e_{r+(k+1)/2} = \overline{f}_{(k+1)/2}$ determine the membership of $t(k)$ and $t(2r+k)$, respectively, in $N^+(t(1))$ and $N^-(t(1))$.

Case 1.1. If $f_{(k+1)/2} = 0$, we have $t(k) \in N^-(t(1))$, and $\overline{f}_{(k+1)/2} = 1$ implies $t(2r+k) \in N^+(t(1))$. It follows that $Y' = \{t(4ri+k) \mid 0 \le i \le (n/r-1)/2\} \subseteq N^-(t(1))$ and $Y'' = \{t(4ri+2r+k) \mid 0 \le i \le (n/r-3)/2\} \subseteq N^+(t(1))$. Similarly as above we can prove that the subtournaments $T\langle Y'\rangle$ and $T\langle Y''\rangle$ are transitive.

Case 1.2. If $f_{(k+1)/2} = 1$, then $t(k) \in N^+(t(1))$ and $\overline{f}_{(k+1)/2} = 0$ which implies that $t(2r+k) \in N^-(t(1))$. Since the sequence e has the form $f\overline{f}\ldots\overline{f}f$ it follows that $Y' \subseteq N^+(t(1))$ and $Y'' \subseteq N^-(t(1))$. As in the previous case we can show that the subtournaments $T\langle Y'\rangle$ and $T\langle Y''\rangle$ are transitive. A change in the value of $f_{(k+1)/2}$ results in the reversal of arcs associated with $t(1)$. However, the arcs between vertices of Y' depend on f_k only. The same reasoning applies to Y''.

Case 2. Let k be even. This implies that $e_{k/2} = f_{k/2}$ and $e_{r+k/2} = \overline{f}_{k/2}$ determine the membership of $t_{(k)}$ and $t_{(2r+k)}$, respectively, in $N^+(t_{(1)})$ and $N^-(t_{(1)})$.

Case 2.1. If $f_{k/2} = 0$, then $t_{(k)} \in N^+(t_{(1)})$, and $\overline{f}_{k/2} = 1$ implies $t_{(2r+k)} \in N^-(t_{(1)})$. Similarly as in the previous case we have $Y^{'} \subseteq N^+(t_{(1)})$, $Y^{''} \subseteq N^-(t_{(1)})$, and the subtournaments $T\langle Y^{'}\rangle$ and $T\langle Y^{''}\rangle$ are transitive.

Case 2.2. Using similar arguments as above, we can prove that if $f_{k/2} = 1$, then the sets $Y^{'}$ and $Y^{''}$ determine transitive subtournaments $T\langle Y^{'}\rangle$ and $T\langle Y^{''}\rangle$, respectively. This completes the proof for $f_k = 0$.

Assume now $f_k = 1$. This implies $O_{\zeta^{f_k}(k)} = O_{r+k} = \{t_{(2ri+r+k)} \mid 0 \leq i \leq n/r-1\}$. In a way similar to the previous case we define $Y^{'} = \{t_{(4ri+r+k)} \mid 0 \leq i \leq (n/r-1)/2\}$ and $Y^{''} = \{t_{(4ri+3r+k)} \mid 0 \leq i \leq (n/r-3)/2\}$, and prove that $T\langle Y^{'}\rangle$ and $T\langle Y^{''}\rangle$ are transitive subtournaments. The proof is similar to the case $f_k = 0$, however, the direction of all arcs considered is reversed since $e_k = f_k = 1$. This completes the proof for orbits $O_{\zeta^{f_k}(k)} \subseteq N^+(t_{(0)})$. The result for orbits $O_{\zeta^{\overline{f}_k}(k)} \subseteq N^-(t_{(0)})$ follows since $T \cong \overline{T}$. $\square$

Next we consider the subtournaments induced by outsets and insets of vertices in a Walecki tournament with odd signature $e = f\overline{f}\ldots\overline{f}f \in E_n$, whose defining sequence is $f = (0, 0, \ldots, 0) \in E_r$. We show that if the vertex is distinct from $t_{(0)}$ then its outset induces a subtournament that is not regular for n odd. However, the outset of $t_{(0)}$ induces a regular subtournament. Similarly, for n even the outset of $t_{(0)}$ induces an almost regular subtournament but the outset of any other vertex induces a subtournament that is not almost regular. This implies that $t_{(0)}$ must be fixed for any automorphism of a Walecki tournament with an odd signature $e = f\overline{f}\ldots\overline{f}f$ where $f = (0, 0, \ldots, 0)$.

Theorem 4.7. *Let $T = W(e)$ for $e = f\overline{f}\ldots\overline{f}f \in E_n$, $n \geq 5$, n/r odd, and $f = (0, 0, \ldots, 0) \in E_r$. For $v \in V(W(e)) - \{t_{(0)}\}$, the tournaments $T\big\langle N^+(v)\big\rangle$ are not regular and not almost regular subtournaments of T for n odd and n even, respectively.*

Proof. Since $W(e) \cong \overline{W(e)}$, it suffices to prove the theorem for vertices in $N^+(t_{(0)})$. Furthermore, since $\tau^m \in \mathrm{Aut}(T)$, it is sufficient to prove the theorem for the vertices in $N^+(t_{(0)}) \cap M_1$. Let $M' = M_1 \cup M_3 \cup \cdots \cup M_{n/r}$ and $M'' = M_2 \cup M_4 \cup \cdots \cup M_{n/r-1}$.

We first assume $r > 1$ and consider $t_{(1)} \in N^+(t_{(0)}) \cap M_1$. We will count the vertices in $N^+(t_{(1)}) \cap N^+(t_{(2n)})$. First we determine the vertices in $N^+(t_{(1)})$. Since $f = (0, 0, \ldots, 0)$, Theorem 4.1 implies

$$N^+(t_{(1)}) \cap M_1 = \{t_{(2i+2)} \mid 0 \leq i \leq r-1\}. \tag{4.5}$$

Using Lemma 2.5 we have

$$N^+(t_{(1)}) \cap M_2 = \{t_{(2r+2i+1)} \mid 0 \leq i \leq r-1\}. \tag{4.6}$$

Let $X' = N^+(t_{(1)}) \cap M'$ and $X'' = N^+(t_{(1)}) \cap M''$. The odd signature of the sequence e and equalities (4.5) and (4.6) imply

$$X' = \{t_{(4rj+2i+2)} \mid 0 \leq i \leq r-1, 0 \leq j \leq (n/r-1)/2\} \tag{4.7}$$

and

$$X'' = \{t_{(4rj+2r+2i+1)} \mid 0 \leq i \leq r-1, 0 \leq j \leq (n/r-3)/2\}. \tag{4.8}$$

Clearly, $N^+(t_{(1)}) = X' \cup X''$. Next we determine the vertices in $N^+(t_{(2n)})$. We have

$$N^+(t_{(2n)}) \cap M_1 = \{t_{(2i+1)} \mid 1 \leq i \leq r-1\} \tag{4.9}$$

and

$$N^+(t_{(2n)}) \cap M_2 = \{t_{(2r+1)}\} \cup \{t_{(2r+2i+2)} \mid 0 \leq i \leq r-1\}. \tag{4.10}$$

Let Y' denote $N^+(t_{(2n)}) \cap M'$ and let Y'' denote $N^+(t_{(2n)}) \cap M''$. The odd signature of the sequence e and equalities (4.9) and (4.10) imply

$$Y' = \{t_{(4rj+2i+1)} \mid 1 \leq i \leq r-1, 0 \leq j \leq (n/r-3)/2\}. \tag{4.11}$$

Let $Y'' = \overline{Y}'' \cup \overline{\overline{Y}}'' =$ where

$$\overline{Y}'' = \{t_{(4rj+2r+1)} \mid 0 \leq j \leq (n/r-3)/2\} \tag{4.12}$$

and

$$\overline{\overline{Y}}'' = \{t_{(4rj+2r+2i+2)} \mid 0 \leq i \leq r-1, 0 \leq j \leq (n/r-3)/2\}. \tag{4.13}$$

Clearly, $N^+(t_{(2n)}) = \{t_{(0)}\} \cup Y' \cup Y''$.

Comparing the indices of the vertices in equalities (4.7), (4.8), (4.11), (4.12), and (4.13) for vertices in $N^+(t_{(1)})$ and $N^+(t_{(2n)})$, we deduce $(X' \cup X'') \cap (Y' \cup Y'') = \overline{\overline{Y}}$, which implies $N^+(t_{(1)}) \cap N^+(t_{(2n)}) = \overline{Y}''$. Hence, the score of vertex $t_{(2n)}$ in $T\langle N^+(t_{(1)})\rangle$ equals $|\overline{Y}''| = (n/r-1)/2$. If $r > 1$, then $(n/r-1)/2 < n/2-1$ which implies that $T\langle N^+(t_{(1)})\rangle$ is not regular or almost regular when n is odd or even, respectively. The proofs for the remaining vertices of $N^+(t_{(0)}) \cap M_1$ are similar and we omit them.

The arc structure of $T\langle N^+(t_{(1)})\rangle$ is different in the case when $r = 1$, that is, when $e = (0,1,0,1,\ldots,0,1,0) \in E_n$. Notice that n/r odd implies that n has to be odd. In order to verify non-regularity of $T\langle N^+(t_{(1)})\rangle$, we consider $N^+(t_{(1)}) \cap N^+(t_{(3)})$. The signature of e implies

$$N^+(t_{(1)}) = \{t_{(2n)}\} \cup \{t_{(4i+2)},\ t_{(4i+3)} \mid 0 \leq i \leq (n-3)/2\}. \tag{4.14}$$

Since $\tau^2 \in \mathrm{Aut}(W(e))$ we have

$$N^+(t_{(3)}) = \{t_{(2)}\} \cup \{t_{(4i+4)},\ t_{(4i+5)} \mid 0 \leq i \leq (n-3)/2\}. \tag{4.15}$$

Comparing the indices of the vertices in equalities (4.7), (4.8), (4.14), (4.15), for vertices in $N^+(t_{(1)})$ and $N^+(t_{(3)})$ we deduce that $N^+(t_{(1)}) \cap N^+(t_{(3)}) = \{t_{(2)}\}$. Hence, the score of vertex $t_{(3)}$ in $T\langle N^+(t_{(1)})\rangle$ equals 1 implying that $T\langle N^+(t_{(1)})\rangle$ is not regular. This completes the proof. $\square$

4.1.1 Regular subtournaments for n odd

Next we determine the structure of arcs in the subtournaments induced by $N^+(t_{(0)})$ and $N^-(t_{(0)})$. There are two cases to be considered depending on the parity of n.

Let $e = f\overline{f}\ldots\overline{f}f \in E_n$, n odd, be an odd signature sequence with a zero subsignature $f = (0,0,\ldots,0) \in E_r$, and let T denote $W(e)$. We will consider the subtournaments $T\langle N^+(t_{(0)})\rangle$ and $T\langle N^-(t_{(0)})\rangle$. We know that the out-neighbours and in-neighbours of $t_{(0)}$ are determined by f and $\overline{f}$. Therefore, r vertices of each m-set belong to $N^+(t_{(0)})$ and the other r of them to $N^-(t_{(0)})$. On the other hand, the construction of Walecki tournaments implies that out of two consecutive vertices $t_{(j)}$ and $t_{(j+1)}$ exactly one is an out-neighbour of the vertex $t_{(i)}$, whenever $j-i$ is even. Therefore one would hope that the score of each vertex in $T\langle N^+(t_{(0)})\rangle$ is no more than $2n/4 = n/2$. This would imply the regularity of the subtournaments $T\langle N^+(t_{(0)})\rangle$ and $T\langle N^-(t_{(0)})\rangle$.

Theorem 4.8. *Let n be odd and let T denote the Walecki tournament $W(e)$ for $e = f\overline{f}\ldots\overline{f}f \in E_n$, n/r odd, and $f = (0,0,\ldots,0) \in E_r$. If e has period $m < 2n$, then the subtournaments $T\langle N^+(t_{(0)})\rangle$ and $T\langle N^-(t_{(0)})\rangle$ are regular.*

Proof. The result is clearly true for $n \le 3$. Let T be a tournament as stated in the conditions of the theorem and $n \ge 5$. In order to prove that $T\langle N^+(t_{(0)})\rangle$ is regular, we first determine the score of the vertex $t_{(1)}$ in $T\langle N^+(t_{(0)})\rangle$. Let Y denote the set $N^+(t_{(0)}) \cap N^+(t_{(1)})$. We are interested in the cardinality of Y. Since $m < 2n$, Lemma 1.2 implies that $m = 2r$ and n/r is odd. Now, n odd implies that r is also odd. We proceed by proving that $|Y \cap (M_i \cup M_{i+1})| = r$, for $1 \le i \le n/r - 1$. We use Lemma 4.2 and Lemma 4.3 extensively.

Let us consider the cardinality of $Y \cap (M_1 \cap M_2)$. We first determine the vertices in $N^+(t_{(1)}) \cap M_1$. If i is an integer such that $1 \le i \le r-1$, then $e_{i+1} = f_{i+1}$. Because $f_{i+1} = 0$, we have

$$t_{(2i+1)} \in N^-(t_{(1)}) \quad \text{and} \quad t_{(2i+2)} \in N^+(t_{(1)}). \tag{4.16}$$

Since $T \cong \overline{T}$, we may assume that $e_1 = f_1 = 0$. Thus, $t_{(2)} \in N^+(t_{(1)})$. Next we consider $N^+(t_{(0)}) \cap M_1$. If j is an integer such that $1 \le j \le r-1$, then $e_{j+1} = f_{j+1}$. Since $f_{j+1} = 0$, we have

$$t_{(j+1)} \in N^+(t_{(0)}) \quad \text{and} \quad t_{(j+1+r)} \in N^-(t_{(0)}). \tag{4.17}$$

Being $0 \le i \le r-1$, we have $2r \le 2(r+i) \le 4r-2$. The neighbours of the vertex $t_{(1)}$ in the set M_2 are given by

$$t_{(2(r+i)+2)} \in N^-(t_{(1)}) \quad \text{and} \quad t_{(2(r+i)+1)} \in N^+(t_{(1)}). \tag{4.18}$$

If k is an integer such that $0 \le k \le r-1$, then $2r \le 2r+k \le 3r-1$. The neighbours of the vertex $t_{(0)}$ in the set M_2 are given by

$$t_{(2r+k+1)} \in N^+(t_{(0)}) \quad \text{and} \quad t_{(2r+k+1+r)} \in N^-(t_{(0)}). \tag{4.19}$$

We use (4.16), (4.17), (4.18), and (4.19) in the following case study. Let i be an integer such that $1 \le i \le (r-3)/2$. Since $e_{i+1} = f_{i+1} = 0$, it follows that $t_{(2i+2)}, t_{(2r+2i+1)} \in N^+(t_{(1)})$. Similarly, $e_{i+(r+1)/2} = f_{i+(r+1)/2} = 0$ implies $t_{(r+2i+1)} \in N^+(t_{(1)})$, and $e_{i+(r+3)/2} = f_{i+(r+3)/2} = 0$ implies $t_{(3r+2i+2)} \in N^+(t_{(1)})$. Also $e_{2i+1} = f_{2i+1} = 0$ implies $t_{(2i+1)}, t_{(2r+2i+1)} \in N^+(t_{(0)})$, and $e_{2i+2} = f_{2i+2} = 0$ implies $t_{(2i+2)}, t_{(2r+2i+2)} \in N^+(t_{(0)})$. Let $1 \le i \le (r-3)/2$. Since $f_{i+1}, f_{2i+1}, f_{2i+2}, f_{i+(r+1)/2}$, and $f_{i+(r+3)/2}$ are all zero, it follows that exactly two of the vertices $t_{(2i+1)}, t_{(2i+2)}, t_{(r+2i+1)}, t_{(r+2i+2)}$, $t_{(2r+2i+1)}, t_{(2r+2i+2)}, t_{(3r+2i+1)}$, and $t_{(3r+2i+2)}$ belong to $Y \cap (M_1 \cup M_2)$.

We have yet to consider vertices $t_{(1)}, t_{(r)}, t_{(r+1)}, t_{(2r)}, t_{(2r+1)}, t_{(3r)}, t_{(3r+1)}$, and $t_{(4r)}$. Their membership in $N^+(t_{(1)}) \cap N^+(t_{(0)})$ is determined by the values of f_1, f_r and $f_{(r+1)/2}$, which are all zero. Notice that $e_r = f_r$, which implies $t_{(r)}, t_{(3r)} \in N^+(t_{(0)})$, and $t_{(2r)}, t_{(4r)} \in N^+(t_{(1)})$. Similarly, $e_{(r+1)/2} = f_{(r+1)/2}$ implies that if $f_{(r+1)/2} = 0$, then $t_{(r+1)}, t_{(3r)} \in N^+(t_{(1)})$. Since $f_1 = 0$, we have $e_{r+1} = \overline{f}_1 = 1$, which implies $t_{(2r+1)} \in N^+(t_{(1)})$ and $t_{(1)}, t_{(2r+1)} \in N^+(t_{(0)})$. Clearly, $t_{(1)} \notin N^+(t_{(1)})$. It follows that exactly two of the vertices $t_{(r)}, t_{(r+1)}, t_{(2r)}, t_{(2r+1)}, t_{(3r)}, t_{(3r+1)}$, and $t_{(4r)}$ belong to $Y \cap (M_1 \cup M_2)$.

We have considered all vertices in $M_1 \cup M_2$ except $t_{(2)}, t_{(r+2)}, t_{(2r+2)}$, and $t_{(3r+2)}$. Their membership in $N^+(t_{(1)}) \cap N^+(t_{(0)})$ is determined by the values of f_1, f_2 and $f_{(r+3)/2}$, which are all zero. Now, $e_1 = f_1 = 0$ implies $t_{(2)} \in N^+(t_{(1)})$, and $e_{r+1} = \overline{f}_1 = 1$ implies $t_{(2r+2)} \in N^-(t_{(1)})$. Notice that $e_2 = f_2 = 0$ implies $t_{(2)}, t_{(2r+2)} \in N^+(t_{(0)})$. Also, $e_{(r+3)/2} = f_{(r+3)/2} = 0$ implies $t_{(3r+2)} \in N^+(t_{(1)})$. Hence, exactly one of the vertices $t_{(2)}$, $t_{(r+2)}, t_{(2r+2)}$, and $t_{(3r+2)}$ belongs to $Y \cap (M_1 \cup M_2)$. It follows by above observations that

$$|Y \cap (M_1 \cup M_2)| = 2(r-3)/2 + 2 + 1 = r. \tag{4.20}$$

Similar to the previous case we can show that

$$|Y \cap (M_i \cup M_{i+1})| = 2(r-1)/2 + 1 = r,$$

for $2 \leq i \leq n/r - 1$, and

$$|Y \cap (M_1 \cup M_{n/r})| \leq 2(r-3)/2 + 1 + 1 = r - 1. \tag{4.21}$$

Let α denote $|Y \cap M_1|$. Since $|Y \cap (M_1 \cup M_2)| = r$, it follows that $|Y \cap M_2| = r - \alpha$. Since n/r is odd, we have $|Y \cap M_{n/r-1}| = r - \alpha$ and $|Y \cap M_{n/r}| = \alpha$ which implies $|Y \cap (M_1 \cup M_{n/r})| = 2\alpha \leq r - 1$. Now, r is odd implies $|Y \cap (M_1 \cup M_{n/r})| \leq r - 1$. Therefore, $2|Y| \leq (r-1) + (n-r) = n - 1$ which implies

$$s(t_{(1)}) = |N^+(t_{(0)}) \cap N^+(t_{(1)})| \leq \frac{n-1}{2} < \frac{n}{2}. \tag{4.22}$$

Similarly, we can prove that

$$s(t_{(i+rf_i)}) = |N^+(t_{(0)}) \cap N^+(t_{(i+rf_t)})| \leq \frac{n-1}{2},$$

for $2 \leq i \leq r$. That is, every vertex in $N^+(t_{(0)}) \cap M_1$ has score at most $(n-1)/2$. Since τ^m is an automorphism of T, the score of every vertex in the tournament $T\langle N^+(t_{(0)})\rangle$ is at most $(n-1)/2$. Now,

$$\binom{n}{2} = \sum_{v \in N^+(t(0)} s(v) \leq \frac{n(n-1)}{2}$$

implies $s(v) = (n-1)/2$ for every vertex $v \in N^+(t_{(0)})$. Therefore, the subtournament $T\langle N^+(t_{(0)})\rangle$ is regular. Regularity of the tournament $T\langle N^-(t_{(0)})\rangle$ follows since $T \cong \overline{T}$. □

4.1.2 Almost regular subtournaments for n even

When n is even, $T\langle N^+(t_{(0)})\rangle$ can not be regular. However, one can prove that in the case of $f = (0, 0, \ldots, 0) \in E_r$ it is almost regular. We follow an analog of the proof of Theorem 4.8. Oddly enough, the fact that n is even simplifies the proof.

Theorem 4.9. *Let n be even and let T denote the Walecki tournament $W(e)$ for $e = f\overline{f}\ldots\overline{f}f \in E_n$, n/r odd, and $f = (0,0,\ldots,0) \in E_r$. If e has period $m < 2n$, then the subtournaments $T\langle N^+(t_{(0)})\rangle$ and $T\langle N^-(t_{(0)})\rangle$ are almost regular.*

Proof. The result is clearly true for $n \le 4$. Let T be a tournament as stated in the conditions of the theorem. We first prove that $T\langle N^+(t_{(0)})\rangle$ is almost regular. In order to do so we determine the score of the vertex $t_{(1)}$ in $T\langle N^+(t_{(0)})\rangle$. Let Y denote the set $N^+(t_{(0)}) \cup N^+(t_{(1)})$. We are interested in the cardinality of Y. Since $m < 2n$, we have $m = 2r$ and n/r is odd. Now, n even implies that r is also even. We proceed by considering sets $Y \cap (M_i \cup M_{i+1})$ for $1 \le i \le n/r - 1$. Similar to the proof of Theorem 4.8 we can prove $|Y \cap (M_i \cup M_{i+1})| = r$, for $1 \le i \le n/r - 1$, and $|Y \cap (M_{n/r} \cup M_1)| \le r$. Let α denote $|Y \cap M_1|$. Since n/r is odd, $|Y \cap M_{n/r-1}| = r - \alpha$ and $|Y \cap M_{n/r}| = \alpha$ which implies $|Y \cap (M_1 \cup M_{n/r})| = 2\alpha$. Hence, $2\alpha \le r$. Since r is even, we have $\alpha \le r/2$ and $|Y \cap (M_1 \cup M_{n/r})| \le r$. Therefore, $2|Y| \le n$ which implies $s(t_{(1)}) = |N^+(t_{(0)}) \cap N^+(t_{(1)})| \le n/2$. Similarly, we can prove that $s(t_{(i+rf_i)}) = |N^+(t_{(0)}) \cap N^+(t_{(i+rf_i)})| \le n/2$, for $2 \le i \le r$. That is, every vertex in $N^+(t_{(0)}) \cap M_1$ has score at most $n/2$. Since $\tau^m \in \mathrm{Aut}(T)$, the score of every vertex in the subtournament $T\langle N^+(t_{(0)})\rangle$ is at most $n/2$.

Since $T \cong \overline{T}$ with anti-automorphism $\eta = \tau^n \in \mathbb{S}_{2n+1}$, where

$$\eta = (v_{(1)}v_{(2n)})(v_{(2)}v_{(2n-1)})\ldots(v_{(n)}v_{(n+1)})$$
$$= (t_{(1)}t_{(n+1)})(t_{(2)}t_{(n+2)})\ldots(t_{(n)}t_{(2n-1)}),$$

(see Figure 16), we have $\overline{T\langle N^-(t_{(0)})\rangle} \cong T\langle N^+(t_{(0)})\rangle$. Now, $\eta(t_{(1)}) = t_{(3)}$ implies that $|N^-(t_{(0)}) \cap N^+(t_{(3)})| = s(t_{(3)}) \le n/2$ in $T\langle N^-(t_{(0)})\rangle$. Therefore, $|N^+(t_{(0)}) \cap N^-(t_{(1)})| \le n/2$ in $T\langle N^+(t_{(0)})\rangle$. Since

$$N^+(t_{(0)}) = (N^+(t_{(0)}) \cap N^+(t_{(1)})) \cup (N^+(t_{(0)}) \cap N^-(t_{(1)})) \cup \{t_{(1)}\},$$

we have $s(t_{(1)}) = |N^+(t_{(0)}) \cap N^+(t_{(1)})| \ge n/2 - 1$ in $T\langle N^+(t_{(0)})\rangle$. Using a similar argument we can prove that the score of every vertex in $T\langle N^+(t_{(0)})\rangle$ is either $n/2$ or $n/2 - 1$.

If k denotes the number of vertices with score $n/2$ in $T\langle N^+(t_{(0)})\rangle$, then the number of vertices of degree $n/2 - 1$ equals $n - k$. The equation

$$\binom{n}{2} = \sum_{(v \in N^+ t(1))} s(v) = k\frac{n}{2} + (n-k)\frac{n-2}{2}$$

implies that $k = n/2$. In other words, the subtournament $T\langle N^+(t_{(0)})\rangle$ is almost regular. Furthermore, $T\langle N^-(t_{(0)})\rangle$ is also almost regular since $T \cong \overline{T}$. □

4.2 Automorphism groups of odd signature Walecki tournaments with a zero subsignature

Theorem 4.10. *Let n be odd, $n \ge 5$, and let T denote the Walecki tournament $W(e)$ for $e = f\overline{f}\ldots\overline{f}f \in E_n$, n/r odd, and $f = (0,0,\ldots,0) \in E_r$, then $\mathrm{Aut}(W(e)) = \mathbb{Z}_{n/r}$.*

Proof. Let us assume that n is odd, $n \ge 5$, $e = f\overline{f}\ldots\overline{f}f \in E_n$, n/r odd, and $f = (0,0,\ldots,0) \in E_r$. Let T denote the Walecki tournament $W(e)$ and let G denote its automorphism group $\mathrm{Aut}(T)$. We use Orbit Stabilizer Theorem two times to get

$$|G| = |\mathcal{O}(t_{(0)})|\,|G_{t(0)}| = |\mathcal{O}(t_{(0)})|\,|\mathcal{O}(t_{(1)})|\,|G_{t(0),t(1)}|, \tag{4.23}$$

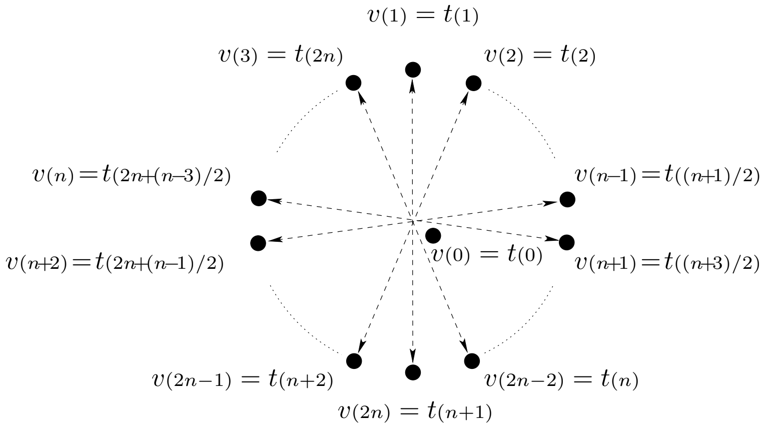

Figure 16: The diagram shows the action of the permutation $\eta = \tau^n \in \mathbb{S}_{2n+1}$ on vertices of the Walecki tournament $W(e)$, for $e \in E_n$, n odd, and $n \geq 1$. Vertex $v(0)$ is fixed by the permutation η which is an *involution* represented by two-way arrows.

where $\mathcal{O}(t(1))$ denotes the orbit of vertex $t(1)$ for the subgroup $G_{t(0)}$ of G.

We first consider the cardinality of $\mathcal{O}(t(0))$. $T\langle N^+(t(0))\rangle$ is a regular tournament by Theorem 4.8. On the other hand $T\langle N^+(t(i))\rangle$ is *not* regular for $t(i) \in N^+(t(0))$ (see Theorem 4.7). Thus, $t(0)$ cannot be mapped to a vertex from $N^+(t(0))$ by elements of G. Since $T \cong \overline{T}$ with the graph anti-automorphism τ^n, $t(0)$ cannot be mapped to a vertex from $N^-(t(0))$ by elements of G. We have proven that $t(0)$ must be fixed under the action of G, and thus

$$|\mathcal{O}(t(0))| = 1. \tag{4.24}$$

Next we determine $|\mathcal{O}(t(1))|$. Since $t(0)$ is a fixed point for any element ρ in G, $\rho(N^+(t(0))) = N^+(t(0))$. Hence, $\rho(t(1)) \in N^+(t(0))$ and $\mathcal{O}(t(1)) \subseteq N^+(t(0))$, implying

$$|\mathcal{O}(t(1))| \leq |N^+(t(0))| = n. \tag{4.25}$$

We proved that the permutation $\tau^{2r} \in \mathbb{S}_{2n+1}$ is an element of G. Since $\tau^{2r}(t(0)) = t(0)$, $\tau^{2r} \in G_{t(0)}$. Hence, $\langle \tau^{2r} \rangle \subseteq G_{t(0)}$. The orbit of $t(1)$ for $\langle \tau^{2r} \rangle$ is O_1, which implies

$$|\mathcal{O}(t(1))| \geq |O_1| = n/r. \tag{4.26}$$

If $r = 1$ then Equations (4.25) and (4.26) imply $|\mathcal{O}(t(1))| = n$. We now assume $r > 1$. We will prove that $|\mathcal{O}(t(1))| = n/r$. Suppose the contrary, $|\mathcal{O}(t(1))| > n/r$. Hence, there exists a vertex $t(i) \in \mathcal{O}(t(1)) - O_1$. Let us assume that $t(i) \in O_i$ where $1 < i \leq 2r$. Since τ^{2r} is an automorphism, we may assume $t(i) \in O_i \cap M_1$. Moreover, $f = (0, 0, \dots, 0)$ implies $t(1), t(i) \in N^+(t(0))$, therefore, $1 < i \leq r$.

It follows that there exist $k > 1$ such that $\tau^{k(i-1)} t(i) = t(i+k(i-1)+1)$ where $r < i + k(i-1) + 1 \leq 2r$. This is a contradiction, for $t(i+k(i-1)+1)$ belongs to $N^-(t(0))$ because $e_{i+k(i-1)+1} = \overline{f}_{i+k(i-1)+1-r} = \overline{0} = 1$, however, it should belong to $N^+(t(0))$ because $t(i) \in N^+(t(0))$. Therefore,

$$|\mathcal{O}(t(1))| = n/r. \tag{4.27}$$

Last we prove that $G_{v(0),v(1)} = id$. The subtournaments $T\langle N^+(t_{(0)})\rangle$ are regular for n odd and almost regular for n even. However, the subtournaments $T\langle N^+(t_{(1)})\rangle$ are not regular and not almost regular for n odd and n even, respectively, implying that any automorphism $\rho \in G_{t(0),t(1)}$ fixes all other vertices. Therefore, $G_{v(0),v(1)} = id$, that is,

$$|G_{t(0),t(1)}| = 1. \tag{4.28}$$

Equations (4.23), (4.24), (4.27), and (4.28) imply that $|G| = n/r$. Now, $\langle \tau^{2r} \rangle \subseteq G_{t(0)} \subseteq G$ and since $\langle \tau^{2r} \rangle \cong \mathrm{Z}_{n/r}$ we have

$$G \cong \mathrm{Z}_{n/r}$$

as required. □

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Parallelism of stable traces

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Abstract

A parallel d-stable trace is a closed walk which traverses every edge of a graph exactly twice in the same direction and for every vertex v, there is no subset $X \subseteq N(v)$ with $1 \leq |N| \leq d$ such that every time the walk enters v from X, it also exits to a vertex in X. In the past, d-stable traces were investigated as a mathematical model for an innovative biotechnological procedure – self-assembling of polypeptide structures. Among other, it was proven that graphs that admit parallel d-stable traces are precisely Eulerian graphs with minimum degree strictly larger than d. In the present paper we give an alternative, purely combinatorial proof of this result.

Keywords: Eulerian graph, parallel d-stable trace, nanostructure design, self-assembling, polypeptide.

Math. Subj. Class.: 05C45, 05C85, 94C15

1 Introduction

All graphs considered in this paper will be connected, finite, and simple, that is, without loops and multiple edges. If v is a vertex of a graph G, then its degree will be denoted by $d_G(v)$ or $d(v)$ for short if G will be clear from the context. The *minimum* and the *maximum* degree of G are denoted with $\delta(G)$ and $\Delta(G)$, respectively. A *directed graph* is a graph where edges have a direction associated with them. In formal terms a directed graph is a pair $G = (V, A)$, where V is a set of vertices and A is a set of ordered pairs of vertices, called *arcs*. A maximal connected subgraph of G is called a *component* of G, while a vertex which separates two other vertices of the same component is a *cutvertex*, and an edge separating its ends is a *bridge*. A maximal connected subgraph without a cutvertex is

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called a *block*. Thus, every block of a graph G is either a maximal 2-connected subgraph, or a bridge (with its ends), or an isolated vertex. A *subtree* T of a graph G is a subgraph of G that is also a tree (any pair of vertices $u, v \in V(T) \subseteq V(G)$ are connected by exactly one path in T). For other general terms and concepts from graph theory not recalled here we refer to [12].

A *circuit* is a closed walk allowing repetitions of vertices and edges. An *Eulerian circuit* in G is a circuit which traverses every edge of G exactly once. G is called *Eulerian* if it admits an Eulerian circuit. A *double trace* in a graph G is a circuit that traverses every edge exactly twice. For a set of vertices $X \subseteq N(v)$, we say that a double trace W has an *X-repetition* at vertex v (nontrivial X-repetition in [3]), if X is nonempty, $X \neq N(v)$, and whenever W comes to v from a vertex in X it also continues to a vertex in X. An X-repetition (at v) is a *d-repetition* if $|X| = d$ (repetition of *order* d), see Figure 1. Clearly if W has an X-repetition at v, then it also has an $(N(v) \setminus X)$-repetition at v (*symmetry of repetitions*). We call a double trace without any repetition of order $\leq d$ a *d-stable trace*. Note, that for every $d' \leq d$, a d-stable trace is also a d'-stable trace.

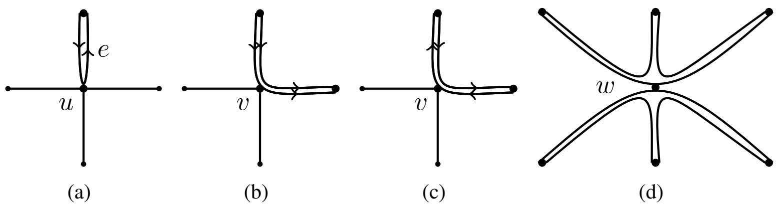


Figure 1: Possible 1-, 2- and 3-repetitions at vertices w, u and w, respectively.

In order to present a mathematical model for the biotechnological procedure from [6] graphs that admit d-stable traces were characterized in [3] (thus generalizing results of Sabidussi [11] and Eggleton and Skilton [2] about 1-stable traces and Klavžar and Rus [8] about 2-stable traces) as follows:

Proposition 1.1 ([3, Proposition 3.4])**.** *A connected graph G admits a d-stable trace if and only if $\delta(G) > d$.*

Let now W be a double trace of a graph G. Then every edge $e = uv$ of G is traversed exactly twice. If in both cases e is traversed in the same direction (either both times from u to v or both times from v to u) we say that e is a *parallel edge* (with respect to W). If this is not the case we say that e is an *antiparallel edge*. The condition that all the edges of G are of the same type is called a *parallelism*. A double trace W is a *parallel double trace* if every edge of G is parallel and an *antiparallel double trace* if every edge of G is antiparallel.

By replacing every edge of a graph with two new edges we can quickly prove that every graph (resp. every Eulerian graph) admits an antiparallel (resp. parallel) double trace, observation made by several authors, Klavžar and Rus in [8] among others. While graphs admitting antiparallel d-stable traces were thoroughly studied in [10], the characterization of parallel d-stable traces was only mentioned as a consequence in [3]:

Theorem 1.2 ([3, Theorem 5.4])**.** *A graph G admits a parallel d-stable trace if and only if G is Eulerian and $\delta(G) > d$.*

In the present paper we will give an alternative proof of this result. Instead of graph embeddings (heavily used in [3]), our approach to the problem will be purely combinatorial. Characterizing graphs that admit parallel d-stable traces also represents a new problem related with forbidden transitions in Eulerian tours of Eulerian graphs (further related problems can be found, among others in [4, 5]).

We can note right away that parallel double traces do not contain 1-repetitions. Note also that none of the operations that we will use on double traces (concatenations, contractions, deletions, inductive constructions, and reordering) will change the orientation of the edges.

1.1 Biotechological background

In 2013 Gradišar et al. [6] presented a novel self-assembly strategy for polypeptide nanostructure design. Their strategy relied on routing a single polypeptide chain consisting of 12 segments through 6 edges of the tetrahedron in such a way that every edge was traversed exactly twice. The required mathematical support for the particular case of the tetrahedron and the general case of a polyhedron was already given in [3, 6, 8], where the authors explained that polyhedron P that is composed from a single polymer chain can be naturally represented by a graph $G(P)$ of the polyhedron. Circuits that traverse every edge of $G(P)$ precisely twice, called double traces of $G(P)$, play a key role in modeling the construction process.

The stability of the constructed polyhedra depends on an additional property whether in the double trace the neighborhoods of vertices can be split. The reader interested in the biotehological procedures that motivated our research may also consult the references [7, 9], where the authors also exposed the use of parallel d-stable traces.

2 Graphs admitting parallel 2-stable traces

The first mathematical model for the biotechnological procedure from [6], introduced in [8], stated that a polyhedral graph P can be realized by interlocking pairs of polypeptide chains if its corresponding graph $G(P)$ contains a 2-stable trace. Two important deficiencies of this model were later found in [3]:

(i) it does not account for vertices of degree ≤ 2, and

(ii) it does not successfully model vertices of degree ≥ 6 (because a polyhedron could split into two parts in a vertex of degree ≥ 6, as can be seen at Figure 1 and therefore the structure would not be stable).

Since until now, a construction of a polyhedron whose graph would have such properties, has not yet been attempted, we first study parallel 2-stable traces in this section.

To make the arguments in this section more transparent, we explain how the reader can graphically imagine 1-repetitions and 2-repetitions in double traces. We say that a double trace contains a 1-repetition if it has an immediate succession of an edge e by its antiparallel copy. If v is a vertex of a graph G with a double trace W and u and w are two different neighbors of v, then we can say that W contains a 2-repetition (through) v if the vertex sequence $u \to v \to w$ appears twice in W in any direction ($u \to v \to w$ or $w \to v \to u$), see Figure 1.

We will need the next lemma in the proof of Theorem 2.3.

Lemma 2.1. *Let G be a graph and let T a subtree of G such that every vertex $v \in V(G) \setminus V(T)$ has at most one neighbor in T. Construct a graph G' from G by contracting T into a single vertex t. If G admits a 2-stable trace W then G' admits a 2-stable trace W' that traverses edges from $E(G) \cap E(G')$ in the same direction as W.*

Proof. Suppose that the graph G admits a 2-stable trace W. Construct a double trace W' from W as follows. Start in an arbitrary vertex of $V(G) \setminus V(T)$ and follow W. Let $a = xy$ be an arc of W that we are currently traversing on our walk along W. If $x, y \in V(G) \setminus V(T)$, then we put xy into W' so that the order of arcs from W is preserved. If $x \in V(T)$ and $y \notin V(T)$ then we put ty in W' instead of a. Similarly, we replace arcs where $x \notin V(T)$ and $y \in V(T)$ with xt. Finally, the occurrences of the arcs from T are ignored in W'.

We claim that W' is a 2-stable trace of G'. Since every edge is traversed twice in W, every edge is traversed twice in W'. Hence W' is a double trace. If W' is not a 2-stable trace, there exists a vertex $x \in V(G')$ such that W' has a 1-repetition or a 2-repetition at x. Denote the neighborhood of vertex t in G' with $N(t)$. We have to consider three cases.

Case 1: $x \notin N(t)$.

It is clear from the construction that if W' had a 1-repetition or a 2-repetition at x, then W would have a 1-repetition or a 2-repetition at x, a contradiction.

Case 2: $x \in N(t)$.

It is again clear from the construction that if W' had a 1-repetition yxy or a 2-repetition yxz, where $y, z \neq t$, then W would have a 1-repetition or a 2-repetition at x, a contradiction.

Assume first that W' has a 1-repetition txt. It follows that W should contain hxg, where $h, g \in T$. Since every vertex in $V(G) \setminus V(T)$ has at most one neighbor in T, $h = g$. Therefore W should contain a 1-repetition hxh, a contradiction.

Assume next that W' has a 2-repetition txy for some neighbor y of x. It follows that W should contain hxy and gxy, where $h, g \in T$. Since every vertex in $V(G) \setminus V(T)$ has at most one neighbor in T, $h = g$. Therefore W should contain a 2-repetition hxy, a contradiction.

Case 3: $x = t$.

Assume first that W' has a 1-repetition yty for some neighbor y of t. It follows that W should contain $yhAhy$, where h is the unique neighbor of y in T and A is a circuit in T. Since T is a tree, the only possibility that circuit appears in a part of a double trace W that is completely included in T is with a 1-repetition, a contradiction.

Assume next that W' has a 2-repetition ytz for some neighbors y and z of t. It follows that W should contain $yhBgz$ and $yhCgz$, where h is a unique neighbor of y in T, g is a unique neighbor of z in T, while B and C are hg-paths in T. Considering the fact that in a tree any two vertices are connected with a unique path, we can argue that $B = C$ and therefore that then W should have a 2-repetition (1-repetition if $h = g$), a contradiction.

We have thus proved that W' is a 2-stable trace in G'. During the construction of W' we did not change the direction of any arc from W. □

Note that Lemma 2.1 is, by repetition of the procedure described above, also true for forests (any number of disjoint subtrees).

The following was proven in [8], where it was also observed that a graph G admits a parallel double trace if and only if G is Eulerian.

Proposition 2.2 ([8, Proposition 5.4])**.** *A connected graph G admits a parallel 1-stable trace if and only if G is Eulerian.*

Proof. Parallelism of any stable trace of a graph G implies that all the vertices of G are of even degree and traversing an arbitrary Eulerian circuit of G twice in the same direction constructs a parallel 1-stable trace. □

We next prove Theorem 2.3 about parallel 2-stable traces and then use it in Section 3 to present an alternative proof of Theorem 1.2.

Theorem 2.3. *A graph G admits a parallel 2-stable trace if and only if G is Eulerian and $\delta(G) > 2$.*

Note that for Eulerian graphs the constraint on the minimal degree of a graph from Theorem 2.3 is equivalent to $\delta(G) \geq 4$.

Proof. Suppose that a graph G admits a parallel 2-stable trace. By definition, every 2-stable trace is a 1-stable trace. Thus by Proposition 2.2, G is Eulerian and hence by Proposition 1.1 we infer that $\delta(G) \geq 4$.

For the converse assume that G fulfills the conditions of the theorem. We proceed by induction on $\Delta = \Delta(G)$.

Let $\Delta = 4$. Then $\delta(G) = \Delta(G) = 4$. By Proposition 2.2, G admits a parallel 1-stable trace W'. If W' is not already a 2-stable trace, W' contains at least one 2-repetition. We proceed with the second induction on the number k of vertices where W' has 2-repetitions. Let $k \geq 1$ and let v be one of the vertices where W' has a 2-repetition. If a 1-stable trace W' has a 2-repetition through v, where v is a vertex with $d_G(v) = 4$, then it is not difficult to see that W' has two 2-repetitions through v. Let v_1, v_2, v_3, and v_4 be the neighbors of v. Without loss of generality, we can assume that $A = v_1 \to v \to v_2$ is the first and $B = v_3 \to v \to v_4$ is the second 2-repetition through v in W'. That means that sequences A and B appear twice in W'. Because W' is a parallel 1-stable trace, there are only two possibilities how occurrences of A and B are arranged in W'. These possibilities are $AABB$ (Figure 2, left) and $ABAB$ (Figure 3, left). Note that we left out all the other vertices in Figures 2 and 3.

In the first case we construct a double trace W from W' in G as follows. We start in an arbitrary vertex of $V(G) \setminus \{v\}$ and follow W'. Let $a = xy$ be an arc of W' that we are currently traversing on our walk along W'. If $x, y \in V(G) \setminus \{v, v_1, v_2, v_3, v_4\}$, then we put xy into W so that the order of arcs from W' is preserved. Put one occurrence of $v_1 \to v \to v_2$ and one occurrence of $v_3 \to v \to v_4$ in W as well. Replace the remaining occurrence of $v_1 \to v \to v_2$ with $v_1 \to v \to v_4$ and the remaining occurrence of $v_3 \to v \to v_4$ with $v_3 \to v \to v_2$, so that W stays connected, see Figure 2, right.

We construct W analogously in the second case, see Figure 3, right.

We claim that in both cases W is a parallel 1-stable trace of G with at least one vertex with 2-repetition less than W'. Note first that any edge $e = xy$ that appears in W (arcs xy or yx appears in W) has its unique corresponding edge e' in W'. Any edge $e = xy$ in W, where $x \neq v$ and $y \neq v$, is traversed twice in the same direction in W because it is traversed twice in the same direction in W'. Four remaining edges (vv_1, vv_2, vv_3, and vv_4)

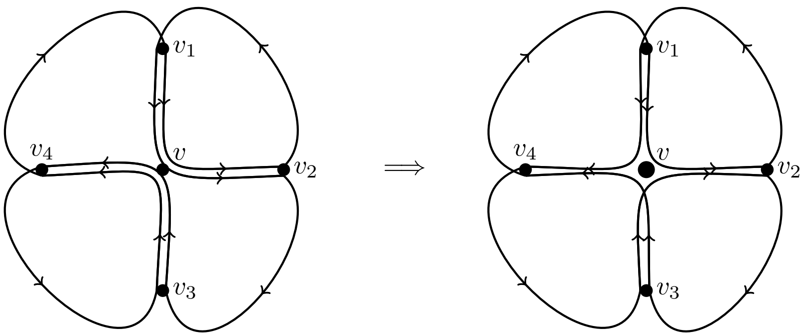


Figure 2: Removing 2-repetition through v (case $AABB$).

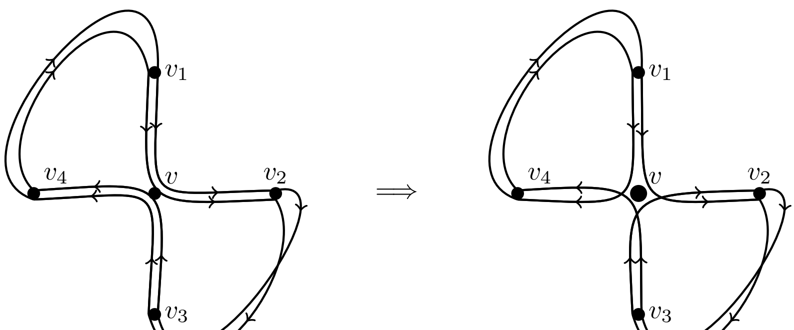


Figure 3: Removing 2-repetition through v (case $ABAB$).

are traversed twice in the same direction by construction. Hence W is a parallel double trace. It is also clear from the construction that W is a 1-stable trace. Finally we need to verify that W has at least one vertex with 2-repetition less than W'. Let x be an arbitrary vertex of G in which W has a 2-repetition. We have to consider three cases.

Case 1: $x \notin \{v, v_1, v_2, v_3, v_4\}$.

It is clear from the construction that if W has a 2-repetition through x, then also W' has a 2-repetition through x.

Case 2: $x \in \{v_1, v_2, v_3, v_4\}$.

It is again clear from the construction that if W has a 2-repetition yxz, where $y, z \neq v$, then also W' has a 2-repetition through x.

Similarly, if W has a 2-repetition vxy for some neighbor y of x, then also W' has a 2-repetition through x since the order of arcs adjacent to $\{v_1, v_2, v_3, v_4\}$ did not change in W.

Case 3: $x = v$.

The 1-stable trace W' had a 2-repetition (two 2-repetitions to be more accurate) through v but during the construction of W we manage to remove them both.

We have thus constructed a 1-stable trace W which have at least one vertex with 2-repetition less than W'. Hence, it follows by induction assumption that any 4-regular graph admits a parallel 2-stable trace.

Assume now that $\Delta \geq 6$ and that any graph H with $\Delta(H) < \Delta$ that fulfills the conditions of Theorem 2.3 admits a parallel 2-stable trace. We have to again consider two cases.

Case 1: $\Delta \equiv 2 \pmod 4$.

Construct the graph G' from G as follows. For every vertex v of degree Δ (temporary denote its neighbors with $v_1, \dots, v_\Delta$) repeat the following procedure. Remove v from G. Add two new vertices v' and v'', connect them by an edge, connect v' with $v_1, \dots, v_{\frac{\Delta}{2}}$, and connect v'' with the remaining neighbors of v, see Figure 4.

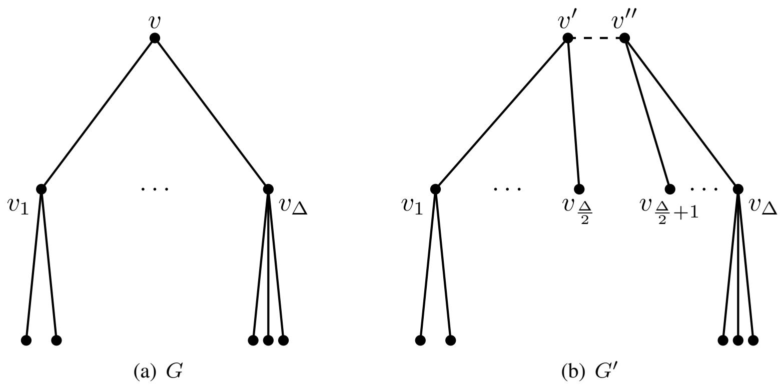


Figure 4: Construction from the proof of Theorem 2.3 for the case $\Delta \equiv 2 \pmod 4$.

Note that in G' all except the newly added vertices are of the same degree as in G, while $d_{G'}(v') = \frac{\Delta}{2} + 1$ and $d_{G'}(v'') = \frac{\Delta}{2} + 1$ (the last two statements are true for all new vertices). It follows that $\Delta(G') < \Delta$. Since $\Delta \geq 6$, we then also infer that $\delta(G') \geq 4$. Because $\Delta \equiv 2 \pmod 4$, the degrees $d_{G'}(v') = d_{G'}(v'') = \frac{\Delta}{2} + 1$ are even, hence G is Eulerian and by the induction assumption on Δ, the graph G' admits a parallel 2-stable trace. If we use a path containing vertices v' and v'' as subtree T, it follows from a repeated application of Lemma 2.1 that G admits a parallel 2-stable trace.

Case 2: $\Delta \equiv 0 \pmod 4$.

Construct the graph G' from G as follows. For every vertex v of degree Δ (temporary denote its neighbors with $v_1, \ldots, v_\Delta$) repeat the following procedure. Remove v from G, and add three new vertices v', v'', and v'''. Connect v'' with v' and v''' by an edge, connect v' with $v_1, \ldots, v_{\frac{\Delta}{2}-1}$, connect v'' with $v_{\frac{\Delta}{2}}$ and $v_{\frac{\Delta}{2}+1}$, and connect v''' with the remaining neighbors of v, see Figure 5.

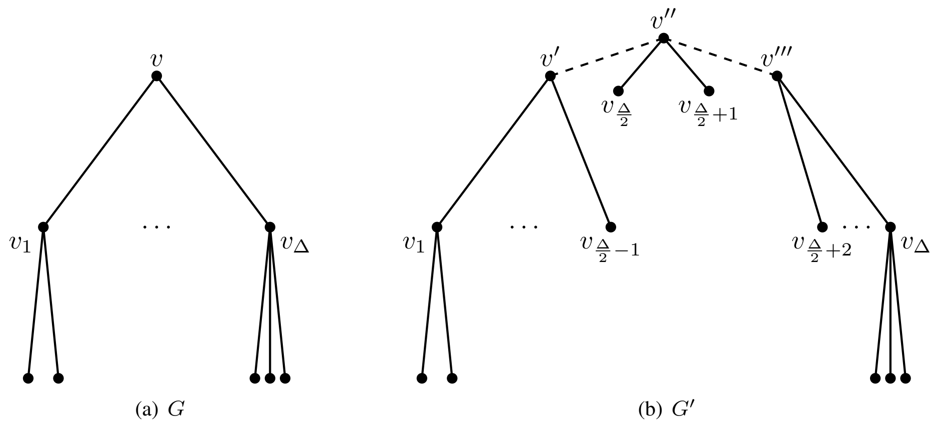


Figure 5: Construction from the proof of Theorem 2.3 for the case $\Delta \equiv 0 \pmod 4$.

Analogously as in the first case, note that in G' all except the newly added vertices are of the same degree as in G, while $d_{G'}(v') = d_{G'}(v''') = \frac{\Delta}{2}$ and $d_{G'}(v'') = 4$ (the last two statements are true for all new vertices). It follows that $\Delta(G') < \Delta$. Since $\Delta \geq 6$, we then also infer that $\delta(G') \geq 4$. Because $\Delta \equiv 0 \pmod 4$, the degrees $d_{G'}(v') = d_{G'}(v''') = \frac{\Delta}{2}$ are even, hence G is Eulerian. By the induction assumption on Δ, the graph G' admits a parallel 2-stable trace. Similarly as in previous case, if we use a path containing vertices v', v'' and v'' as subtree T, it follows from repeated application Lemma 2.1 that G admits a parallel 2-stable trace.

We have thus proved Theorem 2.3. $\square$

3 Alternative proof of Theorem 1.2

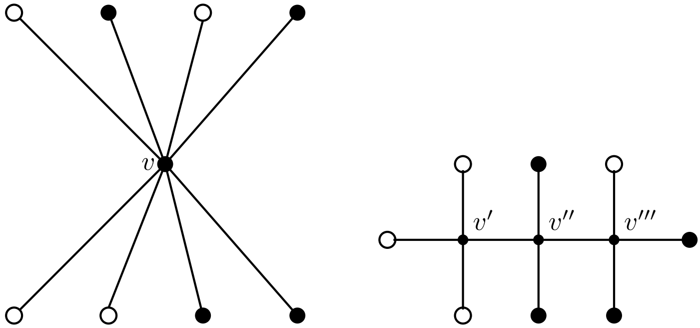
We now extend the results from previous section to present an alternative proof of Theorem 1.2 (Theorem 5.4 from [3]).

Proof. Assume first that the graph G admits a parallel d-stable trace. From Proposition 1.1 it follows that $\delta(G) > d$ for every graph G that admits a d-stable trace. Assume that there exists an vertex v of odd degree in G. Since every edge of a parallel double trace is used twice in the same direction, input and output degree of a parallel double trace W would not match at v, which is absurd. Therefore it follows that G is Eulerian and $\delta(G) > d$.

For the converse assume that graph G is Eulerian and $\delta(G) > d$. Since G is Eulerian, $\delta(G)$ is an even number. Furthermore, since for parallel 1-stable traces and 2-stable traces the theorem follows from Proposition 2.2 and Theorem 2.3, respectively, we can assume that $d \geq 3$. Let G' be a graph obtained from G by replacing every vertex v of degree $d_G(v) > 4$ with $(d_G(v) - 2)/2$ new vertices, connected into a path P_v and additionally connecting two endvertices of P_v with three different neighbors of v and each inner vertex of P_v with two different remaining neighbors, so that each of the vertices from $N(v)$ is connected to exactly one vertex in P_v. It is not difficult to see that G' is a 4-regular graph and therefore by Theorem 2.3 admits a parallel 2-stable trace W'. Construct a parallel double trace W in G from W' as follows. We start in an arbitrary vertex of G' and follow W'. Let $a' = xy$ be an arc of W' that we are currently traversing on our walk along W'. If for every v, $d_G(v) > 4$, $x, y \notin V(P_v)$, then we put xy into W so that the order of arcs from W' is preserved. If for some v, $d_G(v) > 4$, $x \in P_v$ or $y \in P_v$, we replace a' with vy or xv, respectively. Finally, occurrences of the arcs with both endvertices contained in some P_v are ignored in W.

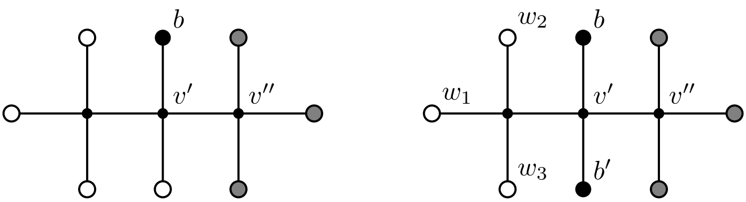
We claim that the parallel double trace W is a parallel d-stable trace of the graph G. We assume conversely and denote an arbitrary vertex in which W has a repetition of order $\leq d$ with v. Denote the maximal order of $(\leq d)$-repetition at v with d'. Since we used the same construction as in the proof of Theorem 2.3, it follows that W is a parallel 2-stable trace (and $d' > 2$). From the symmetry of repetitions it then also follows that $d_G(v) > d' + 2$, since otherwise W would have at least one 1-repetition or one 2-repetition at v (therefore also $d_G(v) \geq 8$). It is then also not difficult to see that every repetition in a parallel double trace is of even order. Let X be a subset of $N(v)$ containing vertices from a maximal repetition at v (note that $|X| = d'$). There exists a path P_v in G' that during the construction replaced v from G. To make the argument more transparent, we imagine vertices from P_v arranged in a horizontal line with all the neighbors of v except for two, lying directly above or below vertices of P_v. The remaining two neighbors of vertex v are aligned at the beginning and at the end of the horizontal line containing vertices from P_v. Figure 6(b) shows P_v with vertices from $N(v)$ in G' for $d_G(v) = 8$ (v', v'', and v''' are the vertices replacing v in G'). Next, we color vertices from $N(v)$ with two colors—black and white, so that vertices from X are colored black while vertices from $N(v) \setminus X$ are colored white. Example of such a coloring can be seen at Figure 6.

Since the subset $N(v)\setminus X$ is also a repetition, the arguments used hereinafter are true for black and white vertices and we can, without loss of generality, assume that the neighbor of $N(v)$, lying farmost to the left in the above mentioned horizontal line is colored white. We next move along this horizontal line and denote the first black vertex that we meet (below or above the line) with b. Denote its neighbor in P_v with v'. Since there are at least four black vertices, v' is not the farmost right vertex from P_v. Therefore, we can also denote the right neighbor of v' from P_v with v'' and consider two cases. In the first case b is the only neighbor of v' ($\notin P_v$) colored black (Figure 7(a)), while in the second case also the second neighbor of v' ($\notin P_v$) is colored black (Figure 7(b)). In both cases we can, without loss of generality, assume that an edge bv' is traversed twice in the direction toward v' in W' (that is, arc bv' is traversed twice in W, while arc $v'b$ does not appear in W'). The fact that W has an X-repetition implies that every time double trace W comes to v from a



(a) v and $N(v)$ in G (b) P_v and $N(v)$ in G'

Figure 6: Structures of $N(v)$ in G and P_v in G'. Vertices contained in X are colored black.



(a) b is the only black neighbor of v' (b) Both neighbors of v' from $N(v)$ are black

Figure 7: Two cases of the structure of P_v (of v' and b to be more precise). Vertices for which the color is not determined are colored grey.

vertex in X it also continues to a vertex in X and, consequently, that every time a double trace W' comes to a vertex in P_v from a (black colored) vertex in X it also leaves to a (black colored) vertex in X. Note that in between W' can traverse other vertices from P_v and that this applies for all appearances of verb *continue* from now on until the end of this section. Analogously is true for (white colored) vertices from $N(v) \setminus X$. Therefore, in W' there exist two subsequences which start with bv', continue on some other vertices from P_v and end in two from b different vertices from X. In the first case, when b is the only black colored neighbor of v', the subsequence $b \to v' \to v''$ has to appear twice in W', since otherwise W' can not continue (twice) from b to a black colored vertex without previously traversing white vertex. This contradicts the fact that W' is a parallel 2-stable trace, since $bv'v''$ is a 2-repetition at v'. In the second case, we denote the set of white vertices that appear to the left of b with $\mathcal{W} = \{w_1, \ldots, w_l\}$. (Note that l is an odd integer.) For an example, see Figure 7(b), where those vertices are denoted with w_1, w_2, and w_3. Next, we denote the second black colored neighbor of v' from $N(v)$ with b'. The subsequence $b \to v' \to b'$ can appear at most once in W' (otherwise W' would have a 2-repetition at v'). Assume next that for every $w \in \mathcal{W}$, w continues to a vertex in $\mathcal{W}$. Then vertices from $\mathcal{W}$ form an odd repetition in W', which can not appear in a parallel 2-stable trace. Therefore, at least one vertex w from $\mathcal{W}$ has to continue to a white colored vertex not included in $\mathcal{W}$ (that is, w continues to a white colored vertex to the right of b). If subsequence $b \to v' \to b'$ does not appear in W' it follows that edge $v'v''$ (arc $v'v''$ and $v''v'$) is used more than twice in W': at least once to connect a vertex from $\mathcal{W}$ to a white colored vertex not in $\mathcal{W}$, twice to connect b to a (black colored) vertex in X different from b', and twice to connect b' to a (black colored) vertex in X different from b, which is absurd. If subsequence $b \to v' \to b'$ does appear in W' it (in addition to multiple appearances of $v'v''$) follows that edge $v'v''$ is not parallel in W'. Since all the black colored vertices except b and b' are to the right of v' both $b \to v' \to v''$ and $v'' \to v' \to b'$ have to appear in W', which is also absurd.

Since v was an arbitrary vertex in G and d' was an arbitrary integer, $2 < d' \leq d$, it follows that W is a parallel d-stable trace of G and therefore Theorem 1.2 is proved. □

4 Concluding remarks

In this section we present two concepts which we assumed could be used for constructing parallel 2-stable traces. Unfortunately, it has turned out, when proving Theorem 2.3, that there exist graphs admitting only parallel 2-stable traces which can not be realized using the here described constructions.

The first construction goes as follows. Let G be an Eulerian graph with n vertices (denoted with $v_1, \ldots, v_n$) fulfilling conditions of Theorem 2.3 and let W' be an Eulerian circuit of G. W' induces a set of functions $\Pi' = \{\pi'_1, \ldots, \pi'_n\}$, where $\pi'_i\colon N(v_i) \longrightarrow N(v_i)$, $\pi'_i(v) = u$ if and only if $v \to v_i \to u$ or $u \to v_i \to v$ are sequences in W', for $1 \leq i \leq n$. Note that $u \neq v$, because G is simple and W' traverses every edge exactly once. Suppose that W'' is another Eulerian circuit in G such that W'' induces a set of functions $\Pi'' = \{\pi''_1, \ldots, \pi''_n\}$ with above described characteristics. In addition demand that edges are traversed in the same direction as in W', and that if $\pi'_i(v) = u$ then $\pi''_i(v) \neq u$ and $\pi''_i(u) \neq v$. Concatenate Eulerian circuits W' and W'' into a double trace W in an arbitrary vertex v. It is obvious from the construction that every edge is traversed twice in the same direction in W and that W is without 1-repetitions and 2-repetitions in any vertex other than v. Hence, if a graph G admits two Eulerian circuits with above described characteristics, then G admits parallel 2-stable trace as well.

It turns out that we cannot always construct a parallel 2-stable trace of G by concatenating two Eulerian circuits. For instance, the graph G from Figure 8 has a parallel 2-stable trace:

$$v_1 \to v_2 \to v_3 \to v_1 \to v_2 \to v_4 \to v_1 \to v_5 \to v_2 \to v_3 \to v_4 \to v_6 \to v_5 \to v_2 \to$$
$$v_4 \to v_6 \to v_7 \to v_9 \to v_8 \to v_6 \to v_7 \to v_{10} \to v_8 \to v_{11} \to v_7 \to v_9 \to v_{10} \to$$
$$v_{11} \to v_7 \to v_{10} \to v_{11} \to v_9 \to v_8 \to v_{11} \to v_9 \to v_{10} \to v_8 \to v_6 \to v_5 \to v_3 \to$$
$$v_1 \to v_5 \to v_3 \to v_4 \to v_1,$$

but because of the cut vertex v_6, from any Eulerian circuit W of G we cannot construct another Eulerian circuit with the described properties.

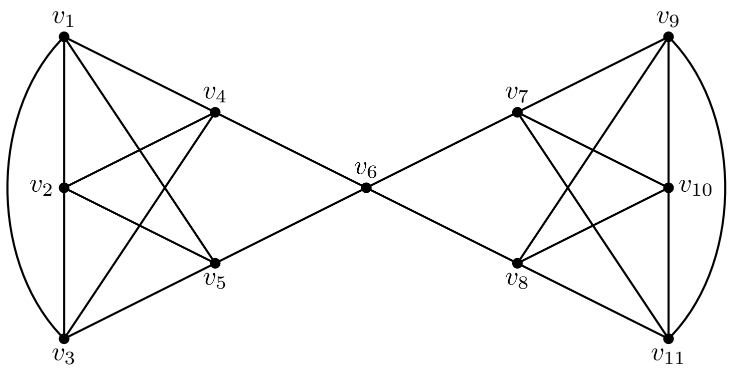


Figure 8: Graph whose parallel 2-stable traces cannot be constructed by concatenating two Eulerian circuits.

The main idea of the second construction is to find a parallel 2-stable trace in each block of a graph G and then concatenate them into a parallel 2-stable trace of the graph G. Let again G be an Eulerian graph fulfilling the conditions of Theorem 2.3. Denote blocks of G with $B_1, \dots, B_k$ and cutvertices with $v_1, \dots, v_l$. Find first a parallel 2-stable trace W_i in block B_i. Concatenate parallel 2-stable traces into a parallel 2-stable trace of G in corresponding cutvertices. When concatenating, one has to be careful that no 1-repetitions and 2-repetitions appear.

Similar as for the first construction, none of the parallel 2-stable traces of the graph G from Figure 8 can not be constructed by concatenating parallel 2-stable traces in its blocks. Vertex v_6 is a unique cutvertex of the graph G and it is contained in both of its blocks. Since v_6 is of degree 2 in both blocks of the graph G, none of them admit parallel 2-stable trace. Similar problem occurs if one or more blocks of G are bridges.

Next possible improvement could instead of parallel 2-stable traces in blocks demand parallel 1-stable traces where 2-repetitions (or 1-repetitions if block is a bridge) would be allowed at cutvertices but are then later removed during the concatenation into a parallel 2-stable trace of the whole graph.

An attempt to find efficient algorithms for constructing and counting stable traces of graphs was made in [1]. It would be of interest to characterize graphs that do not have any of the two above described properties of graphs from Figure 8 and then try to improve the algorithms from [1] by using the above described constructions for those special cases of graphs.

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On primitive geometries of rank two*

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Abstract

In this paper, we describe a new algorithm to classify primitive coset geometries of rank two for a given group G. This algorithm allows us to classify those geometries for the 12 smallest sporadic simple groups.

Keywords: Primitive coset geometries, sporadic groups, codes, designs.

Math. Subj. Class.: 51E24, 20D45

1 Introduction

Primitive coset geometries have been studied since the 1990's, first by a team led by Francis Buekenhout in Brussels [4, 5] and later on by Peter Rowley and Nayil Kilic (see for instance [8, 9, 10, 11, 12]). These geometries may be used to construct codes, designs, graphs, etc. Recently, we had the idea of using rank two primitive geometries to construct new binary codes for the McLaughlin group [13]. More precisely, we examined the binary codes obtained from the row span over $\mathbb{F}_2$ of the adjacency matrices of some strongly regular graphs which occur as subgraphs of the McLaughlin graph, namely those with parameters $(105, 32, 4, 12)$, $(120, 42, 8, 18)$ and $(253, 112, 36, 60)$. These new codes were obtained by computing incidence matrices of rank two geometries whose element-stabilizers are maximal subgroups of the McLaughlin group. In order to be able to generate these geometries, a new approach was needed. Indeed, the previous algorithms described by Dehon and Leemans [7] did not allow for a study of a group such as the Mathieu group

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M_{24} of order roughly $2.4 \cdot 10^8$. We managed to classify such geometries with our new algorithm for the 12 smallest sporadic groups, the largest one being the Rudvalis group, of order roughly $1.4 \cdot 10^{11}$. The geometries obtained are available on the following websites:

- https://data.adam-journal.eu/apg/
- http://homepages.ulb.ac.be/~dleemans/PRI/

Our idea relies on permutation representations of groups. We present in this paper an algorithm that outperforms the previous algorithms by a factor of 1000 at least. It allows to classify rank two primitive coset geometries for the five Mathieu groups, the first three Janko groups, the Higman Sims group, the McLaughlin group, the Held group and the Rudvalis group. It also allows to confirm the classification of rank two primitive geometries of M_{11} given in [5], M_{23} given in [10] and to correct some infelicities in [12] for M_{22}. We also obtained a complete classification for M_{24} while Kilic gives in [11] a partial one. The results for the Janko groups, the Higman Sims group, the McLaughlin group, the Held group and the Rudvalis groups are complete and new.

2 Terminology

The basic concepts about geometries constructed from a group and some of its subgroups are due to Tits [14] (see also [3, Chapter 3]). The following theorem shows how to construct geometries starting from groups.

Theorem 2.1 (Tits, 1956 [14]). *Let n be a positive integer. Let $I := \{1, \ldots, n\}$ be a finite set and let G be a group together with a family of subgroups $(G_i)_{i \in I}$. Let X be the set consisting of all cosets $G_i g$, $g \in G$, $i \in I$. Let $t\colon X \to I$ be defined by $t(G_i g) = i$. Define an incidence relation $*$ on $X \times X$ by:*

$$G_i g_1 * G_j g_2 \text{ iff } G_i g_1 \cap G_j g_2 \text{ is non-empty in } G.$$

Then the 4-tuple $\Gamma := (X, *, t, I)$ is an incidence structure having a chamber. Moreover, the group G acts by right multiplication as an automorphism group on Γ. Finally, the group G is transitive on the flags of rank less than 3.

In the Theorem 2.1 above, a *chamber* is a set containing n cosets that are pairwise non-disjoint. Let G be a group and $\{G_i : i \in \{1, \ldots, n\}\}$ be a set of subgroups of G. We call $\Gamma(G; (G_i)_{i \in I})$ the *coset geometry* associated to G and the subgroups $(G_i)_{i \in I}$ using the above theorem. By Theorem 2.1, we see that the group G acts on Γ as a type-preserving automorphism group.

In this paper, we only deal with geometries of rank two, that is coset geometries constructed from a group G and two subgroups G_1, G_2 of G. Let us denote such a geometry $\Gamma := \Gamma(G; (G_1, G_2))$. We readily have that Γ is *flag-transitive*, that is, G acts transitively on the pairs of non-disjoint cosets of Γ. Moreover, we want Γ to be *primitive*, meaning that G_1 and G_2 must be maximal subgroups of G. Finally, as G_1 and G_2 are maximal subgroups of G, we necessarily have $\langle G_1, G_2 \rangle = G$ provided $G_1 \neq G_2$. This implies that Γ is a firm and connected geometry.

We are thus interested in classifying firm, connected, flag-transitive and primitive coset geometries of rank two for a given group G. Given two coset geometries $\Gamma_1 := \Gamma(G; (G_1, G_2))$ and $\Gamma_2 := \Gamma(G; (H_1, H_2))$, we say that Γ_1 and Γ_2 are *isomorphic* provided there exists an element $g \in \mathrm{Aut}(G)$ such that $g(\{G_1, G_2\}) = \{H_1, H_2\}$. In the next section, we describe an algorithm to classify, up to isomorphism, all firm, connected, primitive geometries of rank 2 for a given group G.

Given a geometry $\Gamma := \Gamma(G; (G_1, G_2))$, its *dual* Γ^* is the geometry

$$\Gamma^* := \Gamma(G; (G_2, G_1)).$$

To a coset geometry of rank two, $\Gamma(G; (G_1, G_2))$ we can associate a graph called the *incidence graph* $\mathcal{G}$ whose vertices are the cosets of G_1 and G_2, two distinct cosets being joined by an edge provided their intersection is nonempty. This graph is bipartite and G acts transitively on the edges of $\mathcal{G}$. Following [2], the *gonality* g of Γ is half the girth of $\mathcal{G}$. The *point-diameter* d_p (resp. *line-diameter* d_l) is the largest distance from the coset G_1 (resp. G_2) to any other coset of Γ. To Γ, we associate the triple $[d_p, g, d_l]$. Finally, we recall that a *design* $S_\lambda(t, k, v)$ is a geometry of rank two with v points and lines of size k such that each set of t points is contained in exactly λ lines.

3 Algorithm

3.1 The old algorithm

The following algorithm was described in [7] (see Section 3, top-down approach) to construct residually weakly primitive geometries. It was the same algorithm that was used by Dehon in [6] to classify primitive geometries. This algorithm constructs primitive geometries of all possible ranks, not only rank two.

Sketch of the Dehon algorithm. Let G be a group for which we want to compute all firm, residually connected, flag-transitive and primitive geometries. Construct a set S containing all maximal subgroups of G and the group $W = \mathrm{Aut}(G)$ acting as a permutation group on S. This group is used to classify geometries up to isomorphism, two geometries (Γ, G) and (Γ', G) being isomorphic if there exists an element g in $\mathrm{Aut}(G)$ such that $g(\Gamma) = \Gamma'$.

Let C_1 be a set of sets containing one representative of each conjugacy class of maximal subgroups of G. Each element $\{G_1\}$ of C_1 (where G_1 is thus a maximal subgroup of G) gives a rank one geometry $\Gamma(G, \{G_1\})$.

If C_1 is nonempty, let C_2 be the empty set and do the following:

For every set $\{G_1\}$ in C_1, determine, up to isomorphism, the subgroups G_2 in S such that $\Gamma(G; G_1, G_2)$ is firm, residually connected and flag-transitive[1]. Store these pairs $\{G_1, G_2\}$ in C_2.

If C_2 is nonempty, let C_3 be the empty set and do the following: for every element $\{G_1, G_2\}$ in C_2, determine, up to isomorphism, the subgroups G_3 in S such that $\Gamma(G; G_1, G_2, G_3)$ is firm, residually connected and flag-transitive. Store these triples $\{G_1, G_2, G_3\}$ in C_3.

And so on, until the set C_{i+1} obtained by adding subgroups to elements of C_i is empty. The sets C_j, $j = 1, \ldots, i$, contain all firm, residually connected, flag-transitive and primitive geometries of rank j of G, up to isomorphism. $\diamondsuit$

In the algorithm above, the bottleneck is the construction of the group W at the very beginning. That task of computing all maximal subgroups of G becomes quickly tedious

[1] In the rank two case, every possible $G_2 \neq G_1$ is good, and the group W is there to make sure we pick only pairwise non-isomorphic pairs of subgroups (G_1, G_2).

and the permutation representation of G on these subgroups has a degree that is quickly too large for MAGMA to work efficiently with it.

Given a rank two coset geometry $\Gamma := \Gamma(G; (G_1, G_2))$ where G_1 and G_2 are maximal subgroups of G, the group G has a faithful primitive permutation representation on the set Ω of cosets of G_1 (and respectively on the cosets of G_2). In that permutation representation, G_2 partitions the cosets into orbits. As G_1 is maximal in G and the representation is faithful, all the conjugates of G_1 correspond to stabilizers of one coset of Ω. Hence, by fixing G_2 and taking stabilizers of representatives of the orbits of G_2 on Ω, we construct all possible rank two geometries $\Gamma(G; (H_1, H_2))$ with H_1 conjugate to G_1 and H_2 conjugate to G_2. One of them is necessarily the starting geometry.

An algorithm follows from the above paragraph: Given a group G and a maximal subgroup M_1 of G, construct the permutation representation of G on the set Ω of right cosets of M_1. This representation is primitive. For any maximal subgroup M_2 of G in that representation, compute the orbits $\mathcal{O}$ of M_2 on Ω. In each orbit $o \in \mathcal{O}$, pick one representative x. The triple $(G; (M_2, G_x))$ gives a primitive geometry of rank 2. This geometry is obviously flag-transitive and it will be firm provided $|o| \neq 1$. This gives an obvious way to produce primitive geometries of rank 2 for a given group G. Any rank two primitive geometry constructed from G can be produced in this way. Therefore, we have a technique to produce all rank two primitive geometries for G. It may happen that we generate several isomorphic copies of the same geometry. To avoid that, every time we generate a geometry with the above technique, we check whether it is isomorphic to one of the geometries obtained so far. We only keep it if it is not isomorphic to any of the previously obtained geometries.

In order to be able to apply the above algorithm, all that is needed now is that we can compute permutation representations of G on all its maximal subgroups and that we can check isomorphism between geometries that may be self-dual. Starting from the Rudvalis group, these permutation representations can become very large. This is where we decided to stop.

We implemented the Algorithm 3.1 in MAGMA [1] and determined all rank two primitive geometries for the twelve smallest sporadic simple groups. Our findings are summarized in the next section.

4 Primitive rank two geometries of sporadic groups

In this section, we summarise the classifications of primitive geometries of rank two we obtained, using the algorithm described in the previous section, for the five Mathieu groups, the first three Janko groups, the McLaughlin group, the Higman-Sims group, the Held group and the Rudvalis group. A summary of the results obtained is available in Table 1. In the last column, the computing time to classify these geometries is given. The computer used was a workstation with 4 Intel Xeon E5 processors with 6 cores each working at 2.9 GHz and 1 TB of RAM. We give the orbit tables for the groups M_{11}, M_{12}, M_{22}, M_{23} and J_1 in the following sections. We omit the tables of the remaining groups since these tables become too large.

4.1 The Mathieu group M_{11}

Table 2 gives the orbit lengths for every primitive permutation representation of M_{11}. Each column corresponds to a given primitive permutation representation and gives the ways

Algorithm 3.1 An algorithm to compute primitive geometries.

Input: G … a group
Output: $geos$ … a sequence containing pairwise non-isomorphic pairs of maximal subgroups of G

Initialize a sequence $geos$ that will be used to store the geometries.
Compute M, a list containing a representative of each conjugacy class of maximal subgroups of G.
for $i := 1$ to $\#M$ **do**
  Let M_1 be the i-th element of M.
  Construct $\phi\colon G \to G/M_1$, the coset action of G on the cosets of M_1.
  Let $\phi(M) := [\phi(x) : x \in M]$.
  for $j := 1$ to $\#M$ **do**
    Let M_2 be the j-th element of $\phi(M)$.
    Compute O, the orbits of K.
    for each orbit o of size > 1 in O **do**
      Let x be a representative of o.
      Let G_x be the stabilizer of x in $\phi(G)$.
      if the pair $\{\phi^{-1}(M_2), \phi^{-1}(G_x)\}$ is not isomorphic to any pair in $geos$ **then**
        add the pair $\{\phi^{-1}(M_2), \phi^{-1}(G_x)\}$ to $geos$
      end if
    end for
  end for
end for
return $geos$

Table 1: The 11 smallest sporadic groups and their rank two primitive geometries.

Group	Order	Degree	Number of geometries	Computing time
M_{11}	7 920	11	37	0.28 s
M_{12}	95 040	12	166	13.79 s
M_{22}	443 520	22	81	3.23 s
M_{23}	10 200 960	23	170	54.04 s
M_{24}	244 823 040	24	5074	106704 s $\sim$ 29 h
J_1	175 560	266	669	146.22 s
J_2	604 800	100	334	71.27 s
J_3	50 232 960	6156	546	5031.72 s
HS	44 352 000	100	339	282.46 s
McL	898 128 000	275	443	2412.12 s
He	4 030 387 200	2058	4074	14.35 days
Ru	145 926 144 000	4060	1511	9.2 days

the points are split into orbits by the corresponding maximal subgroups. So for instance, the entry 12 – 18 – 36 corresponding to the line labelled $M_9 : 2$ and the column labelled 66 means that on the 66-points primitive permutation representation of M_{11} (obtained by looking at the coset action of M_{11} on the cosets of a maximal subgroup isomorphic to S_5), a maximal subgroup $M_9 : 2$ has orbits of length 12, 18 and 36.

Counting the number of orbits of size at least two in the upper triangular half, we get 38 possibilities. In fact, the Mathieu group M_{11} has, up to isomorphism, 37 primitive geometries of rank two as two of them are dual of each other. This confirms the results obtained in [5]. In Table 4, we give for each of the 37 geometries Γ the designs corresponding to Γ and to its dual Γ^*. Some geometries do not appear in that table as a rank two geometry does not necessarily give a design. Entry 28^* is the well known $S_1(4, 5, 11)$, that is the Steiner system associated to the Mathieu group M_{11}.

Table 2: Orbits of primitive permutation representations of M_{11}.

	11	12	55	66	165
M_{10}	1 – 10	12	10 – 45	30 – 36	45 – 120
$L_2(11)$	11	1 – 11	55	11 – 55	55 – 110
$M_9 : 2$	2 – 9	12	1 – 18 – 36	12 – 18 – 36	9 – 12 – 72^2
S_5	5 – 6	2 – 10	10 – 15 – 30	1 – 15 – 20 – 30	10 – 15 – 20 – 60^2
$M_8 : S_3$	3 – 8	4 – 8	3 – 4 – 24^2	4 – 6 – 8 – 24^2	1 – 8 – 12 – 24^4 – 48

4.2 The Mathieu group M_{12}

Table 5 gives the orbit lengths for every primitive permutation representation of M_{12}. Counting the number of orbits of size at least two in the upper triangular half, we get 268 possibilities. In fact, the Mathieu group M_{12} has 166 primitive geometries of rank two as $\mathrm{Aut}(M_{12})$ conjugates several pairs in the 268 possibilities.

4.3 The Mathieu group M_{22}

Table 6 gives the orbit lengths for every primitive permutation representation of M_{22}. Our programs gave 81 geometries up to isomorphism. This corrects the number that was obtained in [12], namely 86.

4.4 The Mathieu group M_{23}

Table 7 gives the orbit lengths for every primitive permutation representation of M_{23}. Our programs gave 170 geometries up to isomorphism. This confirms the results obtained by Kilic in [10].

4.5 The first group of Janko J_1

Table 8 gives the orbit lengths for every primitive permutation representation of J_1. Our programs gave 669 geometries up to isomorphism. This is a completely new result.

Table 3: The 37 rank two primitive geometries of M_{11}.

Nr.	G_1	G_2	$G_1 \cap G_2$	$[d_p, g, d_l]$
1	$\mathrm{GL}_2(3)$	$\mathrm{GL}_2(3)$	S_3	$[5,3,5]$
2	$\mathrm{GL}_2(3)$	$\mathrm{GL}_2(3)$	E_4	$[4,2,4]$
3	$\mathrm{GL}_2(3)$	$\mathrm{GL}_2(3)$	C_2	$[4,2,4]$
4	$\mathrm{GL}_2(3)$	$\mathrm{GL}_2(3)$	C_2	$[5,2,5]$
5	$\mathrm{GL}_2(3)$	$\mathrm{GL}_2(3)$	C_2	$[3,2,4]$
6	$\mathrm{GL}_2(3)$	$\mathrm{GL}_2(3)$	1	$[3,2,3]$
7	$\mathrm{GL}_2(3)$	S_5	D_{12}	$[5,3,5]$
8	$\mathrm{GL}_2(3)$	S_5	D_8	$[4,2,4]$
9	$\mathrm{GL}_2(3)$	S_5	S_3	$[4,2,4]$
10	$\mathrm{GL}_2(3)$	S_5	C_2	$[3,2,3]$
11	$\mathrm{GL}_2(3)$	S_5	C_2	$[3,2,3]$
12	$\mathrm{GL}_2(3)$	$L_2(11)$	D_{12}	$[3,2,4]$
13	$\mathrm{GL}_2(3)$	$L_2(11)$	S_3	$[3,2,3]$
14	$\mathrm{GL}_2(3)$	$M_9:2$	$Q_8:2$	$[6,3,5]$
15	$\mathrm{GL}_2(3)$	$M_9:2$	D_{12}	$[4,3,4]$
16	$\mathrm{GL}_2(3)$	$M_9:2$	C_2	$[3,2,3]$
17	$\mathrm{GL}_2(3)$	$M_9:2$	C_2	$[3,2,3]$
18	$\mathrm{GL}_2(3)$	M_{10}	$Q_8:2$	$[3,2,4]$
19	$\mathrm{GL}_2(3)$	M_{10}	S_3	$[3,2,3]$
20	S_5	S_5	D_8	$[5,2,5]$
21	S_5	S_5	S_3	$[3,2,3]$
22	S_5	S_5	E_4	$[3,2,3]$
23	S_5	$L_2(11)$	A_5	$[3,3,4]$
24	S_5	$L_2(11)$	12	$[3,2,3]$
25	S_5	$M_9:2$	12	$[4,2,3]$
26	S_5	$M_9:2$	8	$[3,2,3]$
27	S_5	$M_9:2$	C_4	$[3,2,3]$
28	S_5	M_{10}	24	$[3,2,3]$
29	S_5	M_{10}	20	$[3,2,3]$
30	$L_2(11)$	$L_2(11)$	A_5	$[3,2,3]$
31	$L_2(11)$	$M_9:2$	D_{12}	$[2,2,2]$
32	$L_2(11)$	M_{10}	A_5	$[2,2,2]$
33	$M_9:2$	$M_9:2$	8	$[3,2,3]$
34	$M_9:2$	$M_9:2$	4	$[3,2,3]$
35	$M_9:2$	M_{10}	M_9	$[3,3,4]$
36	$M_9:2$	M_{10}	16	$[3,2,3]$
37	M_{10}	M_{10}	M_9	$[3,2,3]$

Table 4: Designs $S_\lambda(t,k,v)$ from the rank two primitive geometries of M_{11}.

Nr.	Design
1	$S_8(1,8,165)$
1*	$S_8(1,8,165)$
2	$S_{12}(1,12,165)$
2*	$S_{12}(1,12,165)$
3	$S_{24}(1,24,165)$
3*	$S_{24}(1,24,165)$
4	$S_{24}(1,24,165)$
4*	$S_{24}(1,24,165)$
5	$S_{24}(1,24,165)$
5*	$S_{24}(1,24,165)$
6	$S_{48}(1,48,165)$
6*	$S_{48}(1,48,165)$
7	$S_{10}(1,4,66)$
7*	$S_4(1,10,165)$
8	$S_{15}(1,6,66)$
8*	$S_6(1,15,165)$
9	$S_{20}(1,8,66)$
9*	$S_8(1,20,165)$
10	$S_{60}(1,24,66)$
10*	$S_{24}(1,60,165)$
11	$S_{60}(1,24,66)$
11*	$S_{24}(1,60,165)$
12	$S_3(3,4,12)$
12*	$S_4(1,55,165)$
13	$S_{42}(3,8,12)$
13*	$S_8(1,110,165)$
14	$S_3(1,9,165)$
14*	$S_9(1,3,55)$
15	$S_4(1,12,165)$
15*	$S_{12}(1,4,55)$
16	$S_{24}(1,72,165)$
16*	$S_{72}(1,24,55)$
17	$S_{24}(1,72,165)$
17*	$S_{72}(1,24,55)$
18	$S_1(3,3,11)$
18*	$S_3(1,45,165)$
19	$S_1(8,8,11)$
19*	$S_8(1,120,165)$
20	$S_{15}(1,15,66)$
20*	$S_{15}(1,15,66)$
21	$S_{20}(1,20,66)$
21*	$S_{20}(1,20,66)$
22	$S_{30}(1,30,66)$
22*	$S_{30}(1,30,66)$
23	$S_1(2,2,12)$
23*	$S_2(1,11,66)$
24	$S_1(10,10,12)$
24*	$S_{10}(1,55,66)$
25	$S_{10}(1,12,66)$
25*	$S_{12}(1,10,55)$
26	$S_{15}(1,18,66)$
26*	$S_{18}(1,15,55)$
27	$S_{30}(1,36,66)$
27*	$S_{36}(1,30,55)$
28	$S_5(1,30,66)$
28*	$S_1(4,5,11)$
29	$S_6(1,36,66)$
29*	$S_3(4,6,11)$
30	$S_1(11,11,12)$
30*	$S_1(11,11,12)$
33	$S_{18}(1,18,55)$
33*	$S_{18}(1,18,55)$
34	$S_{36}(1,36,55)$
34*	$S_{36}(1,36,55)$
35	$S_1(2,2,11)$
35*	$S_2(1,10,55)$
36	$S_1(9,9,11)$
36*	$S_9(1,45,55)$
37	$S_1(10,10,11)$
37*	$S_1(10,10,11)$

Table 5: Orbits of primitive permutation representations of M_{12}.

	12	12	66	66	144	220	220
M_{11}	1 – 11	12	66	11 – 55	144	220	55 – 165
M_{11}	12	1 – 11	11 – 55	66	144	55 – 165	220
$M_{10}:2$	12	2 – 10	1 – 20 – 45	30 – 36	144	10 – 90 – 120	40 – 180
$M_{10}:2$	2 – 10	12	30 – 36	1 – 20 – 45	144	40 – 180	10 – 90 – 120
$L_2(11)$	12	12	66	66	$1 – 11^2 – 55 – 66$	220	220
$M_9:S_3$	12	3 – 9	3 – 27 – 36	12 – 54	144	1 – 12 – 27 – 72 – 108	4 – 36 – 72 – 108
$M_9:S_3$	3 – 9	12	12 – 54	3 – 27 – 36	144	4 – 36 – 72 – 108	1 – 12 – 27 – 72 – 108
$S_5 \times 2$	12	12	$6 – 30^2$	$6 – 30^2$	$20^3 – 24 – 60$	40 – 60 – 120	40 – 60 – 120
$4^2:D_{12}$	12	12	6 – 12 – 48	6 – 12 – 48	$16^2 – 32^2 – 48$	12 – 48 – 64 – 96	12 – 48 – 64 – 96
$M_8:S_4$	4 – 8	4 – 8	4 – 6 – 24 – 32	4 – 6 – 24 – 32	48 – 96	4 – 16 – 24 – 32 – 48 – 96	4 – 16 – 24 – 32 – 48 – 96
$A_4 \times S_3$	12	12	12 – 18 – 36	12 – 18 – 36	$6^2 – 18^2 – 24 – 36^2$	$4 – 12 – 24 – 36 – 72^2$	$4 – 12 – 24 – 36 – 72^2$

	396	495	495	1320
M_{11}	396	495	165 – 330	1320
M_{11}	396	495	165 – 330	1320
$M_{10}:2$	$36 – 180^2$	45 – 90 – 360	30 – 45 – 180 – 240	240 – 360 – 720
$M_{10}:2$	$36 – 180^2$	45 – 90 – 360	30 – 45 – 180 – 240	240 – 360 – 720
$L_2(11)$	$55^3 – 66 – 165$	$55^2 – 110^2 – 165$	165 – 330	$55^2 – 165^2 – 220 – 330^2$
$M_9:S_3$	72 – 108 – 216	27 – 108 – 144 – 216	9 – 36 – 54 – 72 – 108 – 216	$24 – 72 – 144 – 216 – 432^2$
$M_9:S_3$	72 – 108 – 216	27 – 108 – 144 – 216	9 – 36 – 54 – 72 – 108 – 216	$24 – 72 – 144 – 216 – 432^2$
$S_5 \times 2$	$1 – 10^2 – 15 – 30^2 – 60^3 – 120$	$5 – 15^2 – 20^2 – 60^3 – 120^2$	$15 – 30^2 – 60 – 120^3$	$10 – 30 – 60^4 – 80 – 120^4 – 240^2$
$4^2:D_{12}$	$4 – 12^2 – 16^2 – 48^3 – 96^2$	$1 – 6 – 16 – 24 – 32^2 – 48^2 – 96^3$	$3 – 12 – 48^2 – 96^4$	$16 – 24 – 48^4 – 64^2 – 96^4 – 192^3$
$M_8:S_4$	$12 – 24^2 – 48 – 96^3$	$3 – 12 – 48^2 – 96^4$	$1 – 6 – 16 – 24 – 32^2 – 48^2 – 96^3$	$8 – 48^2 – 64 – 96^4 – 192^4$
$A_4 \times S_3$	$3 – 9 – 18^4 – 24 – 36^4 – 72^2$	$6 – 9 – 18^4 – 24^2 – 36^4 – 72^3$	$3 – 18^2 – 24 – 36^4 – 72^4$	$1 – 8 – 9 – 12 – 18^3 – 24^2 – 36^7 – 72^{13}$

Table 6: Orbits of primitive permutation representations of M_{22}.

	22	77	176	176	231
$L_3(4)$	1 – 21	21 – 56	56 – 120	56 – 120	21 – 210
$2^4 : A_6$	6 – 16	1 – 16 – 60	80 – 96	80 – 96	15 – 96 – 120
A_7	7 – 15	35 – 42	1 – 70 – 105	15 – 35 – 126	21 – 105^2
A_7	7 – 15	35 – 42	15 – 35 – 126	1 – 70 – 105	21 – 105^2
$2^4 : S_5$	2 – 20	5 – 32 – 40	16 – 80^2	16 – 80^2	1 – 30 – 40 – 160
$2^3 : L_3(2)$	8 – 14	7 – 14 – 56	8 – 56 – 112	8 – 56 – 112	7 – 28 – 84 – 112
M_{10}	10 – 12	2 – 30 – 45	20 – 36 – 120	20 – 36 – 120	30 – 36 – 45 – 120
$L_2(11)$	11^2	11^2 – 55	11 – 55 – 110	11 – 55 – 110	55^3 – 66

	330	616	672
$L_3(4)$	120 – 210	280 – 336	336^2
$2^4 : A_6$	30 – 60 – 240	16 – 240 – 360	96^2 – 480
A_7	15 – 105 – 210	70 – 126 – 420	42 – 210 – 420
A_7	15 – 105 – 210	70 – 126 – 420	42 – 210 – 420
$2^4 : S_5$	10 – 40 – 120 – 160	80 – 96 – 120 – 320	160^3 – 192
$2^3 : L_3(2)$	1 – 7 – 42 – 112 – 168	56^2 – 168 – 336	112^3 – 336
M_{10}	30^2 – 90 – 180	1 – 30 – 45 – 180 – 360	72 – 120^2 – 360
$L_2(11)$	55^3 – 165	66 – 110^2 – 330	1 – 55^2 – 66 – 165 – 330

Table 7: Orbits of primitive permutation representations of M_{23}.

	23	253	253	506
M_{22}	1 – 22	77 – 176	22 – 231	176 – 330
$L_3(4) : 2$	7 – 16	1 – 112 – 140	21 – 112 – 120	30 – 140 – 336
$2^4 : A_7$	2 – 21	21 – 112 – 120	1 – 42 – 210	56 – 210 – 240
A_8	8 – 15	15 – 70 – 168	28 – 105 – 120	1 – 15 – 210 – 280
M_{11}	11 – 12	22 – 66 – 165	55 – 66 – 132	66 – 110 – 330
$2^4 : (3 \times A_5) : 2$	3 – 20	5 – 48 – 80 – 120	3 – 30 – 60 – 160	10 – 16 – 120^2 – 240
$23 : 11$	23	253	253	253^2

	1288	1771	40320
M_{22}	616 – 672	231 – 1540	40320
$L_3(4) : 2$	112 – 336 – 840	35 – 336 – 560 – 840	40320
$2^4 : A_7$	280 – 336 – 672	21 – 210 – 420 – 1120	40320
A_8	168 – 280 – 840	35 – 56 – 420^2 – 840	20160^2
M_{11}	1 – 165 – 330 – 792	165 – 220 – 330 – 396 – 660	720 – 7920^5
$2^4 : (3 \times A_5) : 2$	120 – 160 – 240 – 288 – 480	1 – 20 – 60 – 90 – 160 – 480^3	5760^7
$23 : 11$	23 – 253^5	253^7	1 – 23^4 – 253^{159}

Table 8: Orbits of primitive permutation representations of J_1.

	266	1045	1463
$L_2(11)$	$1-11-12-110-132$	$55-110-220-660$	$11-55-110-132-165-330-660$
$2^3:7:3$	$14-28-56-168$	$1-8-28-56^3-168^5$	$7-56^2-84^2-168^7$
$A_5\times 2$	$2-10-20-24-30-60-120$	$5-40^2-60^2-120^7$	$1-12-15^2-20^2-60^9-120^7$
$19:6$	$19-38^2-57^3$	$19^2-38^4-57-114^7$	$19-38^2-57^{10}-114^7$
$11:10$	$2-22^2-55^2-110$	$55-110^9$	$11-22-55^6-110^{10}$
$D_6\times D_{10}$	$5-6-15-30^4-60^2$	$10-15-30^2-60^{16}$	$3-5-15^5-30^{14}-60^{16}$
$7:6$	$7-14^2-21^3-42^4$	$2-7^2-14^3-21-42^{23}$	$7-14^2-21^{10}-42^{29}$

	1540	1596	2926	4180
$L_2(11)$	$110-220^2-330^3$	$12-132^2-330^2-660$	$55-66-165-330^4-660^2$	$110-220^2-330^3-660^4$
$2^3:7:3$	$28^2-56^4-84-168^7$	$84-168^9$	$28-42-84^2-168^{16}$	$8-28^2-56^3-84-168^{23}$
$A_5\times 2$	$20-40^2-60^{10}-120^7$	$12-24-60^6-120^{10}$	$6-10-30^5-60^{14}-120^{16}$	$20-40^2-60^{10}-120^{29}$
$19:6$	$1-19-38^4-57^6-114^9$	57^4-114^{12}	$19-57^{15}-114^{18}$	$19^2-38^4-57^6-114^{32}$
$11:10$	55^4-110^{12}	$1-11-22^2-55^2-110^{13}$	$11-55^9-110^{22}$	55^4-110^{36}
$D_6\times D_{10}$	$10-30^{15}-60^{18}$	$6-30^9-60^{22}$	$1-15^5-30^{27}-60^{34}$	$10-30^{15}-60^{62}$
$7:6$	$7^2-14^4-21^6-42^{32}$	21^4-42^{36}	$7-21^{15}-42^{62}$	$1-7-14^4-21^6-42^{95}$

5 Conclusions

We have described a new algorithm that allows to compute primitive geometries of rank two for much larger groups than the Dehon algorithm [7]. It remains to extend this algorithm to be able to construct geometries of higher ranks as the Dehon algorithm permitted. Since our first aim was to study codes arising from these rank two geometries, we did not try to extend our algorithm and we leave it as an interesting topic for future work.

The problems found in [12] for M_{22} are very likely due to an incorrect determination of non-isomorphic pairs of subgroups.

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Infinite benzenoids

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Abstract

A family of benzenoids, called *convex benzenoids*, was introduced in 2012 by Cruz, Gutman and Rada. In a later paper by the present author *et al.*, several equivalent characterisations of convex benzenoids have been given and their equivalence was proved. Along the way an *infinite* benzenoid called the *half-plane* was used for the purpose of theoretical reasoning. In this short paper, some properties of infinite benzenoids are discussed. It is proved that their boundary consists of countably many connected components. *Convex infinite* benzenoids are classified and it is proved that there are only *countably* many convex infinite benzenoids, whilst there are *uncountably* many infinite (non-convex) benzenoids. We also show that there are countably many infinite benzenoids which have a finite number of 1s in their *boundary-edges code*.

Keywords: Infinite benzenoid, hexagonal system, convex benzenoid, boundary-edges code, half-plane, countable set.

Math. Subj. Class.: 05C10, 92E10, 03E75

1 Introduction

Benzenoids are important compounds in chemistry and have been extensively studied during the past few decades. For an exhaustive treatment of the topic see the classical reference by Cyvin and Gutman [9]. The reader may want to consult references [5, 6] and [7] for advanced treatments. In the present paper, we study their associated *benzenoid graphs* from a purely mathematical viewpoint. Hereinafter, the word benzenoid is used as a synonym for benzenoid graph. We build upon theoretical treatment of benzenoids from [2]. The framework of [2] allows for generalisation to structures called *infinite benzenoids*. In 2012

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a family of *convex benzenoids* was introduced by Cruz, Gutman and Rada [4]. In a recent work [3], we presented several alternative characterisations of convex benzenoids. In this work, we study properties of convex infinite benzenoids. We assume that the reader is familiar with results of elementary set theory (e.g., the union of countably many countable sets is countable). For definitions of set-theoretic terms such as *countable set* and *uncountable set*, consult a standard reference such as [10] or [12]. This paper further develops several ideas already present in the PhD thesis of the author [1].

2 The hexagonal grid

Let us consider the infinite cubic plane graph $\mathcal{H}$, called the *hexagonal grid*. (For an introduction to infinite graphs, consult Chapter 8 of [8].) It comprises infinitely many hexagonal faces each of which is incident with 6 edges and 6 vertices. We say that faces $a, b \in F(\mathcal{H})$ are *adjacent* if they are different and share an edge. The faces of $\mathcal{H}$ will be simply called hexagons. Two hexagons are *neighbours* if they have exactly one edge in common. Sometimes, it is convenient to introduce a coordinate system on the hexagonal grid $\mathcal{H}$, as shown in Figure 1. Let $h \in \mathcal{H}$. Then $\xi(h)$ and $\eta(h)$ will denote the first and second coordinate

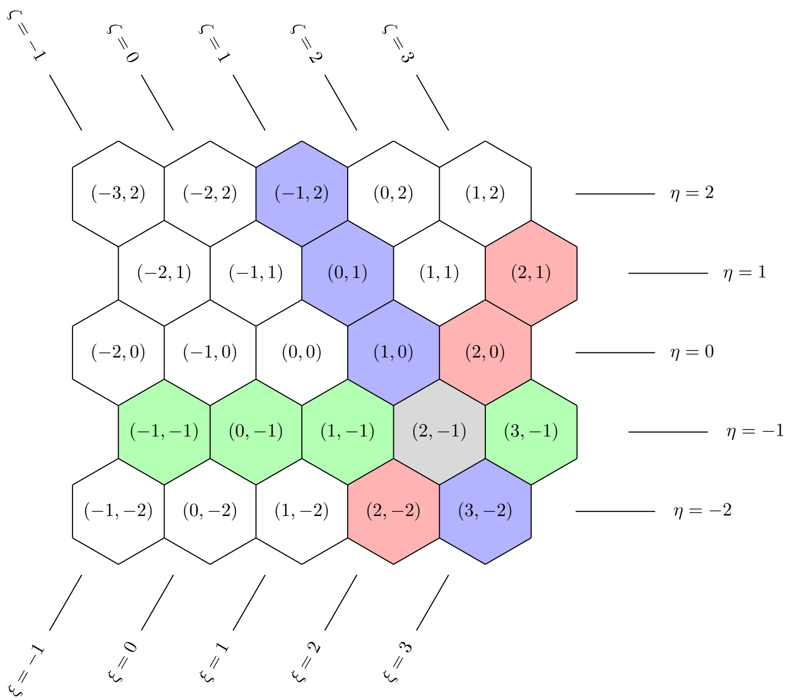


Figure 1: Coordinate system on $\mathcal{H}$.

of h as shown in Figure 1. We may introduce yet another coordinate $\zeta(h)$, but it is not independent of the previous two since $\zeta(h) = \xi(h) + \eta(h)$. For a detailed description of the coordinate system on $\mathcal{H}$, see [1] or [3].

3 Hexagonal systems and benzenoids

An arbitrary subset of faces $\mathcal{K} \subseteq F(\mathcal{H})$, together with all vertices and edges that are incident with at least one member of $\mathcal{K}$, is called a *hexagonal system*. We will denote the corresponding hexagonal system simply by $\mathcal{K}$, even though it is formally a subset of faces. Two hexagonal systems are *isomorphic* if one can be obtained from the other by an isometry of the plane that leaves $\mathcal{H}$ invariant. Hexagons $a \in \mathcal{K}$ and $b \in \mathcal{K}$ belong to the same *connected component* of the hexagonal system if there exists a sequence of hexagons $h_1 = a, h_2, \ldots, h_n = b$ such that h_i and h_{i+1} are adjacent for each $i = 1, \ldots, n-1$ and $\{h_1, \ldots, h_n\} \subseteq \mathcal{K}$. When all hexagons of the sequence are pairwise distinct, it is called a *path* between a and b in $\mathcal{K}$. The *interval* between a and b in $\mathcal{K}$, denoted $I_{\mathcal{K}}(a, b)$, is the set of hexagons which are contained on any of the shortest paths between a and b. A hexagonal system is *connected* if it has a single connected component. A subset of faces $\mathcal{K} \subseteq F(\mathcal{H})$ gives rise to two hexagonal systems: $\mathcal{K}$ and its *complement* $\mathcal{K}^{\complement}$.

We define a benzenoid in the following way:

Definition 3.1. A *benzenoid* is a connected hexagonal system $\mathcal{K}$, such that each connected component of the complement $\mathcal{K}^{\complement}$ is infinite.

A benzenoid is *finite* if it has a finite number of hexagons. Otherwise, it is called an *infinite* benzenoid.

Example 3.2. Let $k \in \mathbb{Z}$. Infinite hexagonal systems

$$\begin{aligned}
\Xi_k &= \{h \in \mathcal{H} \mid \xi(h) = k\}, \\
\mathrm{H}_k &= \{h \in \mathcal{H} \mid \eta(h) = k\}, \text{ and} \\
\mathrm{Z}_k &= \{h \in \mathcal{H} \mid \zeta(h) = k\}
\end{aligned}$$

will be called *lines*. They are all benzenoids and they are all isomorphic to each other.

The hexagonal system $\mathcal{K}_1$ on Figure 2 is defined as

$$\mathcal{K}_1 = \{h \in \mathcal{H} \mid \eta(h) \equiv 0 \pmod 2\} = \bigcup_{k \in \mathbb{Z}} \mathrm{H}_{2k}.$$

$\mathcal{K}_1$ is not a benzenoid, because it is not connected. $\mathcal{K}_1$ consists of infinitely many disjoint

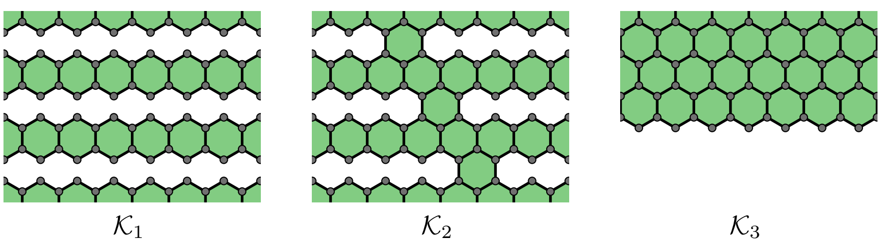


Figure 2: Infinite hexagonal systems $\mathcal{K}_1$, $\mathcal{K}_2$ and $\mathcal{K}_3$.

lines and is isomorphic to its complement $\mathcal{K}_1^{\complement}$.

$\mathcal{K}_2$ is obtained from $\mathcal{K}_1$ by adding another line (with a different slope), i.e., $\mathcal{K}_2 = \mathcal{K}_1 \cup \mathrm{Z}_0$. The hexagonal system $\mathcal{K}_2$ is a benzenoid.

Hexagonal system $\mathcal{K}_3$ is defined as

$$\mathcal{K}_3 = \{h \in \mathcal{H} \mid \eta(h) \geq 0\}.$$

We call it a *convex half-plane*. In the present work, we will simply call it a *half-plane*, since we will not consider other types of (non-convex) half-planes. It is an infinite benzenoid that is isomorphic to its complement $\mathcal{K}_3^{\complement}$. $\diamondsuit$

The following theorem tells us that there are as many (non-isomorphic) infinite benzenoids out there as there are real numbers.

Theorem 3.3. *There exist uncountably many mutually non-isomorphic infinite benzenoids.*

Proof. The interval $[0, 1)$ has the cardinality of the continuum. Each number $x \in [0, 1)$ can be written in its binary representation

$$0.x_1x_2x_3x_4\ldots \tag{3.1}$$

Note that $x_i \in \{0, 1\}$ for each $i \in \mathbb{N}$ and that

$$x = \sum_{i=1}^{\infty} x_i \cdot 2^{-i}. \tag{3.2}$$

The sequence $\{x_i\}_{i=1}^{\infty}$ is uniquely determined if we require that for each $n \in \mathbb{N}$ there exists an integer $m > n$ such that $x_m \neq 1$. For example, the number $\frac{11}{16}$ can be written in binary representation as 0.1011.

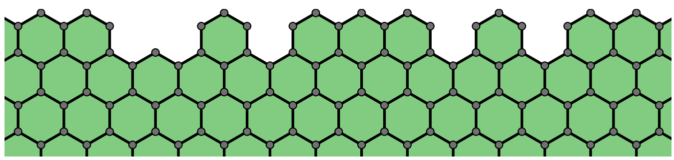


Figure 3: Infinite benzenoid $\mathcal{P}_{\frac{11}{16}}$.

We will assign an infinite benzenoid to every such sequence $\{x_i\}_{i=1}^{\infty}$. Define

$$\mathcal{P}_x = \{h \in \mathcal{H} \mid \eta(h) \leq 0\} \setminus (\{(-2, 0), (-1, 0)\} \cup \{(2i - 1, 0) \mid i \in \mathbb{N} \wedge x_i = 1\}).$$

The infinite benzenoid $\mathcal{P}_x$ is obtained from the half-plane $\mathcal{P} = \{h \in \mathcal{H} \mid \eta(h) \leq 0\}$ by removing hexagons $(-2, 0)$, $(-1, 0)$ and all hexagon $(2i - 1, 0)$ where $i \in \mathbb{N}$ and $x_i = 1$. For example, the infinite benzenoid that corresponds to number $\frac{11}{16}$ is shown in Figure 3.

It is not hard to see that $\mathcal{P}_x \not\cong \mathcal{P}_y$ if and only if $x \neq y$. We constructed an injective mapping from the set $[0, 1)$ to the class of infinite benzenoids. Therefore, the class of all infinite benzenoids is uncountable. $\square$

The *boundary* of a hexagonal system $\mathcal{K}$ consists of all edges and all vertices that are indicent to (at least) one hexagon of $\mathcal{K}$ and (at lest) one hexagon of $\mathcal{K}^{\complement}$. Those vertices and edges are called boundary vertices and boundary edges, respectively.

The boundary of a finite benzenoid is isomorphic to a cycle graph. The boundary of an infinite benzenoid is a disjoint union of one or more *infinite paths*. The boundary of $\mathcal{K}_3$ in Figure 2 is a single infinite path. The boundary of $\mathcal{K}_2$ in Figure 2 consists of infinitely many connected components (that are all infinite paths).

Proposition 3.4. *Let $\mathcal{B}$ be an arbitrary benzenoid. The boundary of $\mathcal{B}$ consists of countably many connected components.*

Proof. The edges of $\mathcal{H}$ can be labeled with natural numbers in a spiral fashion as shown in Figure 4. Let us define a mapping from the set of connected components of the boundary

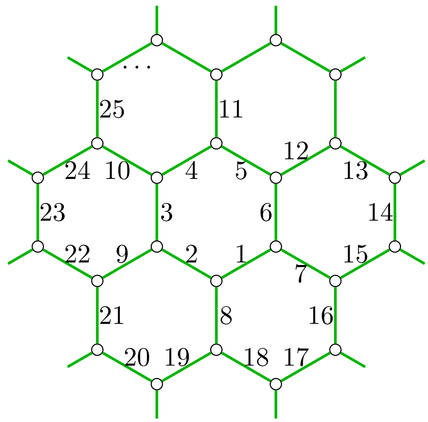


Figure 4: "Spiral" labeling of edges of $\mathcal{H}$.

of $\mathcal{B}$ to natural numbers. Each connected component is mapped to the minimum among all labels of the edges that belong to the component. This mapping to natural numbers is injective and the result follows. □

3.1 The boundary-edges code

Several combinatorial descriptions of finite benzenoids are readily available. In [11], Hansen et al. presented the *boundary-edges code* (abbreviated as BEC). The boundary of a finite benzenoid (which is a cycle graph) is described as a cyclic sequence of numbers, each of which counts the number of edges between two consecutive boundary vertices of degree 3. All those numbers are from the set $\{1, 2, 3, 4, 5\}$. The only exception here is *benzene*, which has BEC 6. In Figure 5, there are several finite benzenoids together with their BECs. The boundary-edges code of $\mathcal{B}$ is denoted $\mathrm{BEC}(\mathcal{B})$.

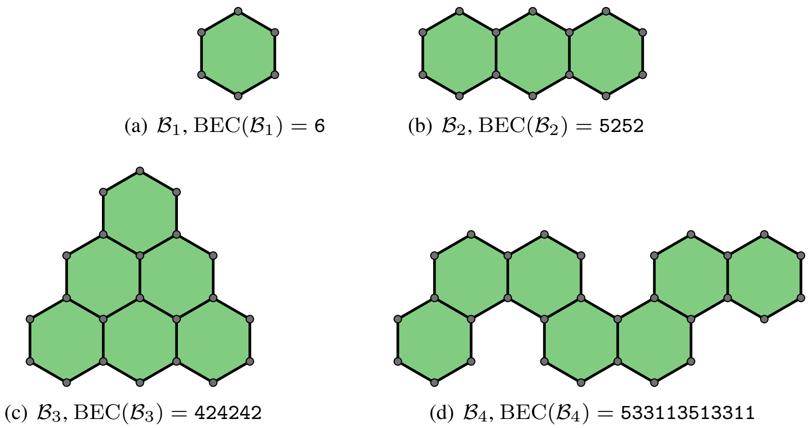
The code $\mathrm{BEC}(\mathcal{B}_3) = 424242$ of $\mathcal{B}_3$ from Figure 5 can also be written as $(42)^3$, where s^k stands for $\underbrace{ss\ldots s}_{k}$.

It is possible to generalise the definition of the BEC to infinite benzenoids. Each connected component of the boundary will be assigned its own BEC. Since a connected component of the boundary of an infinite benzenoid is an infinite path, the BEC can be formally defined as a mapping $\mathbb{Z} \to \{1, 2, 3, 4, 5\}$, i.e. a *doubly infinite sequences*.

Example 3.5. The boundary of a half-plane has a single connected component with the BEC $\ldots 22222 \ldots$, which can simply be written as 2^∞.

The boundary of benzenoid $\mathcal{K}_2$ in Figure 2 has infinitely many connected components. They all have the same BEC, namely $2^\infty 1^3 2^\infty$.

The boundary of benzenoid $\mathcal{P}_{\frac{11}{16}}$ in Figure 3 has a single connected component with BEC $2^\infty 312141^2 3231^2 41^2 32^\infty$. ◊



(a) $\mathcal{B}_1$, $\mathrm{BEC}(\mathcal{B}_1) = 6$ (b) $\mathcal{B}_2$, $\mathrm{BEC}(\mathcal{B}_2) = 5252$

(c) $\mathcal{B}_3$, $\mathrm{BEC}(\mathcal{B}_3) = 424242$ (d) $\mathcal{B}_4$, $\mathrm{BEC}(\mathcal{B}_4) = 533113513311$

Figure 5: Examples of finite benzenoids together with their BECs.

Infinite benzenoids can be classified with respect to the number of connected components of the boundary.

Proposition 3.6. *Let $n \in \mathbb{N} \cup \{0, \infty\}$. There exists an infinite benzenoid $\mathcal{B}$ with n connected components in the boundary of $\mathcal{B}$. Symbol ∞ means that the boundary of $\mathcal{B}$ has (countably) infinitely many connected components.*

Proof. The benzenoid $\mathcal{H}$, i.e. the one that contains all hexagons of the infinite hexagonal grid, is the only one with 0 connected components in the boundary. The boundary of half-plane $\mathcal{P} = \{h \in \mathcal{H} \mid \eta(h) \geq 0\}$ has exactly 1 connected component.

Let

$$\mathcal{B}_k = \mathcal{P} \cup \Xi_0 \cup \Xi_2 \cup \Xi_4 \cup \cdots \cup \Xi_{2k}.$$

It is easy to see that the boundary of $\mathcal{B}_k$ has $k+2$ connected components. In other words, for every natural number $n \geq 2$ there exist an infinite benzenoid, namely $\mathcal{B}_{n-2}$, with exactly n connected components in its boundary.

For the case $n = \infty$, take $\mathcal{K}_2$ from Figure 2. $\square$

4 Convex (infinite) benzenoids

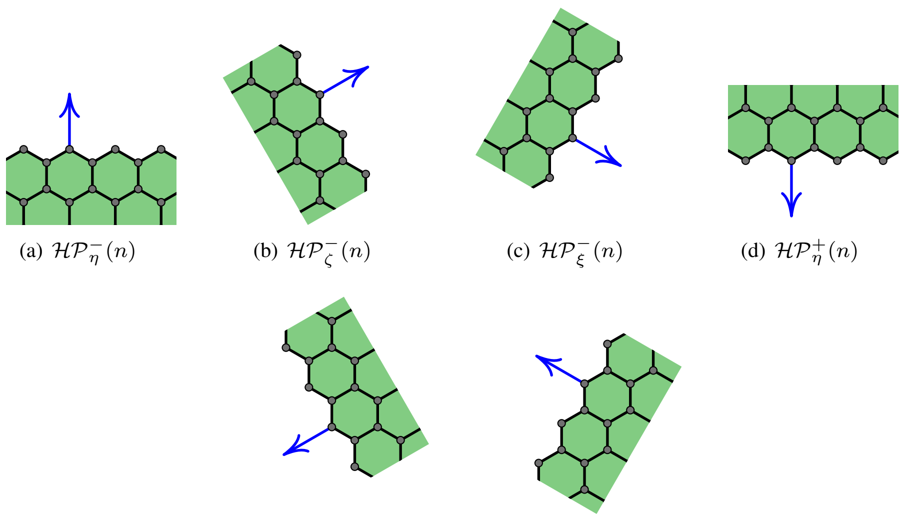
Let us recall the metric definition of a convex hexagonal system from [3]:

Definition 4.1. A hexagonal system $\mathcal{K}$ is *convex* if for any pair of its hexagons a and b the whole interval $I_{\mathcal{H}}(a, b)$ is contained in $\mathcal{K}$.

Theorem 3.3 means that one cannot describe all of the infinite benzenoids algorithmically. This means that there exist infinite benzenoids for which there does not exist a finite computer program for constructing them (even if the program runs infinitely long).

Let us consider convex infinite benzenoids. The whole hexagonal grid $\mathcal{H}$ and the empty set $\emptyset$ are clearly convex. A half-plane is also convex. Each half-plane has a normal which is pointing out of the half-plane (see Figure 6). There are exactly 6 possible directions of half-planes. We will denote them as follows:

$$\mathcal{HP}^+_\xi(n) = \{h \in \mathcal{H} \mid \xi(h) \geq n\}, \tag{4.1}$$
$$\mathcal{HP}^-_\xi(n) = \{h \in \mathcal{H} \mid \xi(h) \leq n\}, \tag{4.2}$$
$$\mathcal{HP}^+_\eta(n) = \{h \in \mathcal{H} \mid \eta(h) \geq n\}, \tag{4.3}$$
$$\mathcal{HP}^-_\eta(n) = \{h \in \mathcal{H} \mid \eta(h) \leq n\}, \tag{4.4}$$
$$\mathcal{HP}^+_\zeta(n) = \{h \in \mathcal{H} \mid \zeta(h) \geq n\}, \tag{4.5}$$
$$\mathcal{HP}^-_\zeta(n) = \{h \in \mathcal{H} \mid \zeta(h) \leq n\}. \tag{4.6}$$



(a) $\mathcal{HP}^-_\eta(n)$ (b) $\mathcal{HP}^-_\zeta(n)$ (c) $\mathcal{HP}^-_\xi(n)$ (d) $\mathcal{HP}^+_\eta(n)$

(e) $\mathcal{HP}^+_\zeta(n)$ (f) $\mathcal{HP}^+_\xi(n)$

Figure 6: The normal of a hexagonal half-plane can point in 6 different directions.

Note that the intersection of two half-planes with the same normal is equal to one of the two. In other words, one is a sub-benzenoid of the other. For example,

$$\mathcal{HP}^+_\xi(3) \cap \mathcal{HP}^+_\xi(5) = \mathcal{HP}^+_\xi(5).$$

Therefore, the interection of any number of half-planes is equal to an intersection of at most 6 of those half-planes. For each direction of the normal that is present in the list, we select the half-plane that is contained in all other half-planes that have the same direction. Also, note that all half-planes (4.1) – (4.6) are isomorphic to each other.

Definition 4.2. Let $\mathcal{B}$ be a benzenoid (finite or infinite). The smallest convex benzenoid containing $\mathcal{B}$ is called the *convex closure* of $\mathcal{B}$ and is denoted $\mathrm{Conv}(\mathcal{B})$.

In [3], the following proposition was proved.

Proposition 4.3. *Any intersection of convex (finite or infinite) benzenoids is a convex benzenoid.* □

Note that the empty set $\emptyset$ can also be considered as a convex benzenoid. To a chemist, this means nothing concrete. To a mathematician, it is clear that every two members of an empty set satisfy the condition in Definition 4.1, i.e., this condition is void.

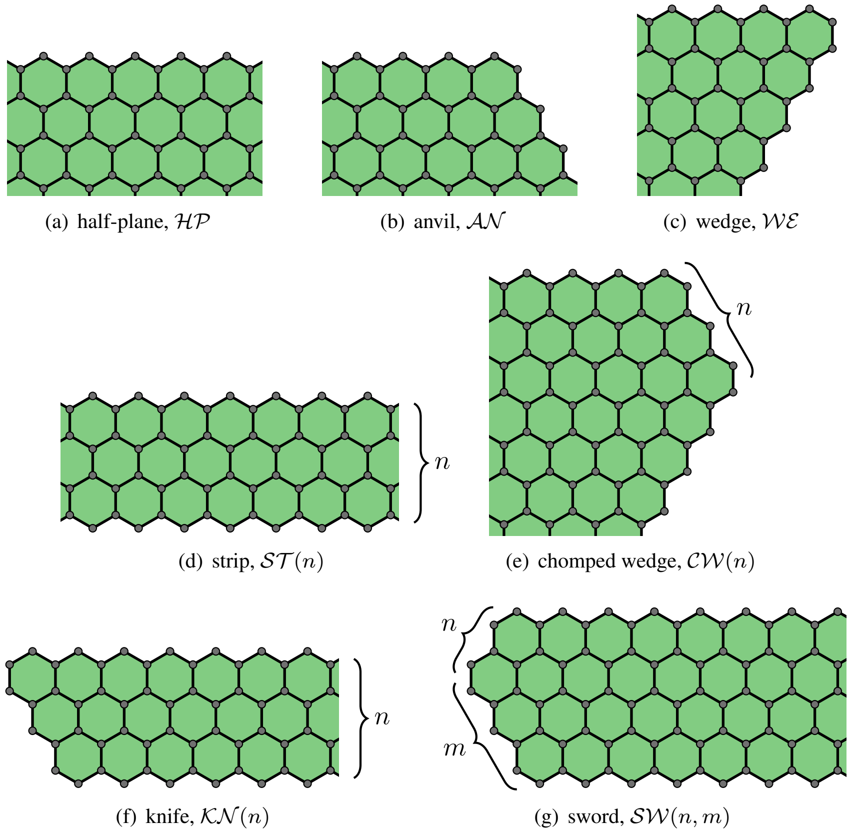


Figure 7: Families of convex infinite benzenoids.

In addition to the hexagonal grid $\mathcal{H}$, the empty set $\emptyset$ and half-plane $\mathcal{HP}$, we introduce the following families of infinite benzenoids (see Figure 7):

(a) The benzenoid $\mathcal{AN}$ in Figure 7(b) is called *anvil* and is uniquely determined (up to isomorphism) by $\mathrm{BEC}(\mathcal{AN}) = 2^\infty 32^\infty$.

(b) The benzenoid $\mathcal{WE}$ in Figure 7(c) is called *wedge* and is uniquely determined (up to isomorphism) by $\mathrm{BEC}(\mathcal{WE}) = 2^\infty 42^\infty$.

(c) A member of the one-parametric family of benzenoids $\mathcal{ST}(n)$, $n \geq 1$, in Figure 7(d) is called a *strip* (of width n) and cannot be uniquely determined by the BEC. However, $\mathcal{ST}(n) \cong \mathcal{HP}^+_\xi(0) \cap \mathcal{HP}^-_\xi(n)$. Note that $\mathcal{ST}(1)$ is called a line.

(d) A member of the one-parametric family of benzenoids $\mathcal{CW}(n)$, $n \geq 2$, in Figure 7(e) is called a *chomped wedge* and is uniquely determined (up to isomorphism) by $\mathrm{BEC}(\mathcal{CW}(n)) = 2^\infty 32^{n-2} 32^\infty$.

(e) A member of the one-parametric family of benzenoids $\mathcal{KN}(n)$, $n \geq 1$, in Figure 7(f) is called a *knife* (of width n) and is uniquely determined (up to isomorphism) by

$$\mathrm{BEC}(\mathcal{KN}(n)) = \begin{cases} 2^\infty 32^{n-2} 42^\infty & \text{if } n \geq 2, \\ 2^\infty 52^\infty & \text{if } n = 1. \end{cases}$$

The benzenoid $\mathcal{KN}(1)$ will also be called a *needle*.

(f) A member of the two-parametric family of benzenoids $\mathcal{SW}(n, m)$, $m \geq n \geq 2$, in Figure 7(g) is called a *sword* and is uniquely determined (up to isomorphism) by $\mathrm{BEC}(\mathcal{SW}(n)) = 2^\infty 32^{n-2} 32^{m-2} 32^\infty$.

All benzenoids on the above list can be obtaned as intersections of half-planes and are therefore convex by Proposition 4.3.

In [3], the following proposition was proved.

Proposition 4.4. *A finite benzenoid $\mathcal{B}$ is convex if and only if it can be obtained as an intersection of half-planes, i.e., if there exist integers n_ξ^+, n_ξ^-, n_η^+, n_η^-, n_ζ^+ and n_ζ^-, such that*

$$\mathcal{B} = \mathcal{HP}_\xi^+(n_\xi^+) \cap \mathcal{HP}_\xi^-(n_\xi^-) \cap \mathcal{HP}_\eta^+(n_\eta^+) \cap \mathcal{HP}_\eta^-(n_\eta^-) \cap \mathcal{HP}_\zeta^+(n_\zeta^+) \cap \mathcal{HP}_\zeta^-(n_\zeta^-). \square$$

Let $\mathcal{B}$ be a benzenoid. We define

$$\eta^+ = \max_{h \in \mathcal{B}} \eta(h) \quad \text{and} \quad \eta^- = \min_{h \in \mathcal{B}} \eta(h).$$

If the set $\{\eta(h) \mid h \in \mathcal{B}\}$ is not bounded from above, we write $\eta^+ = \infty$. Similarly, if the set $\{\eta(h) \mid h \in \mathcal{B}\}$ is not bounded from below, we write $\eta^- = -\infty$. Analogously, we define

$$\xi^+ = \max_{h \in \mathcal{B}} \xi(h), \quad \xi^- = \min_{h \in \mathcal{B}} \xi(h), \quad \zeta^+ = \max_{h \in \mathcal{B}} \zeta(h) \quad \text{and} \quad \zeta^- = \min_{h \in \mathcal{B}} \zeta(h).$$

Lemma 4.5. *Let $\mathcal{B}$ be a convex benzenoid. Then the following statements hold:*

(1) If $\eta^+ < \infty$ and $\xi^+ < \infty$ then $\zeta^+ < \infty$.

(2) If $\eta^- > -\infty$ and $\xi^- > -\infty$ then $\zeta^- > -\infty$.

(3) If $\xi^+ < \infty$ and $\zeta^- > -\infty$ then $\eta^- > -\infty$.

(4) If $\xi^- > -\infty$ and $\zeta^+ < \infty$ then $\eta^+ < \infty$.

(5) If $\eta^+ < \infty$ and $\zeta^- > -\infty$ then $\xi^- > -\infty$.

(6) If $\eta^- > -\infty$ and $\zeta^+ < \infty$ then $\xi^+ < \infty$.

Proof. It is enough to prove statement (1) of the lemma. Other statements will results from the fact that we may use a rotational symmetry of the hexagonal grid $\mathcal{H}$.

Suppose that $\eta^+ < \infty$ and $\xi^+ < \infty$. This implies $\mathcal{B} \subseteq \mathcal{HP}_\eta^-(\eta^+)$ and $\mathcal{B} \subseteq \mathcal{HP}_\xi^-(\xi^+)$. Moreover, $\mathcal{B} \subseteq \mathcal{HP}_\eta^-(\eta^+) \cap \mathcal{HP}_\xi^-(\xi^+)$. But $\mathcal{HP}_\eta^-(\eta^+) \cap \mathcal{HP}_\xi^-(\xi^+)$ is a wedge in which hexagon (ξ^+, η^+) obtains the maximal value of ζ coordinate. Therefore, $\zeta^+ < \infty$. $\square$

The next result generalises Proposition 4.4 to infinite benzenoids.

Proposition 4.6. *An benzenoid $\mathcal{B}$ (finite or infinite) is convex if and only if it can be obtained as an intersection of half-planes.*

Proof. The proof technique used here is similar to the one used in [3] to prove Proposition 4.4. If a benzenoid $\mathcal{B}$ is obtained as an intersection of half-planes then it is convex by Proposition 4.3.

Now let $\mathcal{B}$ be a convex benzenoid. There are several cases to consider, depending on the values of ξ^+, ξ^-, η^+, η^-, ζ^+ and ζ^-.

Suppose that $\xi^- > -\infty$, $\eta^- > -\infty$ and $\zeta^+ < \infty$. Statements (2), (4) and (6) of Lemma 4.5 imply that $\zeta^- > -\infty$, $\eta^+ < \infty$ and $\xi^+ < \infty$, respectively. This means that $\mathcal{B}$ is finite and the result follows from Proposition 4.4.

We need to consider several more cases:

(i) $\xi^- = -\infty$, $\eta^- > -\infty$ and $\zeta^+ < \infty$;

(ii) $\xi^- = -\infty$, $\eta^- = -\infty$ and $\zeta^+ < \infty$;

(iii) $\xi^- = -\infty$, $\eta^- = -\infty$ and $\zeta^+ = \infty$.

Note that because of the symmetry, there are only 3 cases to consider and not 2^3. We provide the proof of case (i). The proofs of (ii) and (iii) are very similar and use the same type of arguments.

(i): Suppose that $\xi^- = -\infty$, $\eta^- > -\infty$ and $\zeta^+ < \infty$. Statements (6) of Lemma 4.5 implies that $\xi^+ < \infty$. Now consider ζ^- and η^+. If $\zeta^- > -\infty$ and $\eta^+ < \infty$ then by statement (5) of Lemma 4.5 we obtain $\xi^- > -\infty$, a contradiction. We have two subcases:

(i.1) $\zeta^- = -\infty$ and $\eta^+ = \infty$;

(i.2) $\zeta^- = -\infty$ and $\eta^+ < \infty$.

Again, by the symmetry argument, we do not need to consider the case $\zeta^- > -\infty$ and $\eta^+ = \infty$. We will now consider case (i.1). The case (i.2) is analogous.

(i.1): From $\eta^- > -\infty$ it follows that there exists a hexagon $h_{\eta^-} \in \mathcal{B}$ such that $\eta(h_{\eta^-}) = \eta^-$. From $\zeta^+ < \infty$ it follows that there exists a hexagon $h_{\zeta^+} \in \mathcal{B}$ such that $\zeta(h_{\zeta^+}) = \zeta^+$. And from $\xi^+ < \infty$ it follows that there exists a hexagon $h_{\xi^+} \in \mathcal{B}$ such that $\xi(h_{\xi^+}) = \xi^+$. See Figure 8 for an illustration. Let $h_1, h_2 \in \mathcal{H}$ such that $\eta(h_1) = \eta^-$, $\xi(h_1) = \xi^+$, $\zeta(h_2) = \zeta^+$ and $\xi(h_2) = \xi^+$. Because $h_1 \in I_{\mathcal{H}}(h_{\eta-}, h_{\xi^+})$ and $h_2 \in I_{\mathcal{H}}(h_{\xi^+}, h_{\zeta^+})$, it follows that $h_1, h_2 \in \mathcal{B}$.

Let n be an arbitrary large integer. From $\zeta^- = -\infty$ it follow that there exists a hexagon $h' \in \mathcal{B}$ such that $\zeta(h') = -n$. Let $h'' \in \mathcal{H}$ be the hexagon with $\zeta(h'') = -n$ and $\eta(h'') = \eta^-$. Since $h'' \in I_{\mathcal{H}}(h', h_1)$ it follow that $h'' \in \mathcal{B}$. This means that $\mathcal{B}$ contains the needle $\{h \in \mathcal{H} \mid \eta(h) = \eta^- \wedge \xi(h) \leq \xi^+\}$. Similarly, $\eta^+ = \infty$ implies that $\mathcal{B}$ also contains the needle $\{h \in \mathcal{H} \mid \zeta(h) = \zeta^+ \wedge \xi(h) \leq \xi^+\}$. The line segment between h_1 and h_2 is also contained in $\mathcal{B}$.

This means that all boundary hexagons of $\mathcal{HP}^+_\eta(\eta^-) \cap \mathcal{HP}^-_\xi(\xi^+) \cap \mathcal{HP}^-_\zeta(\zeta^+)$ are contained in $\mathcal{B}$. But $\mathcal{B} \subseteq \mathcal{HP}^+_\eta(\eta^-) \cap \mathcal{HP}^-_\xi(\xi^+) \cap \mathcal{HP}^-_\zeta(\zeta^+)$ and therefore

$$\mathcal{B} = \mathcal{HP}^+_\eta(\eta^-) \cap \mathcal{HP}^-_\xi(\xi^+) \cap \mathcal{HP}^-_\zeta(\zeta^+).$$

The remaining cases can be proved using the same approach. $\square$

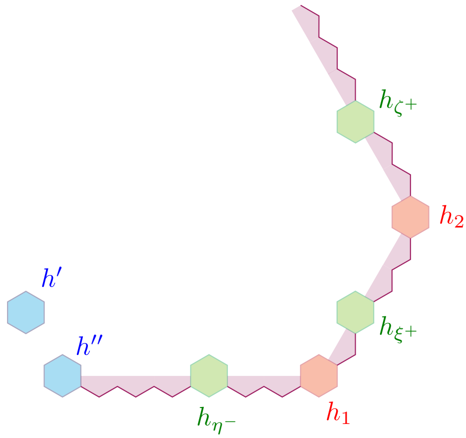


Figure 8: The case (i.1).

We are now able to prove the following theorem.

Theorem 4.7. *An infinite benzenoid is convex if and only if it is isomorphic to one of the following:*

(a) the hexagonal grid $\mathcal{H}$,

(b) the half-plane $\mathcal{HP}$,

(c) the anvil $\mathcal{AN}$,

(d) the wedge $\mathcal{WE}$,

(e) a strip $\mathcal{ST}(n)$ for some $n \geq 1$,

(f) a chomped wedge $\mathcal{CW}(n)$ for some $n \geq 2$,

(g) a knife $\mathcal{KN}(n)$ for some $n \geq 1$,

(h) a sword $\mathcal{SW}(n, m)$ for some $m \geq n \geq 2$.

Moreover, all benzenoids from the above list are pairwise non-isomorphic.

Proof. We already know that all infinite benzenoids listed in the statement of the theorem are convex. It is not hard to see that they are also pairwise non-isomorphic.

Suppose that $\mathcal{B}$ is a convex infinite benzenoid. From Proposition 4.6 it follows that it can be obtained as an intersection of half-planes. We can analyse (case by case) all possibilities for the intersection of (any subset) of the 6 half-planes. In this analysis, we either obtain a finite convex benzenoid (they were classified in [3]), which contradicts the assumption that $\mathcal{B}$ is infinite, or one of the above. □

Let $\mathcal{FO}$ be the class of all such infinite benzenoids $\mathcal{B}$ with the property that the total number of 1s in BECs of all connected components of the boundary of $\mathcal{B}$ is finite.

Theorem 4.8. *There are countably many benzenoids in the class $\mathcal{FO}$.*

Proof. Let $\mathcal{O}_n$, $n \geq 0$, be the finite benzenoid defined by $\mathrm{BEC}(\mathcal{O}_n) = (\mathtt{32}^n)^6$.

Let $\mathcal{B}$ be any benzenoid of the class $\mathcal{FO}$ (see Figure 9 for an example). Because there are finitely many $\mathtt{1}$s in BECs of $\mathcal{B}$, there exists some $\mathcal{O}' = \mathcal{O}_n$ for n large enough, such that $\mathcal{O}'$ contains all edges that correspond to $\mathtt{1}$s in BECs of $\mathcal{B}$ as internal edges (see Figure 10(a)). Then $\mathcal{B} \setminus \mathcal{O}'$ is a hexagonal system that comprises finitely many finite benzenoids and finitely many infinite benzenoids. (In the example in Figure 10(a), there is 1 finite benzenoid and 2 infinite benzenoids.)

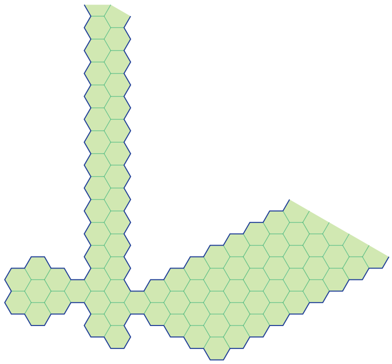
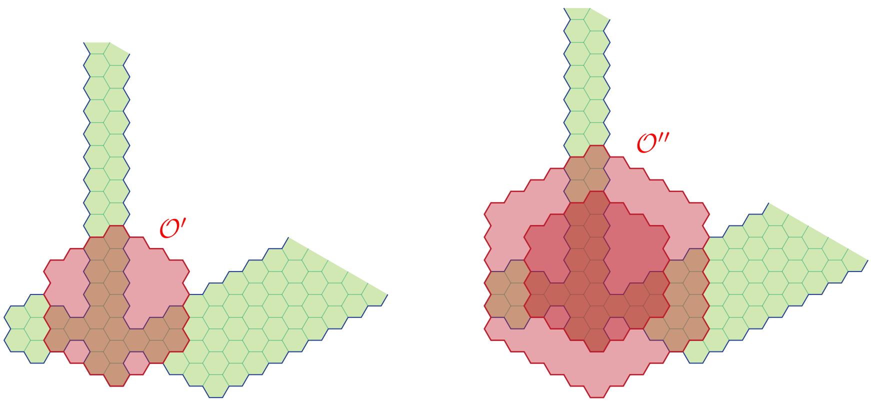


Figure 9: A benzenoid $\mathcal{B} \in \mathcal{FO}$.



(a) (b)

Figure 10: A benzenoid $\mathcal{B} \in \mathcal{FO}$ with $\mathcal{O}'$ and $\mathcal{O}''$.

We can choose a (possibly larger) number $m \geq n$, such that $\mathcal{O}'' = \mathcal{O}_m$ contains $\mathcal{O}'$ and all finite connected components of $\mathcal{B} \setminus \mathcal{O}'$ (see Figure 10(b)). If we remove all edges of $\mathcal{O}''$ from the boundary of $\mathcal{B}$, we obtain an even number of semi-infinite paths. No edge on those semi-infinite paths is an edge that corresponds to a $\mathtt{1}$s in BECs of $\mathcal{B}$, because such edges are all contained in $\mathcal{O}'$. The subsequence of a BEC that corresponds to such a semi-infinite path contains infinitely many 2s, but only a finite number of 3s, 4s and 5s. Those numbers cause bends in the boundary and too many bends would result in a collision of the boundary (see Figure 11), which is impossible. To encode the benzenoid $\mathcal{B}$, we need the

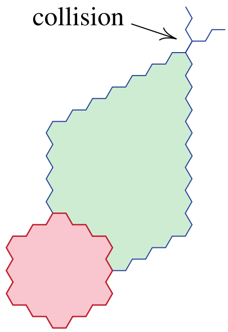


Figure 11: Collision of the boundary of $\mathcal{B}$.

following information:

(i) the number m, which determines the $\mathcal{O}''$ (we have countably many choices),

(ii) the subset of hexagons of $\mathcal{O}''$ that determine $\mathcal{B} \cap \mathcal{O}''$ (there are finitely many such subsets),

(iii) vetices on the boundary of $\mathcal{O}''$ that are starting vertices of semi-infinite paths (finitely many choices),

(iv) positions and types of bends on each semi-infinite path (there are finitely many bends and each type and position can be encoded by a natural number).

From the above encoding of $\mathcal{B}$ it follows that there are countably many different benzenoids in the class $\mathcal{FO}$. □

Corollary 4.9. *There exist countably many mutually non-isomorphic convex infinite benzenoids.*

Proof. By Theorem 4.7, a convex infinite benzenoid is isomorphic to one of those listed in the statement of Theorem 4.7. None of them has a 1 in the boundary-edges code of any connected component of the boundary. Therefore, the class of convex infinite benzenoids is a subclass of $\mathcal{FO}$ and the results follows by Theorem 4.8. □

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Polynomials of degree 4 over finite fields representing quadratic residues*

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Abstract

It is proved that in a finite field F of prime order p, where p is not one of finitely many exceptions, for every polynomial $f(x) \in F[x]$ of degree 4 that has a nonzero constant term and is not of the form $\alpha g(x)^2$ there exists a primitive root $\beta \in F$ such that $f(\beta)$ is a quadratic residue in F. This refines a result of Madden and Vélez from 1982 about polynomials that represent quadratic residues at primitive roots.

Keywords: Finite field, polynomial, quadratic residues.

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1 Introduction

The motivation for this paper is twofold: first refining the result of Madden and Vélez about polynomials that represent quadratic residues at primitive roots [9], and in doing so obtaining a tool with which hamiltonicity of certain families of vertex-transitive graphs of order a product of two primes is proved via a structural analysis of their quotients with respect to an automorphism of prime order. Such a connection between algebraic graph theory and finite fields is not surprising, see, for example, [6, 14] for a similar application of finite fields.

In 1969 Lovász [8] asked for a construction of a finite connected vertex-transitive graph without a Hamilton path, that is, a path containing all vertices of the graph. This problem has spurred quite a bit of interest in the mathematical community, resulting in a number of papers affirming the existence of Hamilton paths and in some cases even Hamilton cycles (see the survey paper [7]). The main obstacle to making a substantial progress with regards to this problem is a lack of structural results for such graphs. Consequently, tools and methods from other areas of mathematics applicable in this context are more than welcome. Such is, for example, the case with the so-called polycirculant conjecture which states that every 2-closed group contains a fixed-point-free automorphism of prime order (see, for example, [3, 4, 10, 12, 13]). Fixed-point-free automorphism of prime order have been of great practical use in constructions of Hamilton cycles in vertex-transitive graphs via the so-called lifting cycle technique [1, 11]. And it is precisely here that the results of this paper are of crucial importance as they allow a successful application of this technique for a complete solution of Lovász problem for connected vertex-transitive graphs of order a product of two primes (see [5]).

More precisely, the goal of this paper is to obtain a novel result on polynomials of degree 4 over finite fields of prime order with regards to a polynomial representation of quadratic residues at primitive roots, thus refining results from [9] (see Theorem 1.1). (The set of nonzero quadratic residues modulo r, that is, nonzero elements of a finite field F of order r that are congruent to a perfect square modulo r, will be called *squares*.)

Theorem 1.1. *Let F be a finite field of prime order p, where p is an odd prime not given in Tables 1 and 2. Then for every polynomial $f(x) \in F[x]$ of degree 4 that has a nonzero constant term and is not of the form $\alpha g(x)^2$ there exists a primitive root $\beta \in F$ such that $f(\beta)$ is a square in F.*

2 Polynomials of degree 4 over finite fields representing quadratic residues

In early eighties, motivated by a question posed by Alspach, Heinrich and Rosenfeld [2] in the context of decompositions of complete symmetric digraphs, Madden and Vélez [9] investigated polynomials that represent quadratic residues at primitive roots. They proved that, with finally many exceptions, for any finite field F of odd characteristic, for every polynomial $f(x) \in F[x]$ of degree $r \geq 1$ not of the form $\alpha g(x)^2$ or $\alpha x g(x)^2$, there exists a primitive root β such that $f(\beta)$ is a nonzero square in F. It is the purpose of this paper to refine their result for polynomials of degree 4. This will then be used in [5] in the constructions of Hamilton cycles for some of the basic orbital graphs arising from the action of $\mathrm{PSL}(2, p)$ on cosets of D_{p-1}. This refinement, stated in Theorem 1.1, will be proved following a series of lemmas.

The following result, proved in [9], is a basis of our argument and will be used throughout this section.

Proposition 2.1 ([9, Corollary 1]). *Let F be a finite field with p^n elements. If s and t are integers such that*

(i) s and t are coprime,

(ii) a prime q divides $p^n - 1$ if and only if q divides st, and

(iii) $2\phi(t)/t > 1 + (rs-2)p^{n/2}/(p^n-1) + (rs+2)/(p^n-1)$,

then, given any polynomial $f(x) \in F[x]$ of degree r, square-free and with nonzero constant term, there exists a primitive root $\gamma \in F$ such that $f(\gamma)$ is a nonzero square in F.

Throughout this section let p be an odd prime and let $q_1 = 2, q_2, \dots, q_m$ be the increasing sequence of prime divisors of $p-1 = q_1^{i_1} q_2^{i_2} \cdots q_m^{i_m}$. As in [9] we define the following functions with respect to this sequence:

$$d(n,m) = 2\left(1 - \frac{1}{q_n}\right)\left(1 - \frac{1}{q_{n+1}}\right)\cdots\left(1 - \frac{1}{q_m}\right), \tag{2.1}$$

$$c_r(n,m) = 2r\sqrt{\frac{q_1 q_2 \cdots q_{n-1}}{q_n q_{n+1} \cdots q_m}}, \tag{2.2}$$

and $k(m)$ as the unique integer such that $d(k(m)-1,m) \le 1 < d(k(m),m)$. Hence $k(m) \ge 2$. Analogously the functions d and c_r can be defined for any positive integers $r \ge 1$, $n < m$ and an arbitrary sequence $\{q_1, \dots, q_m\}$ of primes. The following lemma is a generalization of [9, Lemma 3].

Lemma 2.2. *Let $\{2 = q_1, q_2, \dots, q_m\}$ be a finite sequence of primes satisfying $m \ge 2k(m) + 2$, and let $r = 4$. Then*

$$d(k(m)+1,m) - c_r(k(m)+1,m) > 1. \tag{2.3}$$

Proof. Since $2 \le k(m) \le \frac{m}{2} - 1$, we have $m \ge 6$. Since

$$d(k(m)+1,m) = \left(1 + \frac{1}{q_{k(m)} - 1}\right) d(k(m),m) > 1 + \frac{1}{q_{k(m)} - 1},$$

(2.3) holds if

$$1 + \frac{1}{q_{k(m)} - 1} - 2r\left(\frac{q_1 q_2 \cdots q_{k(m)}}{q_{k(m)+1} q_{k(m)+2} \cdots q_m}\right)^{\frac{1}{2}} > 1,$$

which may be rewritten in the following form

$$q_2 q_3 \cdots q_{k(m)} (q_{k(m)} - 1)^2 < \frac{1}{128} q_{k(m)+1} \cdots q_{m-1} q_m, \tag{2.4}$$

in view of the fact that $r = 4$ and $q_1 = 2$.

We divide the proof into two cases, depending on whether $m \ge 7$ or $m = 6$.

Case 1. $m \geq 7$.

Let Ω be the increasing sequence of all prime numbers and let

$$\mathcal{J}_q = \{q_1 = 2, q_2, q_3, \ldots, q_l = q, q_{l+1}, \ldots, q_m\}$$

be a subsequence of Ω. Then we shall in fact prove a more general result:

$$q_2 q_3 \cdots q_l (q_l - 1)^2 < \frac{1}{128} q_{l+1} \cdots q_{m-1} q_m,$$

where $m \geq 7$ and $l \leq \frac{m}{2} - 1$ is any integer. To show this for the sequence $\mathcal{J}_q$ we define a subsequence $\mathcal{I}_q = \{w_1 = 2, w_2, w_3, \ldots, w_l = q, w_{l+1}, \ldots, w_m\}$ of Ω not missing any prime in Ω from the interval $[w_2, w_m]$. Then the lemma will be proven in case we show that the following holds:

$$w_2 w_3 \cdots w_l (w_l - 1)^2 < \frac{1}{128} w_{l+1} \cdots w_{m-1} w_m, \tag{2.5}$$

where $m \geq 7$ and $l \leq \frac{m}{2} - 1$ is any integer. If $w_m \geq 128$, then (2.5) is clearly true. So we only need to consider primes that are smaller than or equal to 127. If

$$(m - l) - (l - 1 + 2) = m - 2l - 1 \geq 2, \tag{2.6}$$

then (2.5) holds provided $w_{m-1} w_m > 128$ holds. Note that this is true if $w_m \geq 13$, which is the case since $m \geq 7$. Next, note that for either m being even and $l < \frac{m}{2} - 2$ or m being odd, (2.6) holds. So we may assume that m is even and that $l = m/2 - 1 \geq 2$.

Now we prove that (2.5) holds under this assumption for any even integer $m \geq 8$ by induction. Suppose first that $m = 8$. Then $l = 3$ and (2.5) rewrites as

$$w_2 w_3 (w_3 - 1)^2 < \frac{1}{128} w_4 w_5 w_6 w_7 w_8. \tag{2.7}$$

A computer search shows that (2.7) holds for all primes $w_8 \leq 127$. Suppose now that (2.5) is true for an even integer $m \geq 8$. Then we have

$$\begin{aligned} w_2 w_3 w_4 \cdots w_l w_{l+1} (w_{l+1} - 1)^2 &= w_2 (w_3 \cdots w_l w_{l+1} (w_{l+1} - 1)^2) \\ &< w_2 (w_{l+2} w_{l+3} \cdots w_m w_{m+1}) \\ &< (w_{l+2} w_{l+3} \cdots w_m w_{m+1}) w_{m+2}. \end{aligned}$$

Therefore (2.5) is true for all even integers $m \geq 8$ and then for all integers $m \geq 7$. Hence (2.4) holds, and so does (2.3).

Case 2. $m = 6$.

Now $k(m) = 2$. Inserting $l = 2$ and $m = 6$ in (2.5), we have

$$w_2 (w_2 - 1)^2 < \frac{1}{128} w_3 w_4 w_5 w_6. \tag{2.8}$$

A computer search for all the primes less than 131 shows that (2.8) does not hold only for

$$w_{k(m)} = w_2 \in \{11, 13, 17, 19, 23, 29, 31, 37, 41, 43, 53, 59, 61, 67, 71\}.$$

For these exceptional cases, we go back to work on (2.3) directly. Let $l = k(m) = 2$ in $\mathcal{J}_q$. Let $d(n,m)'$ and $c_4(n,m)'$ be the corresponding values for $\mathcal{I}_q$ as defined by functions d and c_r in (2.1) and (2.2). Then one can easily see that $d(3,6)' \le d(3,6)$ and that $c_4(3,6)' \ge c_4(3,6)$, which implies $d(3,6) - c_4(3,6) \ge d(3,6)' - c_4(3,6)'$. Therefore, (2.3) holds for $\mathcal{J}_q$ if it holds for $\mathcal{I}_q$. So it suffices to check (2.3) for $\mathcal{I}_q$. In fact, an additional computer search for the set of primes less than 131 shows that for $w_1 = 2$ and w_2 being each of these exceptional cases, (2.3) holds for $\mathcal{I}_q$. This completes the proof of Lemma 2.2. □

The following result proved in [9] will be needed in the next lemma.

Proposition 2.3 ([9, Lemma 5]). *Let $\{2 = q_1, q_2, \ldots, q_m\}$ be a finite sequence of primes satisfying $m \le 2k(m) + 1$. Then $m \le 9$ and $q_{k(m)-1} \le 5$. In fact the sequence must satisfy one of the following:*

(i) $k(m) = 4$, $q_{k(m)-1} = 5$ *and* $m = 9$,

(ii) $k(m) = 3$, $q_{k(m)-1} = 5$ *and* $m \le 7$,

(iii) $k(m) = 3$, $q_{k(m)-1} = 3$ *and* $m \le 7$, *or*

(iv) $k(m) = 2$, $q_{k(m)-1} = 2$ *and* $m \le 5$.

Lemma 2.4. *Let $\{2 = q_1, q_2, \ldots, q_m\}$ be a finite sequence of primes satisfying $m \le 2k(m) + 1$, and let $p - 1 = q_1^{i_1} q_2^{i_2} \cdots q_m^{i_m}$ with $q_m \ge 131$. Then there exist s and t such that*

(i) *s and t are coprime,*

(ii) *a prime q divides $p-1$ if and only if q divides st, and*

(iii) $2\phi(t)/t > 1 + (4s-2)\sqrt{p}/(p-1) + (4s+2)/(p-1)$.

Proof. Since $m \le 2k(m) + 1$ the four cases (i) – (iv) of Proposition 2.3 need to be considered. In each case, as in [9, Lemma 7], we will prescribe a choice for s (which then determines t uniquely) and use the conditions in each of these four cases to find the lower bound α for the expression $(2\phi(t)t^{-1} - 1)$, that is, $(2\phi(t)t^{-1} - 1) \ge \alpha$. We will then be able to use the assumption $q_m \ge 131$ to show that

$$\alpha > \frac{(4s-2)\sqrt{p} + 4s + 2}{p-1}. \tag{2.9}$$

Suppose first that Proposition 2.3(i) holds, that is, $k(m) = 4$, $q_{k(m)-1} = 5$ and $m = 9$. Then $q_9 \ge 131$. Also, one can easily see that such a sequence of primes must begin with $q_1 = 2$, $q_2 = 3$ and $q_3 = 5$. Let $s = 2 \cdot 3 \cdot 5$ and $t = q_4 q_5 \cdots q_9$. Then

$$\begin{aligned} 2\frac{\phi(t)}{t} - 1 &\ge 2\left(1 - \frac{1}{7}\right)\left(1 - \frac{1}{11}\right)\left(1 - \frac{1}{13}\right)\left(1 - \frac{1}{17}\right)\left(1 - \frac{1}{19}\right)\left(1 - \frac{1}{131}\right) - 1 \\ &\ge 0.27287. \end{aligned}$$

Thus p satisfies (2.9) with $\alpha = 0.27287$ and $s = 30$ if and only if $p > 187899$. Suppose now that there is a prime $p \le 187899$ that satisfies the conditions of the case under analysis. We know that $2 \cdot 3 \cdot 5 \cdot q_9$ divides $p - 1$ with $q_9 \ge 131$. However this requires $q_4 q_5 q_6 q_7 q_8 <$

$187899/(2 \cdot 3 \cdot 5 \cdot 131) \leq 48$ which is clearly not possible, since $q_4q_5q_6q_7q_8 \geq 7 \cdot 11 \cdot 13 \cdot 17 \cdot 19 = 323323$.

We now consider the other three cases of Proposition 2.3, that is, suppose that Proposition 2.3(ii), (iii) or (iv) holds. In all three cases $k(m) \leq 3$. By assumption $q_1 = 2$, and we now consider the various possibilities for q_2. First, assume that $q_2 = 3$ (note that this is possible in the last two cases) and therefore $m \leq 7$. We set $s = 2 \cdot 3$ and $t = q_3q_4q_5q_6q_7$. Thus

$$2\frac{\phi(t)}{t} - 1 \geq 2\left(1-\frac{1}{5}\right)\left(1-\frac{1}{7}\right)\left(1-\frac{1}{11}\right)\left(1-\frac{1}{13}\right)\left(1-\frac{1}{131}\right) - 1 \geq 0.14206.$$

Now p satisfies (2.9) with $\alpha = 0.14206$ and $s = 6$ if and only if $p \geq 24351$. If $p < 24351$ we see that $q_3q_4 \cdots q_{m-1} < 24351/(2{\cdot}3{\cdot}131) < 31$. Since $q_i \geq 5$ for $i \in \{3, 4, \dots, m-1\}$ one can see that either $m = 3$ or $m = 4$. In other words, either $t = q_3$ or $t = q_3q_4$, and thus we can improve the value for α with

$$2\frac{\phi(t)}{t} - 1 \geq 2\left(1-\frac{1}{5}\right)\left(1-\frac{1}{131}\right) - 1 \geq 0.58778.$$

In this case p satisfies (2.9) with $\alpha = 0.58778$ if and only if $p > 1490$. If $p \leq 1490$ observe that the assumption that $6q_m$ divides $p-1$ with $q_m \geq 131$ implies that $q_3 < 2$, a contradiction.

We now use the same approach for the case $q_2 = 5$. We choose $s = 2 \cdot 5$ and $t = q_3q_4 \cdots q_m$. Here we have

$$2\frac{\phi(t)}{t} - 1 \geq 2\left(1-\frac{1}{7}\right)\left(1-\frac{1}{11}\right)\left(1-\frac{1}{13}\right)\left(1-\frac{1}{17}\right)\left(1-\frac{1}{131}\right) - 1 \geq 0.34361.$$

Hence p satisfies (2.9) with $\alpha = 0.34361$ if and only if $p > 12475$. If, however, $p \leq 12475$ then since $10q_m$ divides $p-1$ we have that $q_3 < 10$, and so either $m = 3$ or $m = 4$ and $q_3 = 7$. In both cases we can improve the value for α since $t = q_2q_3$ or $t = q_3q_4$. In particular,

$$2\frac{\phi(t)}{t} - 1 \geq 2\left(1-\frac{1}{7}\right)\left(1-\frac{1}{131}\right) - 1 \geq 0.70119956.$$

In this case p satisfies (2.9) with $\alpha = 0.70119956$ if and only if $p > 3057$. If $p \leq 3057$ observe that the assumption that $10q_m$ divides $p-1$ with $q_m \geq 131$ implies that $q_3 < 3$, a contradiction.

Finally we consider the case $q_2 \geq 7$. Then, by Proposition 2.3, we have $k(m) = 2$ and $m \leq 5$. Here we choose $s = 2$ and use the same technique as above to complete the proof. In particular, we have

$$2\frac{\phi(t)}{t} - 1 \geq 2\left(1-\frac{1}{7}\right)\left(1-\frac{1}{11}\right)\left(1-\frac{1}{13}\right)\left(1-\frac{1}{131}\right) - 1 \geq 0.42758.$$

In this case p satisfies (2.9) with $\alpha = 0.42758$ if and only if $p > 243$. If $p \leq 243$ observe that the assumption that $2q_m$ divides $p-1$ with $q_m \geq 131$ implies that $q_3 < 2$, a contradiction.

In summary we have seen that given any finite sequence of primes with $q_m \geq 131$ we can choose n in such a way that when $s = q_1q_2 \cdots q_n$ and $t = q_{n+1}q_{n+2} \cdots q_m$ we have

$$\frac{2\phi(t)}{t} > 1 + \frac{(4s-2)\sqrt{st+1}}{st} + \frac{4s+2}{st}, \tag{2.10}$$

completing the proof of Lemma 2.4. $\square$

In order to proceed with the proof of Theorem 1.1 we now need to identify all those sequences $\{2 = q_1, q_2, \ldots, q_m\}$ with $q_m < 131$ for which one cannot choose $s = q_1 q_2 \cdots q_n$ and $t = q_{n+1} q_{n+2} \cdots q_m$ so as to satisfy (2.10). Since Lemma 2.2 holds for each q_m we can assume that for each of these sequences Proposition 2.3 applies. A computer search of these finitely many sequences yields the exceptional sequences which are listed in Tables 1 and 2. For each of these exceptional sequences we fix $s = q_1 q_2 \cdots q_n$ and $t = q_{n+1} q_{n+2} \cdots q_m$, and we then search for a constant k such that $x > k$ implies the inequality

$$\frac{2\phi(t)}{t} > 1 + \frac{2(2s-1)\sqrt{x}}{x-1} + \frac{4s+2}{x-1}. \tag{2.11}$$

For each of these sequences Tables 1 and 2 give the smallest bound k obtained in this way. The third column of these tables indicates for which choice of t the given bound k is obtained:

Type 1 means that the bound k was obtained with $t = q_{m-1} q_m$,

Type 2 means that the bound was obtained with $t = q_m$, and

Type 3 means that the bound was obtained with $t = 1$.

A computer search then identifies those primes that are smaller than or equal to the bound k, as summarized in the proposition below.

Proposition 2.5. *Let $\{2 = q_1, q_2, \ldots, q_m\}$ be a finite sequence of primes satisfying $m \le 2k(m) + 1$, and let $p - 1 = q_1^{i_1} q_2^{i_2} \cdots q_m^{i_m}$ with $q_m < 131$. If p is not listed in Tables 1 and 2 then there exist s and t such that*

(i) s and t are coprime,

(ii) a prime q divides $p - 1$ if and only if q divides st, and

(iii) $2\phi(t)/t > 1 + (4s-2)\sqrt{p}/(p-1) + (4s+2)/(p-1)$.

We are now ready to prove Theorem 1.1.

Proof of Theorem 1.1. It follows by Proposition 2.1 that a polynomial $f(x)$ represents a nonzero square at some primitive root in F if there exist s and t satisfying the following three conditions:

(i) s and t are coprime,

(ii) a prime q divides $p - 1$ if and only if q divides st, and

(iii) $2\phi(t)/t > 1 + (4s-2)\sqrt{p}/(p-1) + (4s+2)/(p-1)$.

Our goal is therefore to show that such s and t exist for all odd primes p that are not listed in Tables 1 and 2.

Let $\{q_1 = 2, q_2, \ldots, q_m\}$ be an increasing sequence of prime divisors of $p - 1$. If $m \le 2k(m) + 1$ then Lemma 2.4 applies for $q_m \ge 131$, and Proposition 2.5 applies for $q_m < 131$.

Table 1: The list of sequences not satisfying (2.10), part I.

Sequence $\mathcal{T}$	k	Type	$p \leq k$ with $\mathcal{T}$	$p \equiv 1 \pmod 4) \leq k$ with $\mathcal{T}$, $(p+1)/2$ prime
2	55	3	$3, 5, 17$	5
$2, 3, 5, 11$	2458	1	$331, 661, 991, 1321$	$661, 1321$
$2, 3, 5, 43$	1622	1	1291	no
$2, 3, 7, 17$	1372	1	no	no
$2, 3, 5, 7, 13$	7040	$t = 455$	2731	no
$2, 3, 43$	460	1	no	no
$2, 3, 31$	496	1	373	no
$2, 3, 61$	435	1	367	no
$2, 3, 5, 7, 23$	5145	$t = 805$	4831	no
$2, 3, 23$	547	1	$139, 277$	277
$2, 3, 67$	430	1	no	no
$2, 3, 7, 13$	1517	1	$547, 1093$	1093
$2, 3, 17$	632	1	$103, 307, 409, 613$	613
$2, 3, 5, 13$	2238	1	$1171, 1951$	no
$2, 3, 11$	788	2	$67, 199, 397, 727$	397
$2, 7$	99	2	29	no
$2, 3, 13$	739	2	$79, 157, 313$	$157, 313$
$2, 3, 7$	1023	2	$43, 127, 337, 379,$ $673, 757, 883, 1009$	$673, 757$
$2, 23$	65	2	47	no
$2, 3, 5, 37$	1656	1	no	no
$2, 5$	133	2	$11, 41, 101$	no
$2, 3, 5, 41$	1632	1	1231	no
$2, 3, 59$	437	1	no	no
$2, 3, 53$	444	1	no	no
$2, 3, 7, 19$	1327	1	no	no
$2, 3, 5, 29$	1727	1	no	no
$2, 17$	69	2	no	no
$2, 11$	78	2	23	no
$2, 3, 5, 19$	1921	1	571	no
$2, 3, 41$	464	1	no	no

Suppose now that $m \geq 2k(m) + 2$. Then, by Lemma 2.2, we have

$$d(k(m) + 1, m) > 1 + c_4(k(m) + 1, m).$$

If we let $s = q_1 q_2 \cdots q_{k(m)}$ and $t = q_{k(m)+1} \cdots q_m$ we have $2\phi(t)/t = d(k(m) + 1, m)$,

Table 2: The list of sequences not satisfying (2.10), part II.

Sequence $\mathcal{T}$	k	Type	$p \le k$ with $\mathcal{T}$	$p \equiv 1 \pmod 4) \le k$ with $\mathcal{T}$, $(p+1)/2$ prime
$2,3,5,7,11$	8160	$t = 385$	$2311, 4621$	4621
$2,3,5$	1432	2	$31, 61, 151, 181, 241, 271, 541, 601, 751, 811, 1201$	$61, 541, 1201$
$2,3,5,47$	1604	1	no	no
$2,3,5,31$	1705	1	no	no
$2,3,7,23$	1265	1	967	no
$2,5,17$	180	1	no	no
$2,3,11,13$	1130	1	859	no
$2,13$	74	2	53	no
$2,5,11$	218	1	no	no
$2,5,13$	200	1	131	no
$2,3,37$	475	1	223	no
$2,3,5,7$	3649	1	$211, 421, 631, 1051, 1471, 2521, 3361$	421
$2,3,5,7,19$	5580	$t = 665$	no	no
$2,3$	384	2	$7, 13, 19, 37, 73, 97, 109, 163, 193$	$13, 37, 73, 193$
$2,5,7$	315	1	$71, 281$	no
$2,3,5,23$	1819	1	$691, 1381$	1381
$2,3,47$	453	1	283	no
$2,3,5,7,17$	5905	$t = 595$	3571	no
$2,3,29$	506	1	349	no
$2,3,7,11$	1646	1	463	no
$2,3,5,17$	1995	1	$1021, 1531$	no
$2,29$	63	2	59	no
$2,3,19$	596	1	$229, 457$	457
$2,19$	68	2	no	no

and

$$
\begin{aligned}
c_4(k(m)+1, m) &= 8 \cdot \sqrt{\frac{q_1 q_2 \cdots q_{k(m)}}{q_{k(m)+1} q_{k(m)+2} \cdots q_m}} \\
&= \frac{8s}{\sqrt{q_1 q_2 \cdots q_m}} \ge \frac{8s}{\sqrt{p-1}}
\end{aligned}
$$

Since s is even and $4(p-1) \ge 4s \ge 3$ we may apply [9, Lemma 6] to see that

$$
\frac{(4s-2)\sqrt{p}}{p-1} \le \frac{4s}{\sqrt{p-1}}.
$$

It follows that

$$\frac{2\phi(t)}{t} = d(k(m)+1,m) \geq 1 + c_4(k(m)+1,m) \geq 1 + \frac{8s}{\sqrt{p-1}}$$
$$\geq 1 + \frac{(4s-2)\sqrt{p}}{p-1} + \frac{4s+2}{p-1}.$$

(Note that the last inequality holds since $p \geq 7$.) □

For the sake of completeness we would like to add the following proposition (obtained with a computer search) which deals with exceptional primes p not covered by Theorem 1.1 which are congruent to 1 modulo 4 and for which $(p+1)/2$ is also a prime (primes given in the last column of Tables 1 and 2). As is the case with Theorem 1.1 this proposition too is used in the construction of Hamilton cycles in vertex-transitive graphs of order a product of two primes in [5].

Proposition 2.6. *Let F be a finite field of odd prime order p, and let $k \in F$. If*

$$p \in \{5, 13, 37, 61, 73, 157, 193, 277, 313, 397, 421, 457, 541,$$
$$613, 661, 673, 757, 1093, 1201, 1321, 1381, 4621\}$$

then there exists a primitive root β of F such that $f(\beta) = \beta^4 + k\beta^2 + 1$ is a square in F except when

$$(p,k) \in \{(5,4), (13,1), (13,4), (13,5), (13,6), (13,7), (13,10),$$
$$(37,3), (37,28), (37,29), (61,18), (61,37), (61,40)\}.$$

Amongst these exceptions only for $(p,k) \in \{(13,1), (37,28), (61,18)\}$ there exists $\xi \in S^* \cap (S^*+1)$ such that $k = 2(1-2\xi)$. In particular, $\xi = 10$ for $(p,k) = (13,1)$, $\xi = 12$ for $(p,k) = (37,28)$, and $\xi = 57$ for $(p,k) = (61,18)$. Moreover, amongst these exceptions only for $(p,k) \in \{(13,1), (37,28), (61,18)\}$ there exists $\bar{\xi} \in S^* \cap (S^*+1)$ such that $k = -2(1-2\bar{\xi})$. In particular, $\bar{\xi} = 4$ for $(p,k) = (13,1)$, $\bar{\xi} = 26$ for $(p,k) = (37,28)$, and $\bar{\xi} = 5$ for $(p,k) = (61,18)$.

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