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ADAM, An Offspring Journal is Here!

In view of an increased flow of submitted manuscripts the Editors are often faced with a dilemma: should we consider articles that belong to pure graph theory with no connection to other branches of discrete mathematics? At the other extreme, some submissions are very applied, a lot like those from mathematical chemistry or chemical graph theory. Sometimes the topics of submitted manuscripts are somewhat far from the scope of the journal. Should they undergo a refereeing procedure anyway? And finally, the journal is experiencing a very fast growth. While In 2008 only 20 articles were published, eight years later the number of articles has increased to 61 with a backlog of about 100 papers. We are at a crossroads, something needs to be done.

We decided to launch an offspring, a purely electronic journal and we named it: **The Art of Discrete and Applied Mathematics** (ADAM). In the preparation stage it is run by the same editorial board as AMC, on the same OJS platform. We are starting considering papers for ADAM as of now. Until the first articles are reviewed by MathSciNet and Zentralblatt, we will give authors a choice as to which of the two journals they want to consider for their publication. When the first articles from ADAM are listed in the Web of Science, however, the Editors will decide which journal is more appropriate for a particular accepted paper. There is no doubt that initially ADAM will have lower visibility than AMC but the back-log will be much, much lower. In the long run both journals will benefit.

ADAM will be published by the University of Primorska and by the Slovenian Society for Discrete and Applied Mathematics, with the first volume appearing in 2018. Gradually the structure of its editorial board will be adjusted to the submitted topics. Nevertheless we would like to reiterate that our main goal remains the same. We are committed to publishing excellent contemporary mathematics.

Dragan Marušič and Tomaž Pisanski Editors In Chief



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An algebraic proof of the Erdős-Ko-Rado theorem for intersecting families of perfect matchings

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Abstract

In this paper we give a proof that the largest set of perfect matchings, in which any two contain a common edge, is the set of all perfect matchings that contain a fixed edge. This is a version of the famous Erdős-Ko-Rado theorem for perfect matchings. The proof given in this paper is algebraic, we first determine the least eigenvalue of the perfect matching derangement graph and then use properties of the perfect matching polytope to prove the result.

Keywords: Perfect matching derangement graph, independent sets, Erdős-Ko-Rado theorem. Math. Subj. Class.: 05C35, 05C69

1 Introduction

A perfect matching in the complete graph K_{2k} is a set of k vertex disjoint edges. Two perfect matchings intersect if they contain a common edge. In this paper we use an algebraic method to prove that the natural version of the Erdős-Ko-Rado (EKR) theorem holds for perfect matchings. This theorem shows that the largest set of perfect matchings, with the property that any two intersect, is the set of the all perfect matchings that contain a specific edge.

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The algebraic method in this paper is similar to the proof that the natural version of the EKR theorem holds for permutations in [4]. In this paper we determine the least eigenvalue for the perfect matching derangement graph. This, with the Delsarte-Hoffman bound, implies that a maximum intersecting set of perfect matchings corresponds to a facet in the perfect matching polytope. The characterization of the maximum set of intersecting perfect matchings follows from the characterization of the facets of this polytope.

Meagher and Moura [8] proved a version of the EKR theorem holds for intersecting uniform partitions using a counting argument [8]. This result includes the EKR theorem for perfect matchings. It is interesting that the counting argument in [8] is straight-forward, except for the case of perfect matchings; in this case a more difficult form of the counting method is necessary.

2 Perfect matchings

A *perfect matching* is a set of vertex disjoint edges in the complete graph K_{2k} . This is equivalent to a partition of a set of size 2k into k-disjoint classes, each of size 2. The number of perfect matchings in K_{2k} is

$$\frac{1}{k!} \binom{2k}{2} \binom{2k-2}{2} \cdots \binom{2}{2} = (2k-1)(2k-3)\cdots 1$$

For an odd integer n define

$$n!! = n(n-2)(n-4)\cdots 1.$$

With this notation, there are (2k - 1)!! perfect matchings.

We say that two perfect matchings are intersecting if they both contain a common edge. Further, a set of perfect matchings is intersecting if the perfect matchings in the set are pairwise intersecting. If e represents a pair from $\{1, \ldots, 2k\}$, then e is an edge of K_{2k} . Define S_e to be the set of all perfect matchings that include the edge e. For any edge e, the set S_e is intersecting. Any set S_e , where e is a pair from $\{1, \ldots, 2k\}$, is called a *canonically intersecting* set of perfect matchings. For every e

$$|S_e| = (2k - 3)!! = (2k - 3)(2k - 5) \cdots 1.$$

The main result of this paper can be stated as follows.

Theorem 2.1. The largest set of intersecting perfect matchings in K_{2k} has size (2k-3)!!. The only sets that meet this bound are the canonically intersecting sets of perfect matchings.

3 Perfect matching derangement graph

One approach to proving EKR theorems for different objects is to define a graph where the vertices are the objects and two objects are adjacent if and only if they are not intersecting (see [4, 9, 15] for just a few examples of where this is done). This is the approach that we take with the perfect matchings.

We use the standard graph notation. A *clique* in a graph is a set of vertices in which any two are adjacent; a *coclique* is a set of vertices in which no two are adjacent. If X is a graph, then $\omega(X)$ denotes the size of the largest clique, and $\alpha(X)$ is the size of the largest coclique. A graph is *vertex transitive* if its automorphism group is transitive on the vertices. For a vertex-transitive graph, there is a relationship between the maximum clique size and maximum coclique size known as the *clique-coclique bound*. The next result is this bound.

Theorem 3.1. Let X be a vertex-transitive graph, then

$$\alpha(X)\,\omega(X) \le |V(X)|.$$

The *eigenvalues* of a graph are the eigenvalues of the adjacency matrix of the graph. Similarly, the eigenvectors and eigenspaces of the graph are the eigenvectors and eigenspaces of the adjacency matrix.

Define the *perfect matching derangement graph* M(2k) to be the graph whose vertices are all perfect matchings on K_{2k} and vertices are adjacent if and only if they have no common edges. Theorem 2.1 is equivalent to the statement that the size of the maximum coclique in M(2k) is (2k - 3)!! and that only the canonically intersecting sets meet this bound.

The number of vertices in M(2k) is (2k - 1)!!. The degree of M(2k), denoted by d(2k), is the number of perfect matchings that do not contain any the edges from some fixed perfect matching. This number can be calculated using the principle of inclusion-exclusion:

$$d(2k) = \sum_{i=0}^{k-1} (-1)^i \binom{k}{i} (2k-2i-1)!!.$$
(3.1)

In practice, this formula can be tricky to use, but we will make use the following simple lower bound on d(2k).

Lemma 3.2. For any k

$$d(2k) > (2k-1)!! - \binom{k}{1}(2k-3)!!.$$

Proof. For any $i \in \{0, ..., k - 1\}$

$$\binom{k}{i}(2k-2i-1)!! = \frac{i+1}{k-i}\binom{k}{i+1}(2k-2i-1)(2k-2(i+1)-1)!!$$
$$> \binom{k}{i+1}(2k-2(i+1)-1)!!$$

(since $\frac{i+1}{k-i}(2k-2i-1) > 1$ for these values of *i*). This implies that the terms in Equation 3.1 are strictly decreasing in absolute value. Since it is an alternating sequence, the first two terms give a lower bound on d(2k).

Next we give some simple properties of the perfect matching derangement graph, including a simple proof of the bound in Theorem 2.1 that uses the clique-coclique bound.

Theorem 3.3. Let M(2k) be the perfect matching derangement graph.

- 1. The graph M(2k) is vertex transitive, and Sym(2k) is a subgroup of the automorphism group of M(2k).
- 2. The size of a maximum clique in M(2k) is 2k 1.

3. The size of a maximum coclique in M(2k) is (2k-3)!!.

Proof. It is clear that the group Sym(2k) acts transitively on the perfect matchings and, though this action, each permutation in Sym(2k) gives an automorphism of M(2k).

Let C be a clique in M(2k). For every perfect matching in C, the element 1 is matched with a different element of $\{2, 3, ..., 2k\}$. Thus the size of C is no more than 2k - 1. A 1-factorization of the complete graph on 2k vertices is a clique of size $\frac{1}{k} {\binom{2k}{2}}$ in M(2k). Since a 1-factorization of K_{2k} exists for every k, the size of the maximum clique is exactly $\frac{1}{k} {\binom{2k}{2}} = 2k - 1$.

Since M(2k) is vertex transitive, the clique-coclique bound, Theorem 3.1, holds so

$$\alpha(M(2k)) \le \frac{(2k-1)!!}{\frac{1}{k}\binom{2k}{2}} = (2k-3)!!.$$

Since the size of any canonically intersecting set meets this bound, we have that

$$\alpha(M(2k)) = (2k - 3)!!.$$

4 Perfect matching association scheme

We have noted that the group Sym(2k) acts on the set of perfect matchings. Under this action, the stabilizer of a single perfect matching is isomorphic to the wreath product of Sym(2) and Sym(k). This is a subgroup of Sym(2k) and is denoted by $Sym(2) \wr Sym(k)$. Thus the set of perfect matchings in K_{2k} correspond to the set of cosets

$$\operatorname{Sym}(2k)/(\operatorname{Sym}(2) \wr \operatorname{Sym}(k)).$$

This implies that the action of Sym(2k) on the perfect matchings is equivalent to the action of Sym(2k) on the cosets $\text{Sym}(2k)/(\text{Sym}(2) \wr \text{Sym}(k))$. This action produces a permutation representation of Sym(2k). We will not give much detail on the representation theory of the symmetric group, rather we will simply state the results that we need a refer the reader to any standard text on the representation theory of the symmetric group, such as [1, 3, 7, 12].

Each irreducible representation of Sym(2k) corresponds to an integer partition $\lambda \vdash 2k$; these representations will be written as χ_{λ} and the character will be denoted by χ_{λ} . The Sym(2k)-module will be denoted by V_{λ} . Information about the representation is contained in the partition. For example, the dimension of the representation can be found just from the partition using the *hook length formula*.

For any group G, the trivial representation of G is denoted by $\mathbf{1}_G$ (and the character by $\mathbf{1}_G$). If $\boldsymbol{\chi}$ is a representation of a group $H \leq \operatorname{Sym}(n)$, then $\operatorname{ind}_{\operatorname{Sym}(n)}(\boldsymbol{\chi})$ is the representation of $\operatorname{Sym}(n)$ induced by $\boldsymbol{\chi}$. Similarly, if $\boldsymbol{\chi}$ is a representation of $\operatorname{Sym}(n)$, then $\operatorname{res}_H(\boldsymbol{\chi})$ is the restriction of $\boldsymbol{\chi}$ to H. The permutation representation of $\operatorname{Sym}(2k)$ acting on $\operatorname{Sym}(2k)/(\operatorname{Sym}(2) \wr \operatorname{Sym}(k))$ is the representation induced on $\operatorname{Sym}(2k)$ by the trivial representation on $\operatorname{Sym}(2) \wr \operatorname{Sym}(k)$ which is denoted by $\operatorname{ind}_{\operatorname{Sym}(2k)}(\mathbf{1}_{\operatorname{Sym}(2)\wr\operatorname{Sym}(k)})$ (see [5, Chapter 13] for more details).

For an integer partition $\lambda \vdash k$ with $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_\ell)$, let 2λ denote the partition $(2\lambda_1, 2\lambda_2, \dots, 2\lambda_\ell)$ of 2k. It is well-known (see, for example, [13, Example 2.2]) that

decomposition of the permutation representation of Sym(2k) from its action on the perfect matchings is

$$\operatorname{ind}_{\operatorname{Sym}(2k)}(\mathbf{1}_{\operatorname{Sym}(2)\wr\operatorname{Sym}(k)}) = \sum_{\lambda \vdash k} \chi_{2\lambda}.$$

The multiplicity of each irreducible representation in this decomposition is one, this implies that $\operatorname{ind}_{\operatorname{Sym}(2k)}(\mathbf{1}_{\operatorname{Sym}(2)\wr\operatorname{Sym}(k)})$ is a *multiplicity-free representation*. This implies that the adjacency matrices of the orbitals from the action of $\operatorname{Sym}(2k)$ on the cosets $\operatorname{Sym}(2k)/(\operatorname{Sym}(2)\wr\operatorname{Sym}(k))$ defines an association scheme on the perfect matchings (see [5, Section 13.4] for more details and a proof of this result). This association scheme is known as the *perfect matching scheme*. Each class in this scheme is labelled with a partition $2\lambda = (2\lambda_1, 2\lambda_2, \ldots, 2\lambda_\ell)$. Two perfect matchings are adjacent in a class if their union forms a set of ℓ cycles with lengths $2\lambda_1, 2\lambda_2, \ldots, 2\lambda_\ell$ (this association scheme is described in more detail in [5, Section 15.4] and [10]).

The graph M(2k) is the union of all the classes in this association scheme in which the corresponding partition contains no part of size two. This means that each eigenspace of M(2k) is the union of modules of Sym(2k); each module in this union is a Sym(2k)module $V_{2\lambda}$ where $\lambda \vdash k$. If ξ is an eigenvalue of M(2k), and its eigenspace includes the Sym(2k)-module $V_{2\lambda}$, then we say that ξ is the eigenvalue for $V_{2\lambda}$. Conversely, we denote the eigenvalue for $V_{2\lambda}$ by $\xi_{2\lambda}$.

The next lemma contains a formula to calculate the eigenvalue for the Sym(2k)-module $V_{2\lambda}$. This gives considerable information about the eigenvalues of M(2k). For a proof the general form of this formula see [5, Section 13.8], we only state the version specific to perfect matchings. If M denotes a perfect matching and $\sigma \in \text{Sym}(2k)$, we will use M^{σ} to denote the matching formed by the action of σ on M.

Lemma 4.1. Let M be a fixed perfect matching in K_{2k} . Let $H \subseteq \text{Sym}(2k)$ be the set of all elements $\sigma \in \text{Sym}(2k)$ such that M and M^{σ} are not intersecting. The eigenvalue of M(2k) for the Sym(2k)-module $V_{2\lambda}$ is

$$\xi_{2\lambda} = \frac{d(2k)}{2^k k!} \sum_{x \in H} \chi_{2\lambda}(x).$$

The Sym(2k)-module $V_{2\lambda}$ is a subspace of the $\xi_{2\lambda}$ -eigenspace and the dimension of this subspace is $\chi_{2\lambda}(1)$.

This formula can be used to calculate the eigenvalue corresponding to a module for the matching derangement graph, but it is not effective to determine all the eigenvalues for a general matching derangement graph. In Section 6 we will show another way to find some of the eigenvalues.

5 Delsarte-Hoffman bound

In Section 6, we will give an alternate proof of the bound in Theorem 2.1 that uses the eigenvalues of the matching derangement graph. This proof is based on the Delsarte-Hoffman bound, which is also known as the ratio bound. The advantage of this bound is that when equality holds we get additional information about the cocliques of maximum size. This information can be used to characterize all the sets that meet the bound. The Delsarte-Hoffman bound is well-known and there are many references, we offer [5, Theorem 2.4.1] for a proof. **Theorem 5.1.** Let X be a k-regular graph with v vertices and let τ be the least eigenvalue of A(X). Then

$$\alpha(X) \le \frac{v}{1 - \frac{k}{\tau}}$$

If equality holds for some coclique S with characteristic vector v_S , then

$$v_S - \frac{|S|}{|V(X)|} \mathbf{1}$$

is an eigenvector with eigenvalue τ .

If equality holds in the Delsarte-Hoffman bound, we say that the maximum cocliques are ratio tight.

The Delsarte-Hoffman bound can be used to prove the EKR theorem for sets. Similar to the situation for the perfect matchings, the group Sym(n) acts on the subsets of $\{1, \ldots, n\}$ of size k. This action is equivalent to the action of Sym(n) on the cosets $Sym(n)/(Sym(n-k) \times Sym(k))$. This action corresponds to a permutation representation, namelv

$$\operatorname{ind}_{\operatorname{Sym}(n)}(\mathbf{1}_{\operatorname{Sym}(n-k)\times\operatorname{Sym}(k)}) = \sum_{i=0}^{k} \chi_{[n-i,i]}.$$
(5.1)

(Details can be found in any standard text on the representation theory of the symmetric group.) This representation is multiplicity free and the orbital schemes from this action is an association scheme better known as the Johnson scheme.

The *Kneser graph* K(n, k) is the graph whose vertices are all the k-sets from $\{1, \ldots, n\}$ and two vertices are adjacent if and only if they are disjoint. The Kneser graph is a graph in the Johnson scheme, it is the graph that corresponds to the orbitals of pairs of sets that do not intersect. A coclique in K(n, k) is a set of intersecting k-sets. The Kneser graph is very well-studied and all of its eigenvalues are known (see [6, Chapter 7] or [5, Section 6.6] for a proof).

Proposition 5.2. The eigenvalues of K(n, k) are

$$(-1)^i \binom{n-k-i}{r-i}$$

with multiplicities $\binom{n}{i} - \binom{n}{i-1}$ for $i \in \{0, \ldots, k\}$.

If we apply the Delsarte-Hoffman bound to K(n, k) we get the following theorem which is equivalent to the standard EKR theorem. The characterization follows from the second statement in the Delsarte-Hoffman bound, see [5, Section 6.6] for details.

Theorem 5.3. Assume that n > 2k. The size of the largest coclique in K(n,k) is $\binom{n-1}{k-1}$, and the only cocliques of this size consist of all k-sets that contain a common fixed element.

To apply the Delsarte-Hoffman bound to M(2k), we first need to determine the value of the least eigenvalue of M(2k). We do not calculate all the eigenvalues of M(2k), rather we calculate the two eigenvalues with the largest absolute value and then show that all other eigenvalues have smaller absolute value.

6 Eigenvalues of the matching derangement graph

In this section we determine the largest and the least eigenvalue of the matching derangement graph. Further, we identify the modules that the eigenvalues are for. First we will use a simple method to show that these two values are eigenvalues of M(2k).

For any edge e in K_{2k} , the partition $\pi = \{S_e, V(M(2k))/S_e\}$ is an equitable partition of the vertices in M(2k). In fact, π is the orbit partition formed by the stabilizer of the edge e in Sym(2k) (this subgroup is isomorphic to Sym $(2) \times$ Sym(2k - 2)) acting on the set of all vertices of M(2k). Each vertex in S_e is adjacent to no other vertices in S_e (since it is a coclique), and is adjacent to exactly d(2k) vertices in $V(M(2k))/S_e$. A straight-forward counting argument shows that each vertex in $V(M(2k))/S_e$ is adjacent to exactly d(2k)/(2k-2) vertices in S_e , and thus to d(2k) - d(2k)/(2k-2) other vertices in $V(M(2k))/S_e$. This implies that the quotient graph of M(2k) with respect to the partition π is

$$M(2k)/\pi = \begin{pmatrix} 0 & d(2k) \\ \frac{1}{2k-2} d(2k) & \frac{2k-3}{2k-2} d(2k) \end{pmatrix}.$$

The eigenvalues for the quotient graph $M(2k)/\pi$ are

$$d(2k), \qquad -\frac{d(2k)}{2k-2}$$

Since π is equitable, these are also eigenvalues of M(2k). The next result identifies the modules which the eigenvalues are for.

Lemma 6.1. The eigenvalue of M(2k) for the Sym(2k)-module $V_{[2k]}$ is d(2k), and the eigenvalue of M(2k) for the Sym(2k)-module $V_{[2k-2,2]}$ is -d(2k)/(2k-2).

Proof. The first statement is clear using the formula in Lemma 4.1.

To prove the second statement, we will consider the equitable partition π defined above. The partition π is the orbit partition of $\text{Sym}(2) \times \text{Sym}(2k-2)$ acting on the perfect matchings. Let $H = \text{Sym}(2) \times \text{Sym}(2k-2)$ and denote the cosets of H in Sym(2k) by $\{x_0H = H, x_1H, \dots, x_{2k^2-k-1}H\}$.

The -d(2k)/(2k-2)-eigenvector of $M(2k)/\pi$ lifts to an eigenvector v of M(2k). A simple calculation shows that the entries of v are $1 - \frac{1}{2k-1}$ or $-\frac{1}{2k-1}$, depending on if the index of the entry is in S_e , or not. This means that $v = v_e - \frac{1}{2k-1}\mathbf{1}$, where v_e is the characteristic vector of S_e .

The group $\operatorname{Sym}(2k)$ acts on the edges of K_{2k} , and for each $\sigma \in \operatorname{Sym}(2k)$, we can define

$$v^{\sigma} = v_{e^{\sigma}} - \frac{1}{2k-1}\mathbf{1}.$$

Under this action, the vector v is fixed by any permutation in H. If we define

$$V = \operatorname{span}\{v^{\sigma} : \sigma \in \operatorname{Sym}(2k)\},\$$

then V is a subspace of the -d(2k)/(2k-2)-eigenspace. Moreover, V is invariant under the action of Sym(2k), so it is also a Sym(2k)-module. To prove this lemma we need to show that V is isomorphic to the Sym(2k)-module $V_{[2k-2,2]}$.

Let W be the Sym(2k)-module for the induced representation $\operatorname{ind}_{\operatorname{Sym}(2k)}(\mathbf{1}_H)$. By Equation 5.1, W is the sum of irreducible modules of Sym(2k) that are isomorphic to $M_{[2k]}, M_{[2k-1,1]}$ and $M_{[2k-2,2]}$. The vector space W is isomorphic to the vector space of functions $f \in L(\operatorname{Sym}(2k))$ that are constant on H. For each coset xH, let $\delta_{xH}(\sigma)$ be the characteristic function for xH; so $\delta_{xH}(\sigma)$ is defined to be equal to 1 if σ is in xH, and 0 otherwise. Since W is the $\operatorname{Sym}(2k)$ -module for the representation induced by $\mathbf{1}_H$, the functions δ_{xH} form a basis for W (see [5, Section 11.13] for details).

Define the map $f: V \to W$ so that

$$f(v^{\sigma}) = \delta_{\sigma H} - \frac{1}{2k-1} \sum_{i=0}^{2k^2 - k - 1} \delta_{x_i H}.$$

Since $v^{\sigma} = v^{\pi}$ if and only if $\sigma H = \pi H$, this function is well-defined. Further, it is a Sym(2k)-module homomorphism. Thus V is isomorphic to a submodule of W. Since V is not trivial, it must be the Sym(2k)-module $V_{[2k-2,2]}$, since it is the only module (other than the trivial) that is common to both $\operatorname{ind}_{\operatorname{Sym}(2k)}(\mathbf{1}_H)$ and $\operatorname{ind}_{\operatorname{Sym}(2k)}(\mathbf{1}_{\operatorname{Sym}(k)})$. \Box

We have found two of the eigenvalues of M(2k), next we will show that all the remaining eigenvalues are smaller in absolute value. We need the following theorem by Rasala [11] that gives bounds on the dimension of the irreducible representations of Sym(n).

Theorem 6.2. For $n \ge 15$, the irreducible representations with the seven smallest degrees are given in the following table.

Representations	Degree
$[n], [1^n]$	1
$[n-1,1], [2,1^{n-2}]$	n-1
$[n-2,2], [2,2,1^{n-4}]$	$\frac{1}{2}n(n-3)$
$[n-2,1,1], [3,1^{n-3}]$	$\frac{1}{2}(n-1)(n-2)$
$[n-3,3], [2,2,2,1^{n-6}]$	$\frac{1}{6}n(n-1)(n-5)$
$[n-3,1,1,1], [4,1^{n-4}]$	$\frac{1}{6}(n-1)(n-2)(n-3)$
$[n-3,2,1], [3,2,1^{n-5}]$	$\frac{1}{3}n(n-2)(n-4)$

Next we will bound the size of the other eigenvalues. This bound follows from the straightforward fact that if A is the adjacency matrix of a graph, then the trace of the square of A is equal to both the sum of the squares of the eigenvalues of A, and to twice the number of edges in the graph. The proof of this result closely follows the proof of the least eigenvalue of the derangement graph of the symmetric group by Ellis [2].

Theorem 6.3. For $\lambda \vdash k$, the absolute value of the eigenvalue of M(2k) for the Sym(2k)-module $V_{2\lambda}$ is strictly less than d(2k)/(2k-2), unless $\lambda = [k]$ or $\lambda = [k-1,1]$.

Proof. If 2k < 15, this theorem can be checked by directly calculating all the eigenvalues (this can easily be done using a computational algebra program such as GAP [16]), so we will assume that $2k \ge 16$.

Let A be the adjacency matrix of M(2k) and use $\xi_{2\lambda}$ to denote the eigenvalue for the Sym(2k)-module $V_{2\lambda}$. The sum of the eigenvalues of A^2 is twice the number of edges in M(2k), that is

$$\sum_{\lambda \vdash k} \chi_{2\lambda}(1) \xi_{2\lambda}^2 = (2k - 1) !! d(2k).$$

From Lemma 6.1 we know the eigenvalues for two of the modules, so this bound can be expressed as

$$\sum_{\substack{\lambda \vdash k \\ \lambda \neq [k], [k-1,1]}} \chi_{2\lambda}(1)\xi_{2\lambda}^2 = (2k-1)!! d(2k) - d(2k)^2 - (2k^2 - 3k) \left(\frac{d(2k)}{2k-2}\right)^2.$$

Since all the terms in left-hand side of the above summation are positive, any single term is less than the sum. Thus

0

$$\chi_{2\lambda}(1)\xi_{2\lambda}^2 \le (2k-1)!!\,d(2k) - d(2k)^2 - (2k^2 - 3k)\left(\frac{d(2k)}{2k-2}\right)^2,$$

(where $\lambda \vdash k$ and $\lambda \neq [k], [k-1,1]$). If $|\xi_{2\lambda}| \ge d(2k)/(2k-2)$, then this reduces to

$$\chi_{\lambda}(1) \le \frac{(2k-1)!!(2k-2)^2}{d(2k)} - 6k^2 + 11k - 4.$$

Using the bound in Lemma 3.2, this implies that

$$\chi_{\lambda}(1) < 2k^2 - k = \frac{(2k)^2 - (2k)}{2}$$

If $|\xi_{2\lambda}| \ge d(2k)/(2k-2)$, then 2λ must be one of the first four representations in the table of Theorem 6.2. Thus 2λ must be either [2k] or [2k-2,2], which proves the result. \Box

We restate this result in terms of the least eigenvalue of the matching derangement graph; noting that Theorem 6.3 implies that $V_{[2k-2,2]}$ is the only Sym(2k)-module that has -d(2k)/(2k-2) as its eigenvalue.

Corollary 6.4. The smallest eigenvalue of M(2k) is -d(2k)/(2k-2) and the multiplicity of this eigenvalue is $2k^2 - 3k$.

7 The Sym(2k)-module $V_{[2k-2,2]}$

Applying the Delsarte-Hoffman bound with the fact that -d(2k)/(2k-2) is the least eigenvalue of M(2k), proves that any canonical coclique is ratio tight since

$$\frac{|V(M(2k))|}{1 - \frac{d}{\tau}} = \frac{(2k-1)!!}{1 - \frac{d(2k)}{-\frac{d(2k)}{2k-2}}} = (2k-3)!!.$$

For S a maximum coclique in M(2k) we will use v_S to denote the characteristic vector of S. The ratio bound implies that |S| = (2k - 3)!! and, further, that

$$v_s - \frac{1}{2k-1}\mathbf{1}$$

is a -d(2k)/(2k-2)-eigenvector. This vector is called the *balanced* characteristic vector of S, since is it orthogonal to the all ones vector. Since the Sym(2k)-module $V_{[2k-2,2]}$ is the only module for which the corresponding eigenvalue is the least (this follows directly from Theorem 6.3) we have the following result which will be used to determine the structure of the maximum cocliques in M(2k).

Lemma 7.1. The characteristic vector for any maximum coclique in M(2k) is in the direct sum of the Sym(2k)-modules $V_{[2k]}$ and $V_{[2k-2,2]}$.

A perfect matching is a subset of the edges in the complete graph, and thus can be represented as a characteristic vector; this is a vector in $\mathbb{R}^{\binom{2k}{2}}$. Define the *incidence matrix* for the perfect matchings in K_{2k} to be the matrix U whose rows are the characteristic vectors of the perfect matchings of K_{2k} . The columns of U are indexed by the edges in the complete graph and the rows are indexed by the perfect matchings. The column of U corresponding to the edge e is the characteristic vector of S_e .

We will show that the characteristic vector of any maximum coclique of M(2k) is a linear combination of the columns of U.

Lemma 7.2. The characteristic vectors of the canonical cocliques of M(2k) span the direct sum of the Sym(2k)-modules $V_{[2k]}$ and $V_{[2k-2,2]}$.

Proof. Let v_e be the characteristic vector of S_e . From Lemma 7.1, the vector $v_e - \frac{1}{2k-1}\mathbf{1}$ is in the Sym(2k)-module $V_{[2k-2,2]}$, and v_e is in the direct sum of the Sym(2k)-modules $V_{[2k]}$ and $V_{[2k-2,2]}$. So all that needs to be shown is that the span of all the vectors v_e has dimension $2k^2 - 3k + 1$, or equivalently, that the rank of U is $2k^2 - 3k + 1$.

Let I denote the $\binom{k}{2} \times \binom{k}{2}$ identity matrix and A(2k, 2) the adjacency matrix of the Kneser graph K(2k, 2). Then

$$U^{T}U = (2k - 3)!!I + (2k - 5)!!A(2k, 2).$$

By Proposition 5.2, 0 is an eigenvalue of this matrix with multiplicity 2k - 1. Thus the rank of $U^T U$ (and hence U) is $\binom{2k}{2} - (2k - 1) = 2k^2 - 3k + 1$.

This result, and the comments at the beginning of this section, imply the following corollary.

Corollary 7.3. The characteristic vector of a maximum coclique in the perfect matching derangement graph is in the column space of U.

Next we will show that this implies that any maximum coclique is a canonical intersecting set. To do this we will consider a polytope based on the perfect matchings.

8 The perfect matching polytope

The convex hull of the set of characteristic vectors for all the perfect matchings of a graph K_{2k} is called the *perfect matching polytope* of K_{2k} . Let U be the incidence matrix defined in the previous section, then the perfect matching polytope is the convex hull of the rows of U. A *face* of the perfect matching polytope is the convex hull of the rows where Uh achieves its maximum for some vector h. A *facet* is a maximal proper face of a polytope.

If S is a maximum coclique in M(2k), then from Corollary 7.3, we know that $Uh = v_s$ for some vector h. If a vertex of K_{2k} is in S, then the corresponding row of Uh is equal to 1; conversely, if a vertex of K_{2k} is not in S, then the corresponding row of Uh is equal to 0. Thus a maximum intersecting set of perfect matchings is a facet of the perfect matching polytope. In this section, we will give a characterization of the facets of the perfect matching polytope for the complete graph.

Let S be a subset of the vertices of K_{2k} and define the *boundary* of S to be the set of edges that join a vertex in S to a vertex not in S. The boundary is denoted by ∂S and is also known as an *edge cut*. If S is a subset of the vertices of K_{2k} of odd size, then any

perfect matching in K_{2k} must contain at least one edge from ∂S . If S is a single vertex, then any perfect matching contains exactly one element of ∂S . It is an amazing classical result of Edmonds that these two constraints characterize the perfect matching polytope for any graph. For a proof of this result see Schrijver [14].

Theorem 8.1. Let X be a graph. A vector x in $\mathbb{R}^{|E(X)|}$ lies in the perfect matching polytope of X if and only if:

(*a*) $x \ge 0$;

(b) if $S = \{u\}$ for some $u \in V(X)$, then $\sum_{e \in \partial S} x(e) = 1$;

(c) if S is an odd subset of V(X) with $|S| \ge 3$, then $\sum_{e \in \partial S} x(e) \ge 1$.

If X is bipartite, then x lies in the perfect matching polytope if and only if the first two conditions hold. \Box

The constraints in Equation (b) define an affine subspace of $\mathbb{R}^{|E(X)|}$. The perfect matching polytope is the intersection of this subspace with affine half-spaces defined by the conditions in Equation (a) and Equation (c); hence the points in a proper face of the polytope must satisfy at least one of these conditions with equality.

For any graph X (that is not bipartite) the vertices of a facet are either the perfect matchings that miss a given edge, or the perfect matchings that contain exactly one edge from ∂S for some odd subset S.

It follows from Theorem 8.1 that every perfect matching in K_{2k} is a vertex in the perfect matching polytope for the complete graph. But we can also determine the vertices of every facet in this polytope.

Lemma 8.2. In the matching polytope of K_{2k} , the vertices of a facet of maximum size are the perfect matchings that do not contain a given edge.

Proof. Let F be a facet of the polytope of maximum size. From the above comments, equality holds in at least one of equations

$$\sum_{e \in \partial S} x(e) \ge 1$$

for all $x \in F$. Suppose S is the subset that defines such an equation, then S is an odd subset of the vertices in K_{2k} for which $\sum_{e \in \partial S} x(e) = 1$ for all $x \in F$.

Let s be the size of S. Each perfect matching with exactly one edge in ∂S consists of the following: a matching of size (s-1)/2 covering all but one vertex of S; an edge joining this missed vertex of S to a vertex in \overline{S} ; and a matching of size (2k - s - 1)/2covering all but one vertex in \overline{S} . Hence there are

$$(s-2)!! s(2k-s) (2k-s-2)!! = s!!(2k-s)!!$$

such perfect matchings. We denote this number by N(s) and observe that

$$\frac{N(s-2)}{N(s)} = \frac{2k - s + 2}{s}.$$

Hence for all s such that $3 \le s \le k$ we see that the values N(s) are strictly decreasing, so the maximum size of a set of such vertices is N(3) = 3(2k - 3)!!.

On the other hand, the number of perfect matchings in K_{2k} that do not contain a given edge is

$$(2k-1)!! - (2k-3)!! = (2k-2)(2k-3)!!$$

Since this is always larger than N(3), the lemma follows.

We now have all the tools to show that any maximum intersecting set of perfect matchings is the set of all matchings that contain a fixed edge.

Theorem 8.3. The largest coclique in M(2k) has size (2k - 3)!!. The only cocliques that meet this bound are the canonically intersecting sets of perfect matchings.

Proof. Let S be a maximum coclique in M(2k) and let v_S be the characteristic vector of S. Then |S| = (2k-3)!!, by the Delsarte-Hoffman bound and Corollary 6.4. The Delsarte-Hoffman bound, along with Theorem 6.3, further imply that the vector $v_S - \frac{1}{2k-1}\mathbf{1}$ is in the Sym(2k)-module $V_{[2k-2,2]}$.

the Sym(2k)-module $V_{[2k-2,2]}$. By Lemma 7.2, $v_S - \frac{1}{2k-1}\mathbf{1}$ is a linear combination of the balanced characteristic vectors of the canonical cocliques. This also implies that v_S is a linear combination of the characteristic vectors of the canonical cocliques. So there exists a vector x such that $Ux = v_S$ (where U is the matrix defined in Section 7).

Finally, by Lemma 8.2, \overline{S} is a face of maximal size an it consists of all the perfect matching that avoid a fixed edge. This implies that S is a canonical coclique of M(2k). \Box

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Cyclic and symmetric hamiltonian cycle systems of the complete multipartite graph: even number of parts

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Abstract

In this paper, we present a complete solution to the existence problem for a cyclic hamiltonian cycle system for the complete multipartite graph with an even number of parts all of the same cardinality. We also give necessary and sufficient conditions for the system to be symmetric as well.

Keywords: Hamiltonian cycle, cyclic cycle system, symmetric hamiltonian cycle system, complete multipartite graph.

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1 Introduction

Throughout this paper, K_v will denote the complete graph on v vertices and, if v is even, $K_v - I$ will denote the cocktail party graph of order v, namely the graph obtained from K_v by removing a 1-factor I, that is, a set of $\frac{v}{2}$ pairwise disjoint edges. Also $K_{m \times n}$ will denote the complete multipartite graph with m parts of same cardinality n; if n = 1, we

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may identify $K_{m \times 1}$ with K_m , while if n = 2, $K_{m \times 2}$ is nothing but the cocktail party graph $K_{2m} - I$.

For any graph Γ we write $V(\Gamma)$ for the set of its vertices and $E(\Gamma)$ for the set of its edges. We denote by $C = (c_0, c_1, \ldots, c_{\ell-1})$ the cycle of length ℓ whose edges are $[c_0, c_1], [c_1, c_2], \ldots, [c_{\ell-1}, c_0]$. An ℓ -cycle system of a graph Γ is a set \mathcal{B} of cycles of length ℓ whose edges partition $E(\Gamma)$; clearly a graph may admit a cycle system only if the degree of each vertex is even. For general background on cycle systems we refer to the surveys [7, 8]. An ℓ -cycle system \mathcal{B} of Γ is said to be *hamiltonian* if $\ell = |V(\Gamma)|$, and it is said to be cyclic if we may identify $V(\Gamma)$ with the cyclic group \mathbb{Z}_v , and if for any $C = (c_0, c_1, \ldots, c_{\ell-1}) \in \mathcal{B}$, we have also $C + 1 = (c_0 + 1, c_1 + 1, \ldots, c_{\ell-1} + 1) \in \mathcal{B}$. The existence problem for cyclic cycle systems of K_v has generated a considerable amount of interest. Many authors have contributed to give a complete answer in the case $v \equiv 1$ or $\ell \pmod{2\ell}$ (see [10, 11, 19, 20, 21, 22, 26]). We point out in particular that the existence problem of a cyclic hamiltonian cycle system (HCS, for short) for K_v has been solved by Buratti and Del Fra in [11], and that for $K_v - I$ it has been solved by Jordon and Morris [17].

The existence problem for cycle systems of the complete multipartite graph has not been solved yet, but we have many interesting recent results on this topic (see for instance [4, 5, 24, 25]). Still, very little is known about the same problem with the additional constraint that the system be cyclic. We have a complete solution in the following very special cases: the length of the cycles is equal to the cardinality of the parts [12]; the cycles are hamiltonian and the parts have cardinality two [14, 17]. We have also some partial results in [3].

Hamiltonian cycle systems of $K_{m \times n}$ have been shown to exist ([18]) whenever the degree of each vertex of the graph, that is (m-1)n, is even; in this paper we start investigating the existence of cyclic hamiltonian cycle systems of $K_{m \times n}$, and completely solve the problem when m is even.

We also consider the existence of a symmetric HCS for $K_{m \times n}$ with n > 1, a concept recently introduced by Schroeder in [23] generalizing the notion of symmetry given in [6] for cocktail party graphs: in this definition, an HCS for $K_{m \times n}$ is *n*-symmetric if each cycle in the system is invariant under a fixed-point-free automorphism of order *n*. We will show that the cycle systems we shall construct in will turn out to be symmetric in this sense.

The paper is organized as follows: after some preliminary notes in Section 2 on the methods we shall use, in Section 3 we establish a necessary condition in the case n even for the existence of a cyclic cycle system (not necessarily hamiltonian) of $K_{m \times n}$ from which we derive a necessary condition for the existence of a cyclic HCS of $K_{m \times n}$. Then in Section 4 we give a complete solution to the existence problem of a cyclic HCS with an even number of parts, proving that in this case the necessary condition we found is also sufficient. The main result of this paper is the following.

Theorem 1.1. Let m be even; a cyclic and n-symmetric HCS for $K_{m \times n}$ exists if and only if

- (a) $n \equiv 0 \pmod{4}$, or
- (b) $n \equiv m \equiv 2 \pmod{4}$.

The proof of Theorem 1.1 will follow from the various results proved in Sections 3 and 4. First, in Corollary 3.4 we give the necessary condition for the existence of a cyclic HCS

of $K_{m \times n}$. Then, in Proposition 4.2 we study the bipartite case, finally in Theorem 4.3 and in Theorem 4.7 we deal with the case $n \equiv 0 \pmod{4}$, and $n \equiv 2 \pmod{4}$, respectively.

2 Preliminaries

The main results of this paper will be obtained by using the method of *partial differences* introduced by Marco Buratti and used in many papers, see for instance [2, 9, 10, 11, 13, 14, 27]. Here we recall some definitions and results useful in the rest of the paper.

Definition 2.1. Let $C = (c_0, c_1, \dots, c_{\ell-1})$ be an ℓ -cycle with vertices in an abelian group G and let d be the order of the stabilizer of C under the natural action of G, that is, $d = |\{g \in G : C + g = C\}|$. The multisets

$$\Delta C = \{ \pm (c_{h+1} - c_h) \mid 0 \le h < \ell \}, \\ \partial C = \{ \pm (c_{h+1} - c_h) \mid 0 \le h < \ell/d \}.$$

where the subscripts are taken modulo ℓ , are called the *list of differences* from C and the *list of partial differences* from C, respectively.

More generally, given a set \mathcal{B} of ℓ -cycles with vertices in G, by $\Delta \mathcal{B}$ and $\partial \mathcal{B}$ one means the union (counting multiplicities) of all multisets ΔC and ∂C respectively, where $C \in \mathcal{B}$.

We recall the definition of a *Cayley graph on a group* G with connection set Ω , denoted by $Cay[G:\Omega]$. Let G be an additive group and let $\Omega \subseteq G \setminus \{0\}$ such that for every $\omega \in \Omega$ we also have $-\omega \in \Omega$. The Cayley graph $Cay[G:\Omega]$ is the graph whose vertices are the elements of G and in which two vertices are adjacent if and only if their difference is an element of Ω (an analogous definition can be given in multiplicative notation). Note that $K_{m \times n}$ can be interpreted as the Cayley graph $Cay[\mathbb{Z}_{mn} : \mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}]$, where by $m\mathbb{Z}_{mn}$ we mean the subgroup of order n of \mathbb{Z}_{mn} . The vertices of $K_{m \times n}$ will be always understood as elements of \mathbb{Z}_{mn} and the parts of $K_{m \times n}$ are the cosets of $m\mathbb{Z}_{mn}$ in \mathbb{Z}_{mn} . We consider the natural action of \mathbb{Z}_{mn} on the cycles of $K_{m \times n}$: given a cycle $C = (c_0, c_1, \ldots, c_{\ell-1})$ of $K_{m \times n}$ we define C+t as the cycle $(c_0+t, c_1+t, \ldots, c_{\ell-1}+t)$, where $c_0, c_1, \ldots, c_{\ell-1}, t$ are elements of \mathbb{Z}_{mn} . The stabilizer and the orbit of any cycle C of $K_{m \times n}$ will be understood with respect to this action and will be denoted by Stab(C) and Orb(C), respectively. A cyclic HCS of $K_{m \times n}$ is completely determined by a set of *base cycles*, namely, a complete system of representatives for the orbits of its cycles under the action of \mathbb{Z}_{mn} . The next theorem, which is a consequence of the theory of partial differences, will play a fundamental role in this paper.

Theorem 2.2. A set \mathcal{B} of mn-cycles is a set of base cycles of a cyclic HCS of $K_{m \times n}$ if and only if $\partial \mathcal{B} = \mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}$.

In Example 2.4 we will show how to construct a cyclic HCS of $K_{10\times 6}$ applying Theorem 2.2.

For our purposes the following notation will be useful. Let $c_0, c_1, \ldots, c_{r-1}, x$ be elements of an additive group G, with x of order d. The closed trail

$$[c_0, c_1, c_2, \ldots, c_{r-1},$$

$$c_0 + x, c_1 + x, c_2 + x, \dots, c_{r-1} + x, \dots,$$

$$c_0 + (d-1)x, c_1 + (d-1)x, c_2 + (d-1)x, \dots, c_{r-1} + (d-1)x]$$

will be denoted by

$$[c_0, c_1, \ldots, c_{r-1}]_x.$$

For brevity, given $P = [c_0, c_1, \ldots, c_{r-1}]$, we write $[P]_x$ for the closed trail $[c_0, c_1, \ldots, c_{r-1}]_x$. For instance in \mathbb{Z}_{12} $[0, 5, 1]_9$ represents the closed trail (a cycle in this case) (0, 5, 1, 9, 2, 10, 6, 11, 7, 3, 8, 4).

Remark 2.3. Note that $[c_0, c_1, \ldots, c_{r-1}]_x$ is a (dr)-cycle if and only if the elements c_i , for $i = 0, \ldots, r-1$, belong to pairwise distinct cosets of the subgroup $\langle x \rangle$ in G. Also, if $C = [c_0, c_1, \ldots, c_{r-1}]_x$ is a (dr)-cycle, then

$$\partial C = \{ \pm (c_i - c_{i-1}) \mid i = 1, \dots, r-1 \} \cup \{ \pm (c_0 + x - c_{r-1}) \}.$$

We point out that in the case of cyclic HCS of $K_{m \times n}$ we have that dr = mn. Hence, if the list ∂C has no repeated elements, the order of Stab(C) is d, and the length of the \mathbb{Z}_{mn} -orbit of C is r.

Example 2.4. Here we present the construction of a cyclic HCS of $K_{10\times 6}$. Consider the following cycles with vertices in \mathbb{Z}_{60} :

$$\begin{split} C_1 &= [0, 19, 1, 17, 3, 15, 6, 14, 8, 12]_{10}, \quad C_2 &= [0, 29, 1, 28, 2, 27, 3, 26, 4, 25]_{10}, \\ C_3 &= [0, 3]_2, \quad C_4 &= [0, 7]_2, \quad C_5 &= [0, 13]_2, \quad C_6 &= [0]_{17}. \end{split}$$

One can easily check that $\mathcal{B} = \{C_1, \ldots, C_6\}$ is a set of hamiltonian cycles of $K_{10\times 6}$ and that:

$$\partial C_1 = \pm \{19, 18, 16, 14, 12, 9, 8, 6, 4, 2\},$$

$$\partial C_2 = \pm \{29, 28, 27, 26, 25, 24, 23, 22, 21, 15\},$$

$$\partial C_3 = \pm \{3, 1\}, \quad \partial C_4 = \pm \{7, 5\}, \quad \partial C_5 = \pm \{13, 11\}, \quad \partial C_6 = \pm \{17\}$$

Hence $\partial \mathcal{B} = \mathbb{Z}_{60} \setminus 10\mathbb{Z}_{60}$. So, in view of Theorem 2.2, we can conclude that \mathcal{B} is a set of base cycles of a cyclic HCS of $K_{10\times 6}$.

Explicitly the required system consists of the following 27 cycles:

$$\{C_1 + i, C_2 + i \mid i = 0, \dots, 9\} \cup \{C_3 + i, C_4 + i, C_5 + i \mid i = 0, 1\} \cup \{C_6\}.$$

An HCS of the complete graph K_v , v odd, is said to be symmetric if there is an involutory permutation ϕ of the vertices of K_v fixing all its cycles; in the case v is even, an HCS of the cocktail party graph $K_v - I$ is symmetric if all its cycles are fixed by the involution switching all pairs of endpoints of the edges of I. This definition is due to Akiyama, Kobayashi and Nakamura [1] in the case v odd, and to Brualdi and Schroeder [6] in the case v even. Symmetric hamiltonian cycle systems always exist in the odd case: an example is the well-known Walecki construction, and more generally, any 1-rotational HCS is clearly symmetric (an HCS is called 1-rotational if it has an automorphism group G acting sharply transitively on all but one vertex). It was recently proved that the number of nonisomorphic 1-rotational HCSs of order v = 2n + 1 > 9 is bounded below by $2^{\lceil 3n/4 \rceil}$ ([16]), so that in the case v odd symmetric HCSs are quite common.

In the case v even we have the following result.

Theorem 2.5 (Brualdi and Schroeder [6]). A symmetric HCS of $K_v - I$ exists if and only if $\frac{v}{2} \equiv 1$ or 2 (mod 4).

In [14], the authors study the case of an HCS of K_v which is *both* cyclic and symmetric; their result in the case v even is that there exists a cyclic and symmetric HCS of K_v for all values for which a cyclic HCS exists, that is, for $\frac{v}{2} \equiv 1$ or 2 (mod 4) and $\frac{v}{2}$ not a prime power.

Very recently Michael Schroeder [23] studied hamiltonian cycle systems for a graph Γ in which each cycle is fixed by a fixed-point-free automorphism ϕ of Γ of order n > 2, so that $V(\Gamma) = mn$ for some m; we shall call such an HCS *n*-symmetric.

To admit an *n*-symmetric HCS, Γ must be a subgraph of $K_{m \times n}$, and in [23] the existence problem of an *n*-symmetric HCS for $K_{m \times n}$ is completely solved in the following result.

Theorem 2.6 (Schroeder [23]). Let $m \ge 2$ and $n \ge 1$ be integers such that (m - 1)n is even. An n-symmetric HCS for $K_{m \times n}$ always exists except when we have, simultaneously, $n \equiv 2 \pmod{4}$ and $m \equiv 0$ or $3 \pmod{4}$.

Note that we shall see the same non-existence condition later on in Corollary 3.4. It makes sense therefore to study, as done in [14] for the cocktail party graph, hamiltonian cycle systems for the complete multipartite graph that are *both* cyclic and symmetric. As noted above, $K_{m \times n}$ is the Cayley graph $Cay[\mathbb{Z}_{mn} : \mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}]$. Let γ be the morphism $x \mapsto x + 1 \pmod{mn}$ and set $\phi = \gamma^m$. We have the following condition for a cycle in a cyclic cycle system to be ϕ -invariant.

Lemma 2.7. A cycle C in a cyclic HCS of $K_{m \times n}$ is ϕ -invariant if and only if n divides |Stab(C)| - or equivalently, if |Orb(C)| divides $\frac{mn}{n} = m$.

Example 2.8. Let us consider once more the cycles we used in Example 2.4; we can easily see that the cycle system is also 6-symmetric, since the length of the orbit is 10 for cycles C_1 and C_2 , 2 for cycles C_3 , C_4 , C_5 and 1 for C_6 .

3 Non-existence results

In this section we shall present some non-existence results for cycle systems of the complete multipartite graph $K_{m \times n}$; the methods used here will be closely related to those used in [15], where the case of the cocktail party graph is considered. The results will concern general cycle systems; we will then apply these results to the hamiltonian case.

The following lemma is an immediate generalization of Lemma 2.1 of [15], hence we omit the proof.

Lemma 3.1. Let $C = (c_0, c_1, \ldots, c_{\ell-1})$ be a cycle belonging to a cyclic cycle system of $K_{m \times n}$ and let d be the order of Stab(C). Then Orb(C) is an ℓ -cycle system of $Cay[\mathbb{Z}_{mn} : \{\pm (c_{i-1} - c_i) \mid 1 \le i \le \frac{\ell}{d}\}].$

The next result generalizes Theorem 2.2 of [15].

Proposition 3.2. Let *n* be an even integer. The number of cycle orbits of odd length in a cyclic cycle decomposition of $K_{m \times n}$ has the same parity of $\frac{m(m-1)n^2}{8}$.

Proof. Let \mathcal{B} be a cyclic cycle system of $K_{m \times n}$. For every ℓ -cycle $C = (c_0, c_1, \ldots, c_{\ell-1})$ of \mathcal{B} set

$$\sigma(C) = \sum_{i=1}^{\ell/d} (c_{i-1} - c_i) = (c_0 - c_1) + (c_1 - c_2) + \dots + (c_{\ell/d-1} - c_{\ell/d}) = c_0 - c_{\ell/d},$$

where d is the order of Stab(C). It is easy to see that $c_{\ell/d} = c_0 + \rho$ where ρ is an element of \mathbb{Z}_{mn} of order d and hence we have

$$\sigma(C) = \frac{mnx}{d}$$
 with $gcd(x, d) = 1$.

Since n is even, we have that $\sigma(C)$ is even if and only if d is a divisor of $\frac{mn}{2}$; on the other hand, since the length of Orb(C) is $\frac{mn}{d}$, also |Orb(C)| is even if and only if d is a divisor of $\frac{mn}{2}$. For any cycle $C \in \mathcal{B}$, we thus have that

$$\sigma(C) \equiv |Orb(C)| \pmod{2}. \tag{3.1}$$

Let $S = \{C_1, \ldots, C_s\}$ be a set of base cycles of \mathcal{B} , that is, a complete system of representatives for the orbits of the cycles of \mathcal{B} , so that we have

$$\mathcal{B} = Orb(C_1) \cup Orb(C_2) \cup \ldots \cup Orb(C_s).$$

By Lemma 3.1, the cycles of $Orb(C_i)$ form a cycle system of $Cay[\mathbb{Z}_{mn} : \partial C_i]$. Hence it follows that

$$Cay[\mathbb{Z}_{mn}:\mathbb{Z}_{mn}\setminus m\mathbb{Z}_{mn}] = \bigcup_{i=1}^{s} Cay[\mathbb{Z}_{mn}:\partial C_i] = Cay[\mathbb{Z}_{mn}:\partial \mathcal{S}]$$

so that we obtain

$$\partial \mathcal{S} = \mathbb{Z}_{mn} \setminus m \mathbb{Z}_{mn}. \tag{3.2}$$

Note that ∂C_i is a disjoint union of the set of summands of $\sigma(C_i)$ and the set of their additive inverses. Hence, by (3.2), it follows that $\mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}$ is a disjoint union of the set of all summands of the sum $\sum_{i=1}^{s} \sigma(C_i)$ and the set of their additive inverses. Then, considering that additive inverses elements have the same parity and that $\mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn} = \pm(\{1, 2, \dots, \frac{mn}{2} - 1\} \setminus \{m, 2m, \dots, (\frac{n}{2} - 1)m\})$ we can write:

$$\sum_{i=1}^{s} \sigma(C_i) \equiv \sum_{i=1}^{\frac{mn}{2}-1} i - m \sum_{i=1}^{\frac{n}{2}-1} i \pmod{2}$$

and then

$$\sum_{i=1}^{s} \sigma(C_i) \equiv \frac{m(m-1)n^2}{8} \pmod{2}.$$

From (3.1) we have

$$\sum_{i=1}^{s} |Orb(C_i)| \equiv \frac{m(m-1)n^2}{8} \pmod{2}.$$

Hence the number of cycles C_i of S whose orbit has odd length has the same parity as $\frac{m(m-1)n^2}{8}$, and the assertion follows.

Now we are ready to prove the main non-existence result. In the following given a positive integer x by $|x|_2$ we will denote the largest e for which 2^e divides x.

Theorem 3.3. Let n be an even integer. A cyclic ℓ -cycle system of $K_{m \times n}$ cannot exist in each of the following cases:

(a) $m \equiv 0 \pmod{4}$ and $|\ell|_2 = |m|_2 + 2|n|_2 - 1$;

(b) $m \equiv 1 \pmod{4}$ and $|\ell|_2 = |m-1|_2 + 2|n|_2 - 1$;

- (c) $m \equiv 2,3 \pmod{4}$, $n \equiv 2 \pmod{4}$ and $\ell \not\equiv 0 \pmod{4}$; or
- (d) $m \equiv 2,3 \pmod{4}, n \equiv 0 \pmod{4}$ and $|\ell|_2 = 2|n|_2$.

Proof. If \mathcal{B} is an ℓ -cycle system of $K_{m \times n}$, then $|\mathcal{B}| = |E(K_{m \times n})|/\ell = mn^2(m-1)/2\ell$. Hence the number of cycle orbits of odd length of a cyclic ℓ -cycle system of $K_{m \times n}$ has the same parity as $mn^2(m-1)/2\ell$. By Proposition 3.2, we have that $mn^2(m-1)/2\ell \equiv mn^2(m-1)/8 \pmod{2}$. Now the conclusion can be easily proved distinguishing four cases according to the congruence class of m modulo 4.

If the cycles of the system are hamiltonian, that is if $\ell = mn$, we obtain the following corollary.

Corollary 3.4. Let n be an even integer. A cyclic HCS of $K_{m \times n}$ cannot exist if both $m \equiv 0, 3 \pmod{4}$ and $n \equiv 2 \pmod{4}$.

4 Existence of a cyclic and symmetric HCS of $K_{m \times n}$, m even

In this section we present direct constructions of a cyclic and symmetric HCS of the complete multipartite graph with an even number of parts. Since (m - 1)n must be even, if mis even then n is even too; the condition in Corollary 3.4 tells us that when $n \equiv 2 \pmod{4}$, m should also be congruent to 2 modulo 4. If these two requirements are met, we will show that a cyclic and symmetric HCS of $K_{m \times n}$ always exists, and therefore we prove Theorem 1.1.

As observed in the Introduction, $K_{m \times 2} = K_{2m} - I$ is the cocktail party graph; thus we can suppose n > 2, since for n = 2 we can rely on the following result.

Theorem 4.1 (Jordon, Morris [17]; Buratti, Merola [14]). For an even integer $v \ge 4$ there exists a cyclic and symmetric HCS of $K_v - I$ if and only if $v \equiv 2, 4 \pmod{8}$ and $v \ne 2p^{\alpha}$, where p is an odd prime and $\alpha \ge 1$.

We start by considering the complete bipartite graph.

Proposition 4.2. For any even integer n there exists a cyclic and n-symmetric HCS of $K_{2\times n}$.

Proof. For $n = 2\ell$ we need a set \mathcal{B} of base cycles such that $\partial \mathcal{B} = \pm \{1, 3, \dots, 2\ell - 1\}$. Let us first assume ℓ even. For $i = 0, 1, \dots, \ell/2 - 1$ consider the cycle $C_i = [0, 4i + 3]_2$. We have $\partial C_i = \pm \{4i + 1, 4i + 3\}$, and thus $\mathcal{B} = \{C_0, C_1, \dots, C_{\ell/2-1}\}$ is a set of hamiltonian cycles of $K_{2 \times n}$ such that $\partial \mathcal{B} = \mathbb{Z}_{2n} \setminus 2\mathbb{Z}_{2n}$. Now assume that ℓ is odd. For $i = 0, 1, \dots, \lfloor \ell/2 \rfloor - 1$ take $C_i = [0, 4i + 3]_2$ as above, and add the cycle $C' = [0]_{2\ell-1}$. Now $\mathcal{B} = \{C_0, C_1, \dots, C_{\lfloor \ell/2 \rfloor - 1}, C'\}$ is a set of base cycles for a cyclic HCS of $K_{2 \times n}$. This cycle system is also *n*-symmetric by Lemma 2.7 since each cycle belongs to an orbit of length 1 or 2. Now we tackle the case $n \equiv 0 \pmod{4}$.

Theorem 4.3. Let m be an even integer and $n \equiv 0 \pmod{4}$. Then there exists a cyclic and n-symmetric HCS of $K_{m \times n}$.

Proof. We may assume $m \ge 4$, since if m = 2, the statement follows from Proposition 4.2. We shall first give a construction for m a power of 2. Let $m = 2^a$ and n = 4t with a > 1 and $t \ge 1$. We will build a set of $a \cdot t$ base cycles. For all $b = 1, \ldots, a$ and $i = 0, \ldots, t - 1$ consider the following path:

$$P_{i,b} = [0, 2mi + (2^{b+1} - 1), 1, 2mi + (2^{b+1} - 2), 2, 2mi + (2^{b+1} - 3), \dots, (2^{b-1} - 1), 2mi + (2^{b+1} - 2^{b-1})].$$

Note that the elements of $P_{i,b}$ are pairwise distinct modulo 2^b : hence $A_{i,b} = [P_{i,b}]_{2^b}$ is a hamiltonian cycle of $K_{m \times n}$. It is straightforward to check that

$$\partial A_{i,b} = \pm (\{2mi+2^{b-1}\} \cup \{2mi+(2^{b}+1), 2mi+(2^{b}+2), \dots, 2mi+(2^{b+1}-1)\}).$$

Thus $\cup (\partial A_{i,b}) = \mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}$, and the existence of a cyclic HCS of $K_{m \times n}$ follows from Theorem 2.2.

Now assume $m = 2^{a}\overline{m}$ with $a \ge 1$ and $\overline{m} > 1$ odd. Take n = 4t with $t \ge 1$. We start constructing for all $i = 0, \ldots, t - 1$ the following paths:

$$P_{i,j} = \begin{cases} [0, 2mi + (4j-1)] & \text{if } j = 1, \dots, \frac{\overline{m}-1}{2} \\ [0, 2mi + (4j+1)] & \text{if } j = \frac{\overline{m}+1}{2}, \dots, \overline{m}-1 \end{cases}$$
(4.1)

Since 2mi + (4j-1) and 2mi + (4j+1) are odd, $A_{i,j} = [P_{i,j}]_2$ is a hamiltonian cycle of $K_{m \times n}$ for any i, j. Clearly $\partial A_{i,j} = \pm \{2mi + (4j-3), 2mi + (4j-1)\}$ for $j = 1, \ldots, \overline{\frac{m-1}{2}}$ and $\partial A_{i,j} = \pm \{2mi + (4j-1), 2mi + (4j+1)\}$ for $j = \frac{\overline{m+1}}{2}, \ldots, \overline{m} - 1$. Hence for any fixed i we have

$$\bigcup_{j=1}^{\overline{m}-1} \partial A_{i,j} = \pm \left(\{ 2mi+1, 2mi+3, 2mi+5, \dots, 2mi+(2\overline{m}-3) \} \cup \right)$$

 $\{2mi + (2\overline{m} + 1), 2mi + (2\overline{m} + 3), 2mi + (2\overline{m} + 5), \dots, 2mi + (4\overline{m} - 3)\}\$

Now for $i = 0, \ldots, t - 1$ consider the paths

$$Q_{i,1} = [0, 2mi + (4\overline{m} - 1), 1, 2mi + (4\overline{m} - 3), 3, \dots, \overline{m} - 2, 2mi + 3\overline{m}, (4.2) \overline{m} + 1, 2mi + (3\overline{m} - 1), \overline{m} + 3, 2mi + (3\overline{m} - 3), \dots, 2\overline{m} - 2, 2mi + (2\overline{m} + 2)];$$

and finally, if $a \ge 2$, for all $b = 2, \ldots, a$ consider also

$$Q_{i,b} = [0, 2mi + (2^{b+1}\overline{m} - 1), 1, 2mi + (2^{b+1}\overline{m} - 2), 2, \dots, (2^{b-1}\overline{m} - 1), 2mi + (2^{b+1}\overline{m} - 2^{b-1}\overline{m})].$$

Notice that the elements of $Q_{i,b}$ are pairwise distinct modulo $2^b\overline{m}$ and hence $B_{i,b} = [Q_{i,b}]_{2^b\overline{m}}$ is a hamiltonian cycle of $K_{m\times n}$ for any $i = 0, \ldots, t-1$ and $b = 1, \ldots, a$. Also,

$$\partial B_{i,1} = \pm (\{2mi+2, 2mi+4, 2mi+6, \dots, 2mi+2\overline{m}-2\} \cup \\ \{2mi+2\overline{m}+2, 2mi+2\overline{m}+4, 2mi+2\overline{m}+6, \dots, 2mi+4\overline{m}-2\} \cup \\ \{2mi+2\overline{m}-1, 2mi+4\overline{m}-1\})$$

and for $b = 2, \ldots, a$

$$\partial B_{i,b} = \pm (\{2mi+2^{b-1}\overline{m}\} \cup \{2mi+(2^{b}\overline{m}+1), 2mi+(2^{b}\overline{m}+2), \dots, 2mi+(2^{b+1}\overline{m}-1)\}).$$

It turns out that for every fixed i we have

$$\bigcup_{b=1}^{a} \partial B_{i,b} = \pm \left(\{2mi+2, 2mi+4, 2mi+6, \dots, 2mi+4\overline{m}\} \cup \{2mi+(4\overline{m}+1), 2mi+(4\overline{m}+2), 2mi+(4\overline{m}+3), \dots, 2mi+(m-1)\} \cup \{2mi+(m+1), 2mi+(m+2), 2mi+(m+3), \dots, 2mi+(2m-1)\} \right).$$

Let $\mathcal{B} = \{A_{i,j} \mid 0 \le i < t, 1 \le j < \overline{m}\} \cup \{B_{i,b} \mid 0 \le i < t, 1 \le b \le a\}$. From what we have seen above, for every fixed *i* we have

$$\begin{pmatrix} \overline{m}_{-1} \\ \bigcup \\ j=1 \end{pmatrix} \cup \begin{pmatrix} a \\ \bigcup \\ b=1 \end{pmatrix} \otimes B_{i,b} = \pm \left(\{ 2mi+1, 2mi+2, 2mi+3, \dots, 2mi+(m-1) \} \cup \{ 2mi+(m+1), 2mi+(m+2), 2mi+(m+3), \dots, 2mi+(2m-1) \} \right)$$

and so $\partial \mathcal{B} = \mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}$. We conclude that \mathcal{B} is a set of base cycles of a cyclic HCS of $K_{m \times n}$.

It is easily seen from Lemma 2.7 that these cycle systems are also *n*-symmetric, since in all cases the length of the orbit of each cycle divides m.

Example 4.4. Following the proof of Theorem 4.3 we give here the construction of a set of base cycles of a cyclic and 4-symmetric HCS of $K_{18\times4}$. In the notation of the Theorem, a = 1, $\overline{m} = 9$ and t = 1. Take the following cycles:

$$\begin{split} A_{0,1} &= [0,3]_2, \quad A_{0,2} &= [0,7]_2, \quad A_{0,3} &= [0,11]_2, \quad A_{0,4} &= [0,15]_2, \\ A_{0,5} &= [0,21]_2, \quad A_{0,6} &= [0,25]_2, \quad A_{0,7} &= [0,29]_2, \quad A_{0,8} &= [0,33]_2, \\ B_{0,1} &= [0,35,1,33,3,31,5,29,7,27,10,26,12,24,14,22,16,20]_{18}. \end{split}$$

We have

$$\bigcup_{j=1}^{8} \partial A_{0,j} = \pm (\{1, 3, 5, \dots, 15\} \cup \{19, 21, 23, \dots, 33\})$$

and

$$\partial B_{0,1} = \pm (\{2, 4, 6, \dots, 16\} \cup \{20, 22, 24, \dots, 34\} \cup \{17, 35\}).$$

So, given $\mathcal{B} = \{A_{0,1}, A_{0,2}, \dots, A_{0,8}, B_{0,1}\}$, we have $\partial \mathcal{B} = \mathbb{Z}_{72} \setminus 18\mathbb{Z}_{72}$.

Now, we give the construction of a set of base cycles of a cyclic and 8-symmetric HCS of $K_{72\times8}$. Notice that $\overline{m} = 9$ as before, but a = 3 and t = 1, so we need to construct a larger number of cycles. For i = 0 we take

$$A_{0,1} = [0,3]_2, \quad A_{0,2} = [0,7]_2, \quad A_{0,3} = [0,11]_2, \quad A_{0,4} = [0,15]_2,$$

$$A_{0,5} = [0,21]_2, \quad A_{0,6} = [0,25]_2, \quad A_{0,7} = [0,29]_2, \quad A_{0,8} = [0,33]_2,$$

$$\begin{split} B_{0,1} &= & [0,35,1,33,3,31,5,29,7,27,10,26,12,24,14,22,16,20]_{18}, \\ B_{0,2} &= & [0,71,1,70,2,69,3,68,\ldots,17,54]_{36}, \\ B_{0,3} &= & [0,143,1,142,2,141,3,140,\ldots,35,108]_{72}. \end{split}$$

We have

$$\binom{8}{\bigcup_{j=1}^{3}} \partial A_{0,j} \cup \binom{3}{\bigcup_{b=1}^{3}} \partial B_{0,b} = \pm \left(\{1, 2, 3, \dots, 71\} \cup \{73, 74, 75, \dots, 143\} \right).$$

Furthermore, for i = 1:

$$A_{1,1} = [0, 147]_2, \quad A_{1,2} = [0, 151]_2, \quad A_{1,3} = [0, 155]_2, \quad A_{1,4} = [0, 159]_2,$$
$$A_{1,5} = [0, 165]_2, \quad A_{1,6} = [0, 169]_2, \quad A_{1,7} = [0, 173]_2, \quad A_{1,8} = [0, 177]_2,$$

$$\begin{array}{rcl} B_{1,1} &=& [0,179,1,177,3,175,5,173,7,171,10,170,12,168,14,166,16,164]_{18}, \\ B_{1,2} &=& [0,215,1,214,2,213,3,212,\ldots,17,198]_{36}, \\ B_{1,3} &=& [0,287,1,286,2,285,3,284,\ldots,35,252]_{72}. \end{array}$$

We have

$$\binom{8}{\bigcup_{j=1}^{3}} \partial A_{1,j} \cup \binom{3}{\bigcup_{b=1}^{3}} \partial B_{1,b} = \pm (\{145, 146, 147, \dots, 215\} \cup \{217, 218, 219, \dots, 287\}).$$

So, given $\mathcal{B} = \{A_{i,j} \mid i = 0, 1, j = 1, \dots, 8\} \cup \{B_{i,b} \mid i = 0, 1, b = 1, 2, 3\}$, we have $\partial \mathcal{B} = \mathbb{Z}_{576} \setminus 72\mathbb{Z}_{576}$.

The following definition and lemma are instrumental in proving Theorem 4.7, where we shall settle the case $n \equiv 2 \pmod{4}$.

Definition 4.5. For all positive integers s, d and all odd integers $w \ge 3$, set

$$S(s,d,w) = \left\{s + id \mid 0 \le i \le \frac{w-3}{2}\right\}$$

and

$$\varphi(s,d,w) = \left| \left\{ x \in S(s,d,w) : \gcd(x,w) = 1 \right\} \right|.$$

Lemma 4.6. Assume gcd(s, d, w) = 1. If $3 \nmid s$ when w = 3, then $\varphi(s, d, w) > 0$.

Proof. If w = 3 then $\varphi(s, d, 3) = 1$, since $S(s, d, 3) = \{s\}$ and $3 \nmid s$. Suppose now $w \ge 5$. The assertion is trivial for gcd(s, w) = 1, since $s \in S(s, d, w)$. If $gcd(s, w) \neq 1$, consider the set $T = \{p \text{ prime } : p \mid w, p \nmid s\}$ and let $x = \prod_{p \in T} p$ (with the usual convention that

x = 1 if $T = \emptyset$). Since $w \ge 5$ and x < w, we have that $s + dx \in S(s, d, w)$: we claim that that gcd(s + dx, w) = 1. Note that no prime factor of gcd(s, w) divides d, otherwise we would have $gcd(s, d, w) \ne 1$. Let p be any prime divisor of w. By definition of x, p divides either s or x, but not both. So, we have that p divides one summand of s + dx but not both: thus s + dx is coprime with w.

Theorem 4.7. Let m, n be integers with $m, n \equiv 2 \pmod{4}$. Then there exists a cyclic and *n*-symmetric HCS of $K_{m \times n}$.

Proof. In view of Propositions 4.2 and Theorem 4.1 we may assume $m = 2\overline{m} > 2$ and n = 4t + 2 > 2. Using the notation of Definition 4.5 take

$$s = \begin{cases} 3\overline{m} + 2 & \text{if } m \equiv 2 \pmod{8} \\ 3\overline{m} - 2 & \text{if } m \equiv 6 \pmod{8} \end{cases},$$

 $d = 4\overline{m}$ and $w = \frac{n}{2}$. Now Lemma 4.6 guarantees that the set $S(3\overline{m}\pm 2, 4\overline{m}, \frac{n}{2})$ contains an element $\nu = s + 2m\kappa$ coprime with $\frac{n}{2}$, where $0 \le \kappa \le \frac{n-6}{4}$. It is useful for the following to observe that $\gcd(\nu, mn) = 1$, as $\gcd(3\overline{m}\pm 2, \overline{m}) = 1$.

For all $i = 0, ..., \kappa$ consider the paths $Q_{i,1}$ as in (4.2) and, if $\kappa \ge 1$, for all $i = 0, ..., \kappa - 1$ consider the paths $P_{i,j}$ as in (4.1). As we have seen in Theorem 4.3, $A_{i,j} = [P_{i,j}]_2$ and $B_i = [Q_{i,1}]_m$ are hamiltonian cycles of $K_{m \times n}$ for any i, j.

If $t \ge \kappa + 2$, for all $i = \kappa + 1, \ldots, t - 1$, take also the following paths:

$$\widetilde{P}_{i,j} = \begin{cases} [0, (2i+1)m + (4j-1)] & \text{if } j = 1, \dots, \frac{\overline{m}-1}{2} \\ [0, (2i+1)m + (4j+1)] & \text{if } j = \frac{\overline{m}+1}{2}, \dots, \overline{m}-1 \end{cases}; \\ \widetilde{Q}_i = [0, (2i+1)m + (4\overline{m}-1), 1, (2i+1)m + (4\overline{m}-3), 3, \dots, \overline{m}-2, (2i+1)m + 3\overline{m}, \overline{m}+1, (2i+1)m + (3\overline{m}-1), \overline{m}+3, (2i+1)m + (3\overline{m}-3), \dots, 2\overline{m}-2, (2i+1)m + (2\overline{m}+2)]. \end{cases}$$

We define

$$u = \begin{cases} \frac{3\overline{m}+1}{4} & \text{if } m \equiv 2 \pmod{8} \\ \frac{3\overline{m}-1}{4} & \text{if } m \equiv 6 \pmod{8} \end{cases}$$

and take the paths:

$$\widetilde{R}_{j} = \begin{cases} [0, 2m\kappa + (4j-1)] & \text{if } j = 1, \dots, \frac{\overline{m}-1}{2} \\ [0, 2m\kappa + (4j+1)] & \text{if } j = \frac{\overline{m}+1}{2}, \dots, \overline{m}-1 \text{ and } j \neq u \end{cases}; \\ \widetilde{S} = [0, (2\kappa+1)m + (4\overline{m}-1), 1, (2\kappa+1)m + (4\overline{m}-2), 2, \dots, \frac{\overline{m}-1}{2}, (2\kappa+1)m + 3\overline{m}].$$

Now set $C_{i,j} = [\widetilde{P}_{i,j}]_2$, $D_i = [\widetilde{Q}_i]_m$, $E_j = [\widetilde{R}_j]_2$, $F = [\widetilde{S}]_m$ and $G = [0]_{\nu}$: these are all hamiltonian cycles of $K_{m \times n}$, and we have that for $j = 1, \ldots, \frac{\overline{m}-1}{2}$

$$\partial C_{i,j} = \pm \{ (2i+1)m + (4j-3), (2i+1)m + (4j-1) \}$$

and for $j = \frac{\overline{m}+1}{2}, \dots, \overline{m}-1$

$$\partial C_{i,j} = \pm \{(2i+1)m + (4j-1), (2i+1)m + (4j+1)\}$$

Also,

$$\begin{array}{lll} \partial D_i &=& \pm (\{(2i+1)m+2,(2i+1)m+4,(2i+1)m+6,\ldots,(2i+1)m+\\ && +2\overline{m}-2\} \cup \{(2i+1)m+2\overline{m}+2,(2i+1)m+2\overline{m}+4,\ldots,(2i+1)m+\\ && +4\overline{m}-2\} \cup \{(2i+1)m+2\overline{m}-1,(2i+1)m+4\overline{m}-1\}); \end{array}$$

moreover, for $j = 1, \ldots, \frac{\overline{m}-1}{2}$

$$\partial E_j = \pm \{2m\kappa + (4j-3), 2m\kappa + (4j-1)\}$$

and for $j = \frac{\overline{m}+1}{2}, \ldots, \overline{m}-1$ with $j \neq u$

$$\partial E_j = \pm \{ 2m\kappa + (4j-1), 2m\kappa + (4j+1) \}$$

Finally,

$$\partial F = \pm (\{(2\kappa + 2)m + 1, (2\kappa + 2)m + 2, \dots, (2\kappa + 3)m - 1\} \cup \{2m\kappa + 3\overline{m}\})$$

and $\partial G = \pm \{\nu\}.$

Let $\mathcal{B} = \{A_{i,j} \mid 0 \le i < \kappa, 1 \le j < \overline{m}\} \cup \{B_i \mid 0 \le i \le \kappa\} \cup \{C_{i,j} \mid \kappa < i < t, 1 \le j < \overline{m}\} \cup \{D_i \mid \kappa < i < t\} \cup \{E_j \mid 1 \le j < \overline{m}, j \ne u\} \cup \{F, G\}$. It is routine to check that $\partial \mathcal{B} = \mathbb{Z}_{mn} \setminus m\mathbb{Z}_{mn}$, hence we conclude that \mathcal{B} is a set of base cycles of a cyclic HCS of $K_{m \times n}$. Once more, it is easily checked using Lemma 2.7 that this cycle system is also *n*-symmetric, since in all cases the length of the orbit of each cycle divides *m*. \Box

We point out that the base cycles used in Example 2.4 were constructed following the proof of Theorem 4.7. In particular, according to the notation of the theorem we have

$$C_1 = B_0, \quad C_2 = F, \quad C_3 = E_1, \quad C_4 = E_2, \quad C_5 = E_3, \quad C_6 = G.$$

Example 4.8. Here we present a set of base cycles of a cyclic and 14-symmetric HCS of $K_{6\times 14}$. In the notation of Theorem 4.7, $\overline{m} = t = 3$ and we choose $\kappa = 1$ and $\nu = 19$ which is coprime with $6 \cdot 14$. Following the proof of the theorem we have to take the following cycles:

$$\begin{aligned} A_{0,1} &= [0,3]_2, \quad A_{0,2} &= [0,9]_2, \quad B_0 &= [0,11,1,9,4,8]_6, \quad B_1 &= [0,23,1,21,4,20]_6, \\ C_{2,1} &= [0,33]_2, \quad C_{2,2} &= [0,39]_2, \quad D_2 &= [0,41,1,39,4,38]_6, \quad E_1 &= [0,15]_2, \\ F &= [0,29,1,28,2,27]_6, \quad G &= [0]_{19}. \end{aligned}$$

It follows that

$$\begin{split} \partial\{A_{0,1},A_{0,2}\} &= \pm\{1,3,7,9\}, \ \ \partial\{B_0,B_1\} = \pm\{2,4,5,8,10,11,14,16,17,20,22,23\},\\ \partial\{C_{2,1},C_{2,2}\} &= \pm\{31,33,37,39\}, \ \ \ \partial D_2 = \pm\{32,34,35,38,40,41\},\\ \partial E_1 &= \pm\{13,15\}, \ \ \ \partial F = \pm\{21,25,26,27,28,29\}, \ \ \ \partial G = \pm\{19\}. \end{split}$$

So, letting \mathcal{B} be the set of the constructed cycles, we have $\partial \mathcal{B} = \mathbb{Z}_{84} \setminus 6\mathbb{Z}_{84}$.

Now, we give a set of base cycles of a cyclic and 10-symmetric HCS of $K_{10\times10}$. In the notation of Theorem 4.7, $\overline{m} = 5$, t = 2 and we choose $\kappa = 1$ and $\nu = 37$ which is coprime with 100. We have to take the following cycles:

$$A_{0,1} = [0,3]_2, \quad A_{0,2} = [0,7]_2, \quad A_{0,3} = [0,13]_2, \quad A_{0,4} = [0,17]_2,$$

$$B_0 = [0,19,1,17,3,15,6,14,8,12]_{10}, \quad B_1 = [0,39,1,37,3,35,6,34,8,32]_{10},$$

$$E_1 = [0,23]_2, \quad E_2 = [0,27]_2, \quad E_3 = [0,33]_2,$$

$$F = [0, 49, 1, 48, 2, 47, 3, 46, 4, 45]_{10}, \quad G = [0]_{37}.$$

We have:

$$\bigcup_{i=1}^{4} \partial A_{0,i} = \pm \{1, 3, 5, 7, 11, 13, 15, 17\},\$$

 $\partial \{B_0, B_1\} = \pm \{2, 4, 6, 8, 9, 12, 14, 16, 18, 19, 22, 24, 26, 28, 29, 32, 34, 36, 38, 39\},\$

$$\bigcup_{j=1}^{3} \partial E_j = \pm \{21, 23, 25, 27, 31, 33\},\$$

$$\partial F = \pm \{35, 41, 42, 43, 44, 45, 46, 47, 48, 49\}, \quad \partial G = \pm \{37\}.$$

Hence, letting \mathcal{B} be the set of the constructed cycles, we have $\partial \mathcal{B} = \mathbb{Z}_{100} \setminus 10\mathbb{Z}_{100}$.

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Distance labelings: a generalization of Langford sequences

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Abstract

A Langford sequence of order m and defect d can be identified with a labeling of the vertices of a path of order 2m in which each label from d up to d + m - 1 appears twice and in which the vertices that have been labeled with k are at distance k. In this paper, we introduce two generalizations of this labeling that are related to distances. The basic idea is to assign nonnegative integers to vertices in such a way that if n vertices (n > 1) have been labeled with k then they are mutually at distance k. We study these labelings for some well known families of graphs. We also study the existence of these labelings in general. Finally, given a sequence or a set of nonnegative integers, we study the existence of graphs that can be labeled according to this sequence or set.

Keywords: Langford sequence, distance *l*-labeling, distance *J*-labeling, δ -sequence, δ -set.

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1 Introduction

For the graph terminology not introduced in this paper we refer the reader to [14, 15]. For $m \leq n$, we denote the set $\{m, m + 1, \ldots, n\}$ by [m, n]. A *Skolem sequence* [8, 12] of order m is a sequence of 2m numbers $(s_1, s_2, \ldots, s_{2m})$ such that (i) for every $k \in [1, m]$ there exist exactly two subscripts $i, j \in [1, 2m]$ with $s_i = s_j = k$, (ii) the subscripts i and j satisfy the condition |i - j| = k. The sequence (4, 2, 3, 2, 4, 3, 1, 1) is an example of a Skolem sequence of order 4. It is well known that Skolem sequences of order m exist if and only if $m \equiv 0$ or 1 (mod 4).

Skolem introduced in [13] what is now called a *hooked Skolem sequence* of order m, where there exists a zero at the second to last position of the sequence containing 2m + 1 elements. Later on, in 1981, Abrham and Kotzig [1] introduced the concept of *extended Skolem sequence*, where the zero is allowed to appear in any position of the sequence. An extended Skolem sequence of order m exists for every m. The following construction was given in [1]:

$$(p_m, p_m-2, \dots, 2, 0, 2, \dots, p_m-2, p_m, q_m, q_m-2, \dots, 3, 1, 1, 3, \dots, q_m-2, q_m), (1.1)$$

where p_m and q_m are the largest even and odd numbers not exceeding m, respectively. Notice that from every Skolem sequence we can obtain two trivial extended Skolem sequences just by adding a zero either in the first or in the last position.

Let d be a positive integer. A Langford sequence of order m and defect d [11] is a sequence $(l_1, l_2, \ldots, l_{2m})$ of 2m numbers such that (i) for every $k \in [d, d + m - 1]$ there exist exactly two subscripts $i, j \in [1, 2m]$ with $l_i = l_j = k$, (ii) the subscripts i and j satisfy the condition |i - j| = k. Langford sequences, for d = 2, were introduced in [4] and they are referred to as *perfect Langford sequences*. Notice that, a Langford sequence of order m and defect d = 1 is a Skolem sequence of order m. Bermond, Brower and Germa on one side [2], and Simpson on the other side [11] characterized the existence of Langford sequences for every order m and defect d.

Theorem 1.1. [2, 11] A Langford sequence of order m and defect d exists if and only if the following conditions hold: (i) $m \ge 2d - 1$, and (ii) $m \equiv 0$ or 1 (mod 4) if d is odd; $m \equiv 0$ or 3 (mod 4) if d is even.

For a complete survey on Skolem-type sequences we refer the reader to [3]. For different constructions and applications of Langford type sequences we also refer the reader to [5, 6, 7, 9, 10].

1.1 Distance labelings

Let $L = (l_1, l_2, \ldots, l_{2m})$ be a Langford sequence of order m and defect d. Consider a path P with $V(P) = \{v_i : i = 1, 2, \ldots, 2m\}$ and $E(P) = \{v_i v_{i+1} : i = 1, 2, 2m - 1\}$. Then, we can identify L with a labeling $f : V(P) \rightarrow [d, d + m - 1]$ in such a way that, (i) for every $k \in [d, d + m - 1]$ there exist exactly two vertices $v_i, v_j \in [1, 2m]$ with $f(v_i) = f(v_j) = k$, (ii) the distance $d(v_i, v_j) = k$. Motivated by this fact, we introduce two notions of distance labelings, one of them associated with a positive integer l and the other one associated with a set of positive integers J.

Let G be a graph and let l be a nonnegative integer. Consider any function $f: V(G) \rightarrow [0, l]$. We say that f is a *distance labeling* of length l (or *distance l-labeling*) of G if the following two conditions hold, (i) either f(V(G)) = [0, l] or f(V(G)) = [1, l] and (ii)

if there exist two vertices v_i , v_j with $f(v_i) = f(v_j) = k$ then $d(v_i, v_j) = k$. Clearly, a graph can have many different distance labelings. We denote by $\lambda(G)$, the *labeling length* of G, the minimum l for which a distance l-labeling of G exists. We say that a distance l-labeling of G is proper if for every $k \in [1, l]$ there exist at least two vertices v_i , v_j of G with $f(v_i) = f(v_j) = k$. We also say that a proper distance l-labeling of G is regular of degree r (for short r-regular) if for every $k \in [1, l]$ there exist exactly r vertices v_{i_1} , v_{i_2} , ..., v_{i_r} with $f(v_{i_1}) = f(v_{i_2}) = \ldots = f(v_{i_r}) = k$. Clearly, if a graph G admits a proper distance l-labeling then $l \leq D(G)$, where D(G) is the diameter of G.

Let G be a graph and let J be a set of nonnegative integers. Consider any function $f: V(G) \to J$. We say that f is a *distance J-labeling* of G if the following two conditions hold, (i) f(V(G)) = J and (ii) for any pair of vertices v_i, v_j with $f(v_i) = f(v_j) = k$ we have that $d(v_i, v_j) = k$. We say that a distance J-labeling is *proper* if for every $k \in J \setminus \{0\}$ there exist at least two vertices v_i, v_j with $f(v_i) = f(v_j) = k$. We also say that a proper distance J-labeling of G is *regular* of degree r (for short r-regular) if for every $k \in J \setminus \{0\}$ there exist exactly r vertices $v_{i_1}, v_{i_2}, \ldots, v_{i_r}$ with $f(v_{i_1}) = f(v_{i_2}) = \ldots = f(v_{i_r}) = k$. Clearly, a distance l-labeling is a distance J-labeling in which either J = [0, l] or J = [1, l]. Thus, the notion of a J-labeling is more general than the notion of a l-labeling.

In this paper, we provide the labeling length of some well known families of graphs. We also study the inverse problem, that is, for a given pair of positive integers l and r we ask for the existence of a graph of order lr with a regular l-labeling of degree r. Finally, we study a similar question when we deal with J-labelings. The organization of the paper is as follows. Section 2 is devoted to l-labelings; we start calculating the labeling length of complete graphs, paths, cycles and some others families. The inverse problem is studied in the second part of the section. Section 3 is devoted to the inverse problem in J-labelings. There are many open problems that remain to be solved, we end the paper by presenting some of them.

2 Distance *l*-labelings

We start this section by providing the labeling length of some well-known families of graphs. By definition, $\lambda(K_1) = 0$. In what follows, we only consider graphs of order at least 2.

Proposition 2.1. Let $n \ge 2$. The complete graph K_n has $\lambda(K_n) = 1$.

Proof. By assigning the label 1 to all vertices of K_n , we obtain a distance 1-labeling of it.

Proposition 2.2. Let $n \ge 2$. The path P_n has $\lambda(P_n) = \lfloor n/2 \rfloor$.

Proof. By a previous comment, we know that a Skolem sequence of order m exists if $m \equiv 0$ or 1 (mod 4). This fact together with (1.1) guarantees the existence of a proper distance $\lfloor n/2 \rfloor$ -labeling when $n \not\equiv 4, 6 \pmod{8}$. By removing one of the end labels of (1.1), we obtain a (non proper) distance labeling of length $\lfloor n/2 \rfloor$. Thus, we have that $\lambda(P_n) \leq \lfloor n/2 \rfloor$. Since there are no three vertices in the path which are at the same distance, this lower bound turns out to be an equality.

The sequence that appears in (1.1) also works for constructing proper distance labelings of cycles. Thus, we obtain the next result.

Proposition 2.3. Let $n \ge 3$. The cycle C_n has

$$\lambda(C_n) = \begin{cases} (n-2)/2, & n \neq 6, n \text{ is divisible by } 6, \\ \lfloor n/2 \rfloor, & otherwise. \end{cases}$$

Proof. Since, except for n divisible by 3, there are no three vertices in the cycle C_n which are at the same distance, we have that $\lambda(C_n) \ge \lfloor n/2 \rfloor$. The sequence that appears in (1.1) allows us to construct a (proper) distance $\lfloor n/2 \rfloor$ -labeling of C_n when n is odd. Moreover, if n even not divisible by 3 we can obtain a distance $\lfloor n/2 \rfloor$ -labeling of C_n from the sequence that appears in (1.1) just by removing the end odd label. Suppose now that n is divisible by 3. If n is odd or n = 6, at least $\lfloor n/2 \rfloor$ labels are needed to obtain a distance labeling of C_n . Thus, $\lambda(C_n) = \lfloor n/2 \rfloor$.

So, in what follows we will assume that n is divisible by 6. Since there are three vertices in the cycle which are at the same distance, we have that $\lambda(C_n) \ge (n-2)/2$. Let p_m and q_m be the largest even and odd numbers, respectively, not exceeding (n-2)/2. If $n \equiv 0, 4 \pmod{8}$ then the sequence $(p_m, p_m - 2, \ldots, 2, q_m, 2, \ldots, p_m - 2, p_m, 0, q_m - 2, q_m - 4, \ldots, 3, q_m, n/3, 3, 5, \ldots, q_m - 2, 1, 1)$ defines a (proper) distance (n-2)/2-labeling of C_n . If $n \equiv 6 \pmod{8}$ then $(p_m - 2, p_m - 4, \ldots, 2, p_m, 2, \ldots, p_m - 4, p_m - 2, 0, q_m, q_m - 2, \ldots, 3, p_m, n/3, 3, 5, \ldots, q_m - 2, q_m, 1, 1)$ defines a (proper) distance (n-2)/2-labeling of C_n . Finally, if $n \equiv 2 \pmod{8}$, then the sequence $(p_m, p_m - 2, \ldots, 2, n/6 + \lceil n/12 \rceil + 2, n/6 + \lceil n/12 \rceil - 2, n/6 + \lceil n/12 \rceil - 4, \ldots, 3, 0, n/3, 3, 5, \ldots, n/6 + \lceil n/12 \rceil - 2, 1, 1, n/6 + \lceil n/12 \rceil + 2, n/6 + \lceil n/12 \rceil + 4, \ldots, q_m)$ defines a (proper) distance (n-2)/2-labeling of C_n .

Proposition 2.4. The star $K_{1,k}$ has $\lambda(K_{1,k}) = 2$ when $k \ge 3$, and $\lambda(K_{1,k}) = 1$ otherwise.

Proof. For $k \ge 3$, consider a labeling f that assigns the label 1 to the central vertex and to one of its leaves, and that assigns label 2 to the other vertices. Then f is a (proper) distance 2-labeling of $K_{1,k}$. For $1 \le k \le 2$, the sequences 1 - 1 and 0 - 1 - 1, where 0 is assigned to a leaf, give a (proper) distance 1-labeling of $K_{1,1}$ and $K_{1,2}$, respectively.

Proposition 2.5. Let m and n be integers with $2 \le m \le n$. Then, $\lambda(K_{m,n}) = m$. In particular, the graph $K_{m,n}$ admits a proper distance l-labeling if and only if $m \in \{1, 2\}$.

Proof. Let X and Y be the stable sets of $K_{m,n}$, with |X| = m and |Y| = n. We have that $D(K_{m,n}) = 2$, however the maximum number of vertices that are mutually at distance 2 is n. Thus, by assigning label 2 to all vertices, except one, in Y, 1 to the remaining vertex in Y and to one vertex in X, 0 to another vertex of X we still have left m - 2 vertices in X to label.

Proposition 2.6. Let n and k be positive integers with $n \ge 2$ and $k \ge 3$. Let S_k^n be the graph obtained from $K_{1,k}$ by replacing each edge with a path of n edges. Then

$$\lambda(S_k^n) = \begin{cases} 2(n-1), & \text{if } k = n-1, \\ 2n-1, & \text{if } k = n, \\ 2n, & \text{if } k > n. \end{cases}$$

Moreover, for k < n - 1, the graph S_k^n admits an *l*-distance labeling, where $2(n - o) \le l \le 2(n - o) + 1$, and $\lfloor (2n - 1)/(2k + 1) \rfloor \le o \le \lfloor (2n + 2)/(2k + 1) \rfloor$.

Proof. Suppose that S_k^n admits a distance *l*-labeling with l < 2n. Then, all the labels assigned to leaves should be different and they appear at most twice. Moreover, although each even label could appear *k*-times, one for each of the *k* paths that are joined to the star $K_{1,k}$, odd labels also appear at most twice (either in the same or in two of the original forming paths). Thus, once we fix the labels of leaves, we still have to assign a label to at least (k-2)(n-2) + 1 vertices. Thus, at least 2n-2 labels are needed for obtaining a distance labeling of S_k^n , when $k \ge n-1$. The following construction provides a distance 2(n-1)-labeling of S_k^n , when k = n - 1. Suppose that we label the central vertices of each path using the pattern $2 - 4 - \ldots - 2(n-1)$. Then, add odd labels to the leaves. For the case k = n, we need to introduce a new odd label, which corresponds to 2n - 1. Finally, when k > n, we cannot complete a distance *l*-labeling without using 2n labels. Fig. 1 provides a proper 2n-labeling that can be generalized in that case.

The case k < n-1 requires a more detailed study. Consider the labeling of S_k^n obtained by assigning the labels in the sequence $0 - 2 - 4 - \ldots - 2(n - o) - s_1^i - s_2^i - \ldots - s_o^i$ to the vertices of the path P^i , $i = 1, \ldots, k$, where 0 is the label assigned to the central vertex of S_k^n , and $\{s_j^i\}_{i=1,\ldots,k}^{j=1,\ldots,o}$ is the (multi)set of odd labels, if necessary, we replace some of the even labels by the remaining odd labels. By considering the patern 1 - 1, 3 - 1 - 1 - 3, 5 - 3 - 1 - 1 - 3 - 5 to the vertices of one of the paths, it can be checked that, the graph S_k^n admits an *l*-distance labeling with $l \in \{2(n - o), 2(n - o) + 1\}$ and

$$\left\lfloor \frac{2n-1}{2k+1} \right\rfloor \le o \le \lfloor \frac{2n+2}{2k+1} \rfloor.$$

More specifically, if $\lfloor (2n-1)/(2k+1) \rfloor = \lfloor (2n+2)/(2k+1) \rfloor$ then $o = \lfloor (2n-1)/(2k+1) \rfloor$ and l = 2(n-o). If $\lfloor (2n-1)/(2k+1) \rfloor + 1 = \lfloor (2n)/(2k+1) \rfloor$ then $o = \lfloor (2n)/(2k+1) \rfloor$ and l = 2(n-o)+1. Finally, if $\lfloor (2n)/(2k+1) \rfloor + 1 = \lfloor (2n+1)/(2k+1) \rfloor$ then $o = \lfloor (2n+1)/(2k+1) \rfloor$ and l = 2(n-o)+1.

Fig. 2 and Fig. 3 show proper distance labelings of S_4^5 and S_5^5 , respectively, that have been obtained by using the above constructions, and then, combining pairs of paths (whose end odd labels sum up to 8) for obtaining a proper distance 8-labeling and 9-labeling, respectively.



Figure 1: A proper distance 10-labeling of S_6^5 .

Proposition 2.7. For $n \ge 3$, let W_n be the wheel of order n + 1. Then $\lambda(W_n) = \lceil n/2 \rceil$.

Proof. Except for W_3 , all wheels have $D(W_n) = 2$. The maximum number of vertices that are mutually at distance 2 is $\lfloor n/2 \rfloor$ and all of them are in the cycle. Thus, by assigning



Figure 3: A proper distance 9-labeling of S_5^5 .

label 2 to all these vertices, 0 to one vertex of the cycle and 1 to the central vertex and to one vertex of the cycle, we still have to label $\lceil n/2 \rceil - 2$ vertices.

Proposition 2.8. For $n \ge 2$, let F_n be the fan of order n + 1. Then $\lambda(F_n) = \lfloor n/2 \rfloor$.

Proof. Except for F_2 , all fans have $D(F_n) = 2$. The maximum number of vertices that are mutually at distance 2 is $\lceil n/2 \rceil$ and all of them are in the path. Thus, by assigning label 2 to all these vertices, 0 to one vertex of the path, 1 to the central vertex and to one vertex of the path when n is even and to two vertices when n is odd, we still have to label $\lfloor n/2 \rfloor - 2$ vertices.

2.1 The inverse problem

For every positive integer l, there exists a graph G of order l with a trivial l-labeling that assigns a different label in [1, l] to each vertex. In this section, we are interested in the existence of a graph G that admits a proper distance l-labeling.

We are now ready to state and prove the next result.

Theorem 2.9. For every pair of positive integers l and $r, r \ge 2$, there exists a graph G of order lr with a regular l-labeling of degree r.

Proof. We give a constructive proof. Assume first that l is odd. Let G be the graph obtained from the complete graph K_r by identifying r-1 vertices of K_r with one of the end vertices of a path of length $\lfloor l/2 \rfloor$ and the remaining vertex of K_r with the central vertex of the graph $S_{r+1}^{\lfloor l/2 \rfloor}$. That is, G is obtained from K_r by attaching 2r paths of length $\lfloor l/2 \rfloor$ to its vertices, r+1 to a particular vertex v_1 of K_r and exactly one path to each of the remaining vertices $F = \{v_2, v_3, \ldots, v_r\}$ of K_r . Now, consider the labeling f of G that assigns 1 to the vertices of K_r , the sequence $1 - 3 - \ldots - l$ to the vertices of the paths attached to F and one of the paths attached to v_1 , and the sequence $1 - 2 - 4 - \ldots - (l-1)$ to the remaining paths. Then f is a regular l-labeling of degree r of G. Assume now that l is even. Let Gbe the graph obtained in the above construction for l - 1. Then, by adding a leaf to each vertex of G labeled with l-2 we obtain a new graph G' that admits a regular l-labeling f' of degree r. The labeling f' can be obtained from the labeling f of G, defined above, just by assigning the label l to the new vertices.



Figure 4: A regular 5-labeling of degree 4 of a graph G.



Figure 5: A regular 6-labeling of degree 4 of a graph G'.

Notice that, the graph provided in the proof of Theorem 2.9 also has $\lambda(G) = l$. Figs 4 and 5 show examples for the above construction. The pattern provided in the proof of the above theorem, for r = 2, can be modified in order to obtain the following lower bound for the size of a graph G as in Theorem 2.9.

Proposition 2.10. For every positive integer *l* there exists a graph of order 2*l* and size (l+2)(l+1)/2 - 2 that admits a regular distance *l*-labeling of degree 2.

Proof. Let G be the graph of order 2l and size (l+1)l/2 + l - 1, obtained from K_{l+1} and the path P_l by identifying one of the end vertices u of P_l with a vertex v of K_{l+1} . Let f be the labeling of G that assigns the sequence $1 - 2 - 3 - \ldots - l$ to the vertices of P_l and $1 - 1 - 2 - \ldots - l$ to the verticalces of K_{l+1} in such a way that the vertex obtained by identifying u and v is labeled 1. Then, f is a 2-regular l-labeling of G.

Thus, a natural question appears.

Question 2.11. Can we find graphs that admit a regular distance *l*-labeling of degree 2 which have bigger density (where by density we refer the number of edges in relation to the number of vertices) than the one of Proposition 2.10?

We end this section by introducing an open question related to complexity.

Question 2.12. What is the algorithmic complexity of computing $\lambda(G)$ for a general graph *G*? What about for a tree?

3 Distance *J*-labelings

It is clear from the definition that to say that a graph admits a (proper) distance l-labeling is the same as to say that the graph admits either a (proper) distance [0, l]-labeling or a (proper) distance [1, l]-labeling. That is, we relax the condition on the labels, the set of labels is not necessarily a set of consecutive integers. In this section, we study which kind of sets J can appear as the set of labels of a graph that admits a distance J-labeling.

The following easy fact is obtained from the definition.

Lemma 3.1. Let G be a graph with a proper distance J-labeling f. Then $J \subset [0, D(G)]$, where D(G) is the diameter of G.

3.1 The inverse problem: distance *J*-labelings obtained from sequences.

We start with a definition. Let $S = (s_1, s_1, \ldots, s_1, s_2, \ldots, s_2, \ldots, s_l, \ldots, s_l)$ be a sequence of nonnegative integers where, (i) $s_i < s_j$ whenever i < j and (ii) each number s_i appears k_i times, for $i = 1, 2, \ldots, l$. We say that S is a δ -sequence if there is a simple graph G that admits a partition of the vertices $V(G) = \bigcup_{i=1}^l V_i$ such that, for all $i \in \{1, 2, \ldots, l\}$, $|V_i| = k_i$, and if $u, v \in V_i$ then $d_G(u, v) = s_i$. The graph G is said to realize the sequence S.

Let $\Sigma = \{s_1 < s_2 < \ldots < s_l\}$ be a set of nonnegative integers. We say that Σ is a δ -set with n degrees of freedom or a δ_n -set if there is a δ -sequence S of the form $S = (s_1, s_1, \ldots, s_1, s_2, \ldots, s_2, \ldots, s_l, \ldots, s_l)$, in which the following conditions hold: (i) all, except n numbers different from zero, appear at least twice, and (ii) if $s_1 = 0$ then 0 appears exactly once in S. We say that any graph realizing S also realizes Σ . If n = 0 we simply say that Σ is a δ -set. Let us notice that an equivalent definition for a δ -set is the following: Σ is a δ -set if there exists a graph G that admits a proper distance Σ -labeling.

Proposition 3.2. Let $\Sigma = \{1 = s_1 < s_2 < \ldots < s_l\}$ be a set such that $s_i - s_{i-1} \leq 2$, for $i = 1, 2, \ldots, l$. Then Σ is a δ -set. Furthermore, there is a caterpillar of order 2l that realizes Σ .

Proof. We claim that for each set $\Sigma = \{1 = s_1 < s_2 < \ldots < s_l\}$ such that $s_i - s_{i-1} \leq 2$ there is a caterpillar of order 2l that admits a 2-regular distance Σ -labeling in which the label s_l is assigned to exactly two leaves. The proof is by induction on l. For l = 1, the path P_2 admits a 2-regular distance $\{1\}$ -labeling, and for l = 2, the star $K_{1,3}$ and the path P_4 admit a 2-regular distance $\{1,2\}$ -labeling and a 2-regular distance $\{1,3\}$ -labeling, respectively. Assume that the claim is true for l and let $\Sigma = \{1 = s_1 < s_2 < \ldots < s_{l+1}\}$ such that $s_i - s_{i-1} \leq 2$. Let $\Sigma' = \Sigma \setminus \{s_{l+1}\}$. By the induction hypothesis, there is a caterpillar G' of order 2l that admits a regular distance Σ' -labeling of degree 2 in which the label s_l is assigned to leaves, namely, u_1 and u_2 . Let $u \in V(G')$ be the (unique) vertex

in G' adjacent to u_1 . Then, if $s_{l+1} - s_l = 2$, the caterpillar obtained from G' by adding two new vertices v_1 and v_2 and the edges $u_i v_i$, for i = 1, 2, admits a regular distance Σ -labeling of degree 2 in which the label s_{l+1} is assigned to leaves $\{v_1, v_2\}$. Otherwise, if $s_{l+1} - s_l = 1$ then the caterpillar obtained from G' by adding two new vertices v_1 and v_2 and the edges uv_1 and u_2v_2 admits a regular distance Σ -labeling of degree 2 in which the label s_{l+1} is assigned to leaves $\{v_1, v_2\}$. This proves the claim. To complete the proof, we only have to consider the vertex partition of G defined by the vertices that receive the same label. \Box

Proposition 3.2 provides us with a family of δ -sets, in which, if we order the elements of each δ -set, we get that the differences between consecutive elements are at most 2. This fact may lead us to get the idea that the differences between consecutive elements in δ -sets cannot be too large. This is not true in general and we show it in the next result.

Theorem 3.3. Let $\{k_1, k_2, ..., k_n\}$ be a set of positive integers. Then there exists a δ -set $\Sigma = \{s_1 < s_2 < ... < s_l\}$ and a set of indices $\{1 \le j_1 < j_2 < ... < j_n\}$, with $j_n < l-1$, such that

$$s_{j_1+1} - s_{j_1} = k_1, \ s_{j_2+1} - s_{j_2} = k_2, \dots, \ s_{j_n+1} - s_{j_n} = k_n.$$

Moreover, s_1 can be chosen to be any positive integer.

Proof. Choose any number $d_1 \in \mathbb{N}$ and choose any Langford sequence of defect d_1 (such a sequence exists by Theorem 1.1. We let $d_1 = s_1$. (Notice that if $d_1 = 1$ then the sequence is actually a Skolem sequence). Let this Langford sequence be L_1 . Next, choose a Langford sequence L_2 with defect max $L_1 + k_1$. Next, choose a Langford sequence L_3 with defect max $L_2 + k_2$. Continue this procedure until we have used all the values k_1, k_2, \ldots, k_n . At this point create a new sequence L, where L is the concatenation of $L_1, L_2, \ldots, L_{n+1}$ and label the vertices of the path P_r , $r = \sum_{i=1}^{n+1} |L_i|$, with the elements of L keeping the order in the labeling induced by the sequence L. This shows the result.

The next result shows that there are sets that are not δ -sets.

Proposition 3.4. The set $\Sigma = \{2, 3\}$ is not a δ -set.

Proof. The proof is by contradiction. Assume to the contrary that $\Sigma = \{2, 3\}$ is a δ -set. That is to say, we assume that there exists a sequence S consisting of k_1 copies of 2 and k_2 copies of 3 that is a δ -sequence. Let G be a graph that realizes S and $V_1 \cup V_2$ the partition of V(G) defined as follows: if $u, v \in V_i$ then $d_G(u, v) = i + 1$, for i = 1, 2. It is clear that V_1 must be formed by the leaves of a star with center some vertex $a \in V$. Since a is at distance 1 of any vertex in V_1 , it follows that a must be in V_2 and furthermore, all vertices adjacent to a must be in V_1 . Thus, there are no two adjacent vertices in the neighborhood of a. At this point, let $b \in V_2 \setminus \{a\}$. Then, there is a path of the form a, u_1, u_2, b , where $u_1 \in V_1$ and hence, $u_2, b \in V_2$. This contradicts the fact that $d_G(u_2, b) = 1$.

The above proof works for any set of the form $\Sigma = \{2, n\}$, for $n \ge 3$. Thus, in fact, Proposition 3.4 can be generalized as follows.

Proposition 3.5. The set $\Sigma = \{2, n\}$ is not a δ -set.

Notice that, although $\Sigma = \{2, n\}$ is not a δ -set, it is a δ_1 -set, since we can consider a star in which the center is labeled with n and the leaves with 2.

The next result gives a lower bound on the size of δ -sets in terms of the maximum of the set.

Theorem 3.6. Let Σ be a δ -set with $s = \max \Sigma$. Then, $|\Sigma| \ge \lceil (s+1)/2 \rceil$.

Proof. Let G be a graph that realizes Σ and let $V(G) = \bigcup_{i \in \Sigma} V_i$ be the partition defined as follows: if $u, v \in V_i$ then $d_G(u, v) = i$. Let $a_1, a_2 \in V_s$. At this point, let $P = b_1b_2 \dots b_{s+1}$ be a path of length s starting at a_1 and ending at a_2 . We claim that there are no three vertices in V(P) belonging to the same set $V_j, j \in \Sigma$. Assume to the contrary that there exist vertices u, v and $w \in V(P)$ such that $d_G(u, v) = d_G(u, w) = d_G(v, w)$. Then, we also obtain that $d_P(u, v) = d_P(v, w) = d_P(v, w)$ (since they are on a shortest path between two points), a contradiction. Hence, each set in the partition of V(G) can contain at most two vertices of P. Since |V(P)| = s + 1, it follows that we need at least $\lceil (s+1)/2 \rceil$ sets in the partition of V(G). Therefore, we obtain that $|\Sigma| \ge \lceil (s+1)/2 \rceil$. \Box

It is clear that the above proof cannot be improved in general, since from Proposition 3.2 we get that the any set of the form $\{1, 3, 5, ..., 2n + 1\}$ is a δ -set and $|\{1, 3, 5, ..., 2n + 1\}| = \lceil (2n+2)/2 \rceil$. Furthermore, Proposition 3.5 for $n \ge 4$ is an immediate consequence of the above result. It is also worth to mention that there are sets which meet the bound provided in Theorem 3.6, however they are not δ -sets. For instance, the set $\{2, 3\}$ considered in Proposition 3.4. From this fact, it seems that we cannot characterize δ -sets just from a density point of view. Next we want to propose the following open problem.

Problem 3.7. Characterize δ -sets.

Let Σ be a set. By construction, a path of order $|\Sigma|$ in which each vertex receives a different labeling of Σ defines a distance $|\Sigma|$ -labeling. That is, every set is a $\delta_{|\Sigma|}$ -set. So, according to that, we propose the next problem.

Problem 3.8. Given a set Σ is there a construction that provides the minimum r such that Σ is a δ_r -set?

Thus, the above problem is a bit more general than Open problem 3.7.

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Independent sets on the Towers of Hanoi graphs*

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Abstract

The number of independent sets is equivalent to the partition function of the hardcore lattice gas model with nearest-neighbor exclusion and unit activity. In this article, we mainly study the number of independent sets $i(H_n)$ on the Tower of Hanoi graph H_n at stage n, and derive the recursion relations for the numbers of independent sets. Upper and lower bounds for the asymptotic growth constant μ on the Towers of Hanoi graphs are derived in terms of the numbers at a certain stage, where $\mu = \lim_{v \to \infty} \frac{\ln i(G)}{v(G)}$ and v(G) is the number of vertices in a graph G. Furthermore, we also consider the number of independent sets on the Sierpiński graphs which contain the Towers of Hanoi graphs as a special case.

Keywords: Independent sets, the Tower of Hanoi graph, Sierpiński graph, recursion relation, asymptotic growth constant, asymptotic enumeration.

Math. Subj. Class.: 05C30, 05C69

1 Introduction

Counting sets satisfying a fixed property in graphs ranges among the classical tasks of combinatorics. There is a vast amount of literatures on this kind of combinatorial problems for various classes of graphs, especially for Sierpiński graphs, by different authors. We note that the set counting problems such as the number of independent sets and the number of matchings have been studied in the past [2, 4, 9, 10, 11, 26, 35, 36].

On one hand, all these graph invariants reflect the structure of a graph in some way, and therefore, some of them are even of interest in theoretical chemistry for the study of molecular graphs (see [32, 38]). For example, the number of independent sets is called

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Merrifield-Simmons index, the number of matchings is known as Hosoya index in chemistry. It was shown that both correlate well with physicochemical properties of the corresponding molecules (see [23, 30]).

On the other hand, the number of independent sets is equivalent to the partition function of the hard-core lattice gas model with nearest-neighbor exclusion and unit activity. The lattice gas with repulsive pair interaction is an important model in statistical mechanics [3, 13, 16, 33]. For the special case with hard-core nearest-neighbor exclusion such that each site can be occupied by at most one particle and no pair of adjacent sites can be simultaneously occupied, the partition function of the lattice gas coincides with the independence polynomial in combinatorics [14, 34]. This model is a problem of interest in mathematics [39, 15, 24]. The growth of the number of independent sets in the $m \times n$ grid graph is of interest in statistical physics (see [1]). It is known that the number of independent sets in the $m \times n$ grid graph grows with α^{mn} , where $\alpha = 1.503048082\cdots$ is the so-called hard square entropy constant. The bound for this constant was successively improved by Weber [40], Engel [9] and Calkin and Wilf [4].

The number of independent sets and its bounds had been considered on various graphs [27, 29, 41]. It is of interest to consider independent sets on self-similar fractal lattices which have scaling invariance rather than translational invariance [35]. The recursion relations for the numbers of independent sets on the Sierpiński gasket were derived by Chang, Chen and Yan [6]. A special type of self-similar graph that has been of interest is the Hanoi graph, which has been extensively studied in several contexts [5, 7, 8, 12, 17, 18, 19, 20, 22, 25, 28, 31]. This graph, which is also known as the Tower of Hanoi graph, came from the well known Tower of Hanoi puzzle, as the graph is associated to the allowed moves in this puzzle. We shall derive the recursion relations for the numbers of independent sets on the Tower of Hanoi graphs are derived in terms of the numbers at a certain stage, where $\mu = \lim_{v\to\infty} \frac{\ln i(G)}{v(G)}$, i(G) and v(G) are the number of independent sets and the number of vertices in a graph G, respectively. Furthermore, we also consider the Sierpiński graphs which include the Towers of Hanoi graphs as a special case.

2 Preliminaries

We recall some basic definitions about graphs. A graph G = (V, E) with vertex set V and edge set E is always supposed to be undirected, without loops or multiple edges. Vertices x and y are adjacent if xy is an edge in E. Let v(G) = |V| be the number of vertices and e(G) = |E| the number of edges in G. An independent set is a subset of the vertices such that any two of them are not adjacent. When the number i(G) of independent sets in G grows exponentially with v(G) as $v(G) \to \infty$, let us define a constant μ describing this exponential growth:

$$\mu = \lim_{v(G) \to \infty} \frac{\ln i(G)}{v(G)}.$$

We will see that the limit exists for the Towers of Hanoi graphs and some other Sierpiński graphs considered in this paper.

There are many different approaches to construct self-similar graphs. A construction that is specifically geared to be used in the context of enumeration was described in [35], it is no restated and we will also make use of it here. Some examples can be seen in [37].

The Tower of Hanoi graph (or the Hanoi graph), invented in 1883 by the French math-



Figure 1: The Towers of Hanoi graphs H_0 , H_1 , H_2 and the construction of H_n .

ematician Edouard Lucas, has become a classic example in the analysis of algorithms and discrete mathematical structures. There exists an abundant literature on the properties of the Hanoi graph, which includes the study of shortest paths, average eccentricity, to name a few, see [21] and references therein. The Hanoi graph H_n is derived from the Tower of Hanoi puzzle with n discs. The vertices of the graph H_n in this sequence correspond to all possible configurations of the game Tower with n + 1 disks and three rods, whereas the edges describe transitions between configurations, see [17], and these graphs are finite Schreier graphs of the Hanoi tower group in [12]. Note that the Tower of Hanoi graph can be constructed by the following recursive-modular method. For n = 0, H_0 is the complete graph K_3 (also called a 3-clique or triangle). For $n \ge 1$, H_n is obtained from three copies of H_{n-1} joined by three new edges, each one connecting a pair of vertices from two different replicas of H_{n-1} , as show in Figure 1. From the construction rule, we can find that the number of vertices of H_n is $3^{n+2}-3$.

3 The number of independent sets on H_n

In this section, we will derive the asymptotic growth constant for the number of independent sets on the Tower of Hanoi graph H_n in detail.

For the Tower of Hanoi graph H_n , i_n is its number of independent sets, f_n is its number of independent sets such that all three outmost vertices are not in the vertex subset, g_n is its number of independent sets such that only one specified vertex of three outmost vertices is in the vertex subset, h_n is its number of independent sets such that exact two specified vertices of the three outmost vertices are in the vertex subset, p_n is its number of independent sets such that all three outmost vertices are in the vertex subset. They are illustrated in Figures 2–5, where only the outmost vertices are shown and a solid circle is in the independent set and an open circle is not. Because of rotational symmetry, there are three possible g_n and three possible h_n such that

$$i_n = f_n + 3g_n + 3h_n + p_n$$

and $f_0 = g_0 = 1$, $h_0 = p_0 = 0$, $i_0 = f_0 + 3g_0 + 3h_0 + p_0 = 4$.

Lemma 3.1. For any nonnegative integer n, we have

$$\begin{split} f_{n+1} =& f_n^3 + 6f_n^2 g_n + 3f_n^2 h_n + 9f_n g_n^2 + 6f_n g_n h_n + 2g_n^3, \\ g_{n+1} =& f_n^2 g_n + 2f_n^2 h_n + f_n^2 p_n + 4f_n g_n^2 + 8f_n g_n h_n + 2f_n g_n p_n + 2f_n h_n^2 + 3g_n^3 \\ &\quad + 4g_n^2 h_n, \\ h_{n+1} =& f_n g_n^2 + 4f_n g_n h_n + 2f_n g_n p_n + 3f_n h_n^2 + 2f_n h_n p_n + 2g_n^3 + 7g_n^2 h_n + 2g_n^2 p_n \\ &\quad + 4g_n h_n^2, \\ p_{n+1} =& g_n^3 + 6g_n^2 h_n + 3g_n^2 p_n + 9g_n h_n^2 + 6g_n h_n p_n + 2h_n^3. \end{split}$$

Proof. Note that the number f_{n+1} consists of (i) one configuration where all three H_n belong to the class that enumerated by f_n ; (ii) six configurations where one of the H_n belongs to the class that enumerated by g_n and the other two belong to the class that enumerated by f_n ; (iii) three configurations where one of the H_n belongs to the class that enumerated by h_n and the other two belong to the class that enumerated by h_n and the other two belong to the class that enumerated by h_n and the other two belong to the class that enumerated by f_n ; (iv) nine configurations where one of the H_n belongs to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and the other two belong to the class that enumerated by f_n and h_n , respectively; (vi) two configurations where all three H_n belong to the class that enumerated by g_n as illustrated in Figure 2. And

$$f_{n+1} = f_n^3 + 6f_n^2g_n + 3f_n^2h_n + 9f_ng_n^2 + 6f_ng_nh_n + 2g_n^3$$

is verified by adding these configurations.

Similarly, the expressions of g_{n+1} , h_{n+1} and p_{n+1} can be obtained with appropriate configurations of its three H_n as illustrated in Figures 3–5.



Figure 2: Illustration for the expression of f_{n+1} . The multiplication of three on the righthand-side corresponds to the three possible orientations of H_{n+1} , the multiplication of two on the right-hand-side corresponds to reflection symmetry with respect to the central vertical axis and the multiplication of six on the right-hand-side corresponds to the six possible of considering both orientations and reflection symmetry.

In the following, we will estimate the value $\mu = \lim_{v \to \infty} \frac{\ln i(H_n)}{v(H_n)}$ of the asymptotic growth constant for the Tower of Hanoi graph H_n . The values of f_n, g_n, h_n, p_n for small n are listed in Table 1 by Lemma 3.1, and grow exponentially. For the Tower of Hanoi graph H_n , define the ratios

$$\alpha_n = \frac{g_n}{f_n}, \quad \beta_n = \frac{h_n}{g_n}, \quad \gamma_n = \frac{p_n}{h_n}$$

where *n* is a positive integer. Their values for small *n* are listed in Table 2. From the initial values of f_n, g_n, h_n, p_n , it is easy to see that $f_n > g_n > h_n > p_n$ for all positive integer *n* by induction. Alternatively, these inequalities can be obtained by an injection. For instance, if one of the independent sets enumerated by g_n is given, one can remove



Figure 3: Illustration for the expression of g_{n+1} . The multiplication of two on the righthand-side are corresponds to the reflection symmetry with respect to the central vertical axis.



Figure 4: Illustration for the expression of h_{n+1} . The multiplication of two on the righthand-side are corresponds to the reflection symmetry with respect to the central vertical axis.



Figure 5: Illustration for the expression of p_{n+1} . The multiplication of three on the righthand-side corresponds to the three possible orientations of H_{n+1} , the multiplication of two on the right-hand-side corresponds to reflection symmetry with respect to the central vertical axis and the multiplication of six on the right-hand-side corresponds to the six possible of considering both orientations and reflection symmetry.

f_n and f_n and f_n on f_n .					
n	0	1	2	3	
f_n	1	18	38284	342408411795232	
g_n	1	8	15840	141595222762112	
h_n	0	3	6546	58553484583728	
p_n	0	1	2702	24213460330512	
i_n	4	52	108144	967067994163264	

Table 1: The first few values of f_n, g_n, h_n, p_n and i_n on H_n .

the corner vertex to obtain another independent set that are enumerated by f_n such that $f_n > g_n$ is established. Similarly, other two inequalities can be established. It follows that $\alpha_n, \beta_n, \gamma_n \in (0, 1)$.

Table 2. The first few values of $\alpha_n, \beta_n, \gamma_n$ of Π_n .							
n	1	2	3				
α_n	0.444444444444444	0.413749869397137	0.413527290465016				
β_n	0.375	0.41325757575757575	0.413527260606109				
γ_n	0.333333333333333333	0.412771157959058	0.413527230747269				

Table 2: The first few values of $\alpha_n, \beta_n, \gamma_n$ on H_n

Lemma 3.2. For any positive integer n, the ratios satisfy

$$\alpha_n > \beta_n > \gamma_n.$$

When n increases, the ratio α_n decreases monotonically while γ_n increases monotonically. The three ratios in the large n limit are equal to each other

$$\lim_{n \to \infty} \alpha_n = \lim_{n \to \infty} \beta_n = \lim_{n \to \infty} \gamma_n.$$

Proof. By the definition of $\alpha_n, \beta_n, \gamma_n$, we have

$$\alpha_{n+1} = \alpha_n \frac{B_n}{A_n}, \ \beta_{n+1} = \alpha_n \frac{C_n}{B_n}, \ \gamma_{n+1} = \alpha_n \frac{D_n}{C_n}$$

for a positive integer n, where

$$\begin{split} A_n &= 1 + 6\alpha_n + 3\alpha_n\beta_n + 9\alpha_n^2 + 6\alpha_n^2\beta_n + 2\alpha_n^3, \\ B_n &= 1 + 2\beta_n + \beta_n\gamma_n + 4\alpha_n + 8\alpha_n\beta_n + 2\alpha_n\beta_n\gamma_n + 2\alpha_n\beta_n^2 + 3\alpha_n^2 + 4\alpha_n^2\beta_n, \\ C_n &= 1 + 4\beta_n + 2\beta_n\gamma_n + 3\beta_n^2 + 2\beta_n^2\gamma_n + 2\alpha_n + 7\alpha_n\beta_n + 2\alpha_n\beta_n\gamma_n + 4\alpha_n\beta_n^2, \\ D_n &= 1 + 6\beta_n + 3\beta_n\gamma_n + 9\beta_n^2 + 6\beta_n^2\gamma_n + 2\beta_n^3. \end{split}$$

In the following, we show that $\frac{1}{3} \leq \gamma_n < \beta_n < \alpha_n \leq \frac{4}{9}$ by induction on n. It is true for n = 1, 2, 3, 4 from Table 2. Suppose that $\frac{1}{3} \leq \gamma_n < \beta_n < \alpha_n \leq \frac{4}{9}$ for $n \geq 4$.

Let $\varepsilon_n = \alpha_n - \gamma_n$. Then $\varepsilon_n > \alpha_n - \beta_n$, $\varepsilon_n > \beta_n - \gamma_n$ and $\varepsilon_n \in (0, \frac{1}{9})$. Now,

$$\alpha_n - \alpha_{n+1} = \alpha_n - \alpha_n \frac{B_n}{A_n} = \frac{\alpha_n (A_n - B_n)}{A_n}$$
$$= \frac{\alpha_n}{A_n} [(2 + 6\alpha_n + 4\alpha_n\beta_n + 2\alpha_n^2 + \beta_n)(\alpha_n - \beta_n)$$
$$+ (2\alpha_n\beta_n + \beta_n)(\beta_n - \gamma_n)] > 0,$$

$$\alpha_{n+1} - \beta_{n+1} = \frac{\alpha_n (B_n^2 - A_n C_n)}{A_n B_n} > 0.$$

where

$$B_n^2 - A_n C_n = (10\alpha_n^2\beta_n + 5\alpha_n^2 + \alpha_n\beta_n + 4\alpha_n + \beta_n^2 + 1)(\alpha_n - \beta_n)^2 + (4\alpha_n^2\beta_n^2 + 2\alpha_n\beta_n^2 + 6\alpha_n\beta_n + 2\beta_n)(\alpha_n - \beta_n)(\alpha_n - \gamma_n) + (4\alpha_n^3\beta_n + 10\alpha_n^2\beta_n + 2\alpha_n\beta_n^2 + 2\alpha_n\beta_n + 2\alpha_n\beta_n + \beta_n^2)(\beta_n - \gamma_n)(\alpha_n - \beta_n) + (2\alpha_n\beta_n^2 + \beta_n^2)(\alpha_n - \gamma_n)(\beta_n - \gamma_n) + (4\alpha_n^2\beta_n^2 + 2\alpha_n\beta_n^2)(\beta_n - \gamma_n)^2 > 0,$$

$$\begin{split} A_{n}B_{n} =& 10\alpha_{n} + 2\beta_{n} + 23\alpha_{n}\beta_{n} + \beta_{n}\gamma_{n} + 8\alpha_{n}\beta_{n}^{2} + 88\alpha_{n}^{2}\beta_{n} + 133\alpha_{n}^{3}\beta_{n} + 70\alpha_{n}^{4}\beta_{n} \\ &+ 8\alpha_{n}^{5}\beta_{n} + 36\alpha_{n}^{2} + 56\alpha_{n}^{3} + 35\alpha_{n}^{4} + 6\alpha_{n}^{5} + 48\alpha_{n}^{2}\beta_{n}^{2} + 6\alpha_{n}^{2}\beta_{n}^{3} + 78\alpha_{n}^{3}\beta_{n}^{2} \\ &+ 12\alpha_{n}^{3}\beta_{n}^{3} + 12\alpha_{n}^{3}\beta_{n}^{2}\gamma_{n} + 28\alpha_{n}^{4}\beta_{n}^{2} + 12\alpha_{n}^{2}\beta_{n}^{2}\gamma_{n} + 8\alpha_{n}\beta_{n}\gamma_{n} + 3\alpha_{n}\beta_{n}^{2}\gamma_{n} \\ &+ 21\alpha_{n}^{2}\beta_{n}\gamma_{n} + 20\alpha_{n}^{3}\beta_{n}\gamma_{n} + 4\alpha_{n}^{4}\beta_{n}\gamma_{n} + 1 \\ &> 4\alpha_{n}^{4}\beta_{n} + 8\alpha_{n}^{3}\beta_{n}^{2} + 20\alpha_{n}^{3}\beta_{n} + 5\alpha_{n}^{3} + 8\alpha_{n}^{2}\beta_{n}^{2} + 9\alpha_{n}^{2}\beta_{n} + 4\alpha_{n}^{2} + 3\alpha_{n}\beta_{n}^{2} \\ &+ 2\alpha_{n}\beta_{n} + \alpha_{n}. \end{split}$$

Then

$$\begin{aligned} \alpha_{n+1} - \beta_{n+1} &= \frac{\alpha_n (B_n^2 - A_n C_n)}{A_n B_n} \\ &< \frac{\varepsilon_n^2}{A_n B_n} [4\alpha_n^4 \beta_n + 8\alpha_n^3 \beta_n^2 + 20\alpha_n^3 \beta_n + 5\alpha_n^3 + 8\alpha_n^2 \beta_n^2 + 9\alpha_n^2 \beta_n + 4\alpha_n^2 \\ &+ 3\alpha_n \beta_n^2 + 2\alpha_n \beta_n + \alpha_n] \\ &< \varepsilon_n^2, \end{aligned}$$

since $\varepsilon_n > \alpha_n - \beta_n$ and $\varepsilon_n > \beta_n - \gamma_n$. Similarly, we have $\beta_{n+1} - \gamma_{n+1} = \frac{\alpha_n (C_n^2 - B_n D_n)}{B_n C_n} > 0$, where

$$C_{n}^{2} - B_{n}D_{n} = [(10\beta_{n}^{3} + 4\beta_{n}^{2}\gamma_{n}^{2} + 4\beta_{n}^{2} + 4\beta_{n} + 1)(\alpha_{n} - \beta_{n}) + (2\beta_{n}^{3} + 9\beta_{n}^{2} + 2\beta_{n})(\alpha_{n} - \gamma_{n}) + (2\alpha_{n}\beta_{n}^{2} + \alpha_{n}\beta_{n})(\beta_{n} - \gamma_{n})](\alpha_{n} - \beta_{n}) + [(4\alpha_{n}\beta_{n}^{3} + 10\beta_{n}^{3})(\alpha_{n} - \beta_{n}) + (4\alpha_{n}\beta_{n}^{3} + 2\beta_{n}^{3})(\alpha_{n} - \gamma_{n}) + (2\alpha_{n}\beta_{n}^{2} + \beta_{n}^{2})(\beta_{n} - \gamma_{n})](\beta_{n} - \gamma_{n}) > 0,$$

$$\begin{split} B_n C_n = & 16\alpha_n^3 \beta_n^3 + 8\alpha_n^3 \beta_n^2 \gamma_n + 40\alpha_n^3 \beta_n^2 + 6\alpha_n^3 \beta_n \gamma_n + 29\alpha_n^3 \beta_n + 6\alpha_n^3 + 8\alpha_n^2 \beta_n^4 \\ & + 20\alpha_n^2 \beta_n^3 \gamma_n + 58\alpha_n^2 \beta_n^3 + 4\alpha_n^2 \beta_n^2 \gamma_n^2 + 44\alpha_n^2 \beta_n^2 \gamma_n + 101\alpha_n^2 \beta_n^2 + 18\alpha_n^2 \beta_n \gamma_n \\ & + 60\alpha_n^2 \beta_n + 11\alpha_n^2 + 4\alpha_n \beta_n^4 \gamma_n + 6\alpha_n \beta_n^4 + 4\alpha_n \beta_n^3 \gamma_n^2 + 30\alpha_n \beta_n^3 \gamma_n + 40\alpha_n \beta_n^3 \\ & + 6\alpha_n \beta_n^2 \gamma_n^2 + 43\alpha_n \beta_n^2 \gamma_n + 64\alpha_n \beta_n^2 + 14\alpha_n \beta_n \gamma_n + 35\alpha_n \beta_n + 6\alpha_n + 2\beta_n^3 \gamma_n^2 \\ & + 7\beta_n^3 \gamma_n + 6\beta_n^3 + 2\beta_n^2 \gamma_n^2 + 10\beta_n^2 \gamma_n + 11\beta_n^2 + 3\beta_n \gamma_n + 6\beta_n + 1. \end{split}$$

Thus, we have

$$\beta_{n+1} - \gamma_{n+1} = \frac{\alpha_n (C_n^2 - B_n D_n)}{B_n C_n}$$

$$< \frac{\varepsilon_n^2}{B_n C_n} [8\alpha_n^2 \beta_n^3 + 4\alpha_n^2 \beta_n^2 + \alpha_n^2 \beta_n + 24\alpha_n \beta_n^3 + 4\alpha_n \beta_n^2 \gamma_n^2 + 14\alpha_n \beta_n^2$$

$$+ 6\alpha_n \beta_n + \alpha_n] < \varepsilon_n^2.$$

And

$$\gamma_{n+1} - \gamma_n = \frac{1}{C_n} (\alpha_n D_n - \gamma_n C_n)$$

= $\frac{1}{C_n} [(1 + 4\beta_n + 2\beta_n^2 + 2\beta_n^2 \gamma_n)(\alpha_n - \gamma_n) + (2\alpha_n + 7\alpha_n \beta_n + 2\beta_n \gamma_n + 2\alpha_n \beta_n \gamma_n + 2\alpha_n \beta_n^2)(\beta_n - \gamma_n) + 3\beta_n \gamma_n (\alpha_n - \beta_n)] > 0.$

So, we have (i) $\alpha_n - \alpha_{n+1} > 0$, (ii) $0 < \alpha_{n+1} - \beta_{n+1} < \varepsilon_n^2$, (iii) $0 < \beta_{n+1} - \gamma_{n+1} < \varepsilon_n^2$ and (iv) $\gamma_{n+1} - \gamma_n > 0$.

From (ii) and (iii), we can obtain that $\varepsilon_{n+1} = \alpha_{n+1} - \gamma_{n+1} < 2\varepsilon_n^2 < \frac{2}{81}$ for all positive integer n by induction. It follows that for any positive integer $m \leq n$,

$$\varepsilon_n < 2\varepsilon_{n-1}^2 < 2[2\varepsilon_{n-2}^2]^2 < \dots < \frac{1}{2}[2\varepsilon_m]^{2^{n-m}}$$

Since $\varepsilon_m \in (0, \frac{1}{9})$ for any positive integer m, we have that the values of $\alpha_n, \beta_n, \gamma_n$ are close to each other when n becomes large.

Numerically, we can find

$$\lim_{n \to \infty} \alpha_n = \lim_{n \to \infty} \beta_n = \lim_{n \to \infty} \gamma_n = 0.4135272769487595999 \cdots$$

From the lemmas above, we get the bounds for the number of independent sets.

Theorem 3.3. For any positive integer $m \leq n$,

$$f_m^{3^{n-m}}(1+2\gamma_m)^{\frac{3(3^{n-m}-1)}{2}}(1+\gamma_n)^3 < i_n < f_m^{3^{n-m}}(1+2\alpha_m)^{\frac{3(3^{n-m}-1)}{2}}(1+\alpha_n)^3$$

Proof. By Lemmas 3.1 and 3.2 and the definition of $\alpha_n, \beta_n, \gamma_n$, we have

$$f_{n} = f_{n-1}^{3} (1 + 6\alpha_{n-1} + 3\alpha_{n-1}\beta_{n-1} + 9\alpha_{n-1}^{2} + 6\alpha_{n-1}^{2}\beta_{n-1} + 2\alpha_{n-1}^{3})$$

$$< f_{n-1}^{3} (1 + 6\alpha_{n-1} + 12\alpha_{n-1}^{2} + 8\alpha_{n-1}^{3})$$

$$= [f_{n-1}(1 + 2\alpha_{n-1})]^{3} < [f_{n-2}^{3}(1 + 2\alpha_{n-2})^{3}]^{3}(1 + 2\alpha_{n-1})^{3}$$

$$< f_{n-2}^{3^{2}} (1 + 2\alpha_{n-2})^{3^{2} + 3^{1}}$$

$$< \dots < f_{m}^{3^{n-m}} (1 + 2\alpha_{m})^{\frac{3(3^{n-m}-1)}{2}}.$$

And

$$i_n = f_n + 3g_n + 3h_n + p_n = f_n(1 + 3\alpha_n + 3\alpha_n\beta_n + \alpha_n\beta_n\gamma_n)$$

< $f_n(1 + 3\alpha_n + 3\alpha_n^2 + \alpha_n^3) = f_n(1 + \alpha_n)^3 < f_m^{3^{n-m}}(1 + 2\alpha_m)^{\frac{3(3^{n-m}-1)}{2}}(1 + \alpha_n)^3.$
Similarly, the lower bound for i_n can be derived.

Similarly, the lower bound for i_n can be derived.

Theorem 3.4. The asymptotic growth constant for the number of independent sets in H_n is bounded by

$$\frac{\ln f_m}{3^{m+1}} + \frac{\ln(1+2\gamma_m)}{2\times 3^m} \le \mu \le \frac{\ln f_m}{3^{m+1}} + \frac{\ln(1+2\alpha_m)}{2\times 3^m}$$

where m is a positive integer.

Proof. Note that the number of vertices of H_n is $v(H_n) = 3^{n+1}$, by Theorem 3.3, we have

$$\frac{\ln i_n}{v(H_n)} < \frac{\ln f_m}{3^{m+1}} + \frac{\ln(1+2\alpha_m)}{2\times 3^m} - \frac{\ln(1+2\alpha_m)}{2\times 3^n} + \frac{\ln(1+\alpha_n)}{3^n}$$

and

$$\frac{\ln i_n}{v(H_n)} > \frac{\ln f_m}{3^{m+1}} + \frac{\ln(1+2\gamma_m)}{2\times 3^m} - \frac{\ln(1+2\gamma_m)}{2\times 3^n} + \frac{\ln(1+\gamma_n)}{3^n}$$

So, the bounds for $\mu = \lim_{v(H_n) \to \infty} \frac{\ln i_n}{v(H_n)}$ follow.

As *m* increases, the difference between the upper and lower bounder in Theorem 3.4 becomes small and the convergence is rapid. Numerically, the asymptotic growth constant for the number of independent sets of the Tower of Hanoi graph H_n in the large *n* limit is $\mu = 0.42433435855938823\cdots$. In fact, the numerical value of μ can be obtained with more than a hundred significant figures accurate when *m* is equal to seven.

4 The number of independent sets on graphs $S_{k,n}$

The Sierpiński graphs $S_{k,n}$ were introduced by Klavžar and Milutinović in 1997 in [25]. The graph $S_{k,0}$ is simply the complete graph on k vertices, $S_{k,n}$ is constructed from $S_{k,n-1}$ by copying k times $S_{k,n-1}$ and adding exactly one edge between each pair of copies. For the construction, one can easily derive that the total number of vertices and edges in $S_{k,n}$ are $v(S_{k,n}) = k^{n+1}$ and $e(S_{k,n}) = \frac{1}{2}(k^{n+2} - k)$, respectively. In particularly, we can see those graphs are exactly the graphs of the Tower of Hanoi problem for k = 3 and another case as shown in Figure 6 for k = 4.



Figure 6: The graphs $S_{4,0}$, $S_{4,1}$, $S_{4,2}$ and the construction of $S_{4,n}$.

The method given in the previous section can be applied to enumeration the number of independent sets on this Sierpiński graphs with $k \ge 4$, but the items of the recursion relations will become larger and larger with the increase of k.

To seek the number of independent sets on $S_{4,n}$, we use the following definitions: (i) Define $f_{4,n}$ as the number of independent sets such that all four outmost vertices are not in the vertex sets. (ii) Define $g_{4,n}$ as the number of independent sets such that only one certain outmost vertex are in the vertex sets. (iii) Define $h_{4,n}$ as the number of independent sets such that exactly two certain outmost vertex are in the vertex sets. (iv) Define $p_{4,n}$ as the number of independent sets such that exactly three certain outmost vertex are in the vertex sets. (v) Define $p_{4,n}$ as the number of independent sets such that exactly three certain outmost vertex are in the vertex sets. (v) Define $q_{4,n}$ as the number of independent sets such that all four outmost vertex are in the vertex are in the vertex sets.

n	1	2	3
$f_{4,n}$	163	13064274739	497661511371512614009322138806617451967507
$g_{4,n}$	52	3951119257	150487045809089786329485928937399858428184
$h_{4,n}$	15	1194624638	45505530112368879421817904248654649805971
$p_{4,n}$	4	361093492	13760342318790991781550553074012255470504
$q_{4,n}$	1	109115158	4160967243331065589513567798163834387921
$i_{4,n}$	478	37589988721	1431845211800580068573889060142357640786006

Table 3: The first few values of $f_{4,n}$, $g_{4,n}$, $h_{4,n}$, $p_{4,n}$, $q_{4,n}$ and $i_{4,n}$ on $S_{4,n}$.

Table 4: The first few values of $\alpha_{4,n}$, $\beta_{4,n}$, $\gamma_{4,n}$ and $\delta_{4,n}$ on $S_{4,n}$.

		, , , ,	, , ,
n	1	2	3
$\alpha_{4,n}$	0.319018404907975	0.302436938592921	0.302388355077651
$\beta_{4,n}$	0.288461538461538	0.302350944199809	0.302388354211550
$\gamma_{4,n}$	0.266666666666666	0.302265230863252	0.302388353345449
$\delta_{4,n}$	0.25	0.302179796693760	0.302388352479348

The quantities $f_{4,n}$, $g_{4,n}$, $h_{4,n}$, $p_{4,n}$, $q_{4,n}$ of $S_{4,n}$ are lengthy and given in the appendix. Some values of $f_{4,n}$, $g_{4,n}$, $h_{4,n}$, $p_{4,n}$, $q_{4,n}$, $i_{4,n}$ are listed in Table 3. These numbers grow exponentially, and have no integer factorizations. There are four equivalent $g_{4,n}$, six equivalent $h_{4,n}$, and four equivalent p_n . By definition, we have

$$i_{4,n} = f_{4,n} + 4g_{4,n} + 6h_{4,n} + 4p_{4,n} + q_{4,n}.$$

The initial values at stage zero are $f_{4,0} = g_{4,0} = 1$, $h_{4,0} = p_{4,0} = q_{4,0} = 0$ and $i_{4,0} = 5$.

Define ratios $\alpha_{4,n} = g_{4,n}/f_{4,n}$, $\beta_{4,n} = h_{4,n}/g_{4,n}$, $\gamma_{4,n} = p_{4,n}/h_{4,n}$, $\delta_{4,n} = q_{4,n}/p_{4,n}$. As *n* increases, we find $\alpha_{4,n}$ decrease monotonically while $\beta_{4,n}$, $\gamma_{4,n}$ and $\delta_{4,n}$ increase monotonically with the relation $\alpha_{4,n} > \beta_{4,n} > \gamma_{4,n} > \delta_{4,n}$. The values of these ratios for small *n* are listed in Table 4. Numerically, we can find

$$\lim_{n \to \infty} \alpha_{4,n} = \lim_{n \to \infty} \beta_{4,n} = \lim_{n \to \infty} \gamma_{4,n} = \lim_{n \to \infty} \delta_{4,n} = 0.30238835458805297767 \cdots$$

By a similar argument as the Tower of Hanoi graph H_n in the last section, the asymptotic growth constant for the number of independent sets on $S_{4,n}$ is bounded by

$$\frac{\ln f_{4,m}}{4^{m+1}} + \frac{\ln(1+2\delta_{4,m})}{2\times 4^m} \le \mu_4 \le \frac{\ln f_{4,m}}{4^{m+1}} + \frac{\ln(1+2\alpha_{4,m})}{2\times 4^m}$$

where $\mu_4 = \lim_{v(S_{4,n})\to\infty} \frac{\ln i_{4,n}}{v(S_{4,n})}$ and *m* is a positive integer.

Then, we can obtain the asymptotic growth constant for the number of independent sets on the Sierpińsk graph $S_{4,n}$ in the large n limit is $\mu = 0.378737140730676994823835 \cdots$.

We can also continue verify a similarly bound for the asymptotic growth constant on $S_{5,n}$, in order to avoid verbosity, we are not to describe here. However, the recursion relations of the number of independent sets for general k are difficult to obtain. From what has been discussed above, we have the following conjecture for the Sierpiński graphs $S_{k,n}$ with positive integers k and m.

Conjecture 4.1. The asymptotic growth constant for the number of independent sets on the Sierpińsk graph $S_{4,n}$ is bounded by

$$\frac{\ln f_{k,m}}{k^{m+1}} + \frac{\ln(1+2\phi_{k,m})}{2 \times k^m} \le \mu_k \le \frac{\ln f_{k,m}}{k^{m+1}} + \frac{\ln(1+2\alpha_{k,m})}{2 \times k^m}$$

where the ratios are defined as $\alpha_{k,n} = g_{k,n}/f_{k,n}$, $\phi_{k,n} = w_{k,n}/y_{k,n}$, $f_{k,n}$ is the number of independent sets such that all k outmost vertices are not in the vertex subset, $g_{k,n}$ is the number of independent sets such that one certain outmost vertex is in the vertex subset, $y_{k,n}$ is number of independent sets such that all but one certain outmost vertex are in the vertex subset, and $w_{k,n}$ is the number of independent sets such that all k outmost vertices are in the vertex subset.

Appendix: Recursion relation for $S_{4,n}$

We give the recursive relation for the Siepiński graph $S_{4,n}$ here. Since the subscript is k = 4 for all the quantities throughout this section, we will use the simplified notation f_{n+1} to denote $f_{4,n+1}$ and similar notations for other quantities. For any non-negative integer n, we have

$$\begin{split} f_{n+1} &= f_n^4 + 12 f_n^3 g_n + 12 f_n^3 h_n + 48 f_n^2 g_n^2 + 4 f_n^3 p_n + 84 f_n^2 g_n h_n + 72 f_n g_n^3 + 24 f_n^2 g_n p_n + \\ 30 f_n^2 h_n^2 &+ 156 f_n g_n^2 h_n + 30 g_n^4 + 12 f_n^2 h_n p_n + 36 f_n g_n^2 p_n + 84 f_n g_n h_n^2 + 60 g_n^3 h_n + \\ 24 f_n g_n h_n p_n + 8 g_n^3 p_n + 8 f_n h_n^3 + 24 g_n^2 h_n^2, \end{split}$$

$$\begin{split} g_{n+1} &= f_n^3 g_n + 3f_n^3 h_n + 9f_n^2 g_n^2 + 3f_n^3 p_n + 33f_n^2 g_n h_n + 24f_n g_n^3 + f_n^3 q_n + 24f_n^2 g_n p_n + \\ 21f_n^2 h_n^2 + 96f_n g_n^2 h_n + 18g_n^4 + 6f_n^2 g_n q_n + 21f_n^2 h_n p_n + 51f_n g_n^2 p_n + 93f_n g_n h_n^2 + 69g_n^3 h_n + \\ 3f_n^2 h_n q_n + 9f_n g_n^2 q_n + 3f_n^2 p_n^2 + 66f_n g_n h_n p_n + 24g_n^3 p_n + 21f_n h_n^3 + 66g_n^2 h_n^2 + 6f_n g_n h_n q_n + \\ 2g_n^3 q_n + 6f_n g_n p_n^2 + 12f_n h_n^2 p_n + 24g_n^2 h_n p_n + 14g_n h_n^3, \end{split}$$

$$\begin{split} h_{n+1} &= f_n^2 g_n^2 + 6f_n^2 g_n h_n + 6f_n g_n^3 + 6f_n^2 g_n p_n + 8f_n^2 h_n^2 + 38f_n g_n^2 h_n + 8g_n^4 + 2f_n^2 g_n q_n + \\ 14f_n^2 h_n p_n &+ 30f_n g_n^2 p_n + 64f_n g_n h_n^2 + 50g_n^3 h_n + 4f_n^2 h_n q_n + 8f_n g_n^2 q_n + 5f_n^2 p_n^2 + \\ 80f_n g_n h_n p_n &+ 30g_n^3 p_n + 26f_n h_n^3 + 87g_n^2 h_n^2 + 2f_n^2 p_n q_n + 16f_n g_n h_n q_n + 6g_n^3 q_n + \\ 18f_n g_n p_n^2 + 34f_n h_n^2 p_n + 72g_n^2 h_n p_n + 44g_n h_n^3 + 4f_n g_n p_n q_n + 4f_n h_n^2 q_n + 8g_n^2 h_n q_n + \\ 8f_n h_n p_n^2 + 8g_n^2 p_n^2 + 28g_n h_n^2 p_n + 4h_n^4, \end{split}$$

 $p_{n+1} = f_n g_n^3 + 9 f_n g_n^2 h_n + 3g_n^4 + 9 f_n g_n^2 p_n + 24 f_n g_n h_n^2 + 27 g_n^3 h_n + 3 f_n g_n^2 q_n + 42 f_n g_n h_n p_n + 22 g_n^3 p_n + 18 f_n h_n^3 + 75 g_n^2 h_n^2 + 12 f_n g_n h_n q_n + 6 g_n^3 q_n + 15 f_n g_n p_n^2 + 39 f_n h_n^2 p_n + 99 g_n^2 h_n p_n + 69 g_n h_n^3 + 6 f_n g_n p_n q_n + 9 f_n h_n^2 q_n + 21 g_n^2 h_n q_n + 21 f_n h_n p_n^2 + 24 g_n^2 p_n^2 + 96 g_n h_n^2 p_n + 15 h_n^4 + 6 f_n h_n p_n q_n + 6 g_n^2 p_n q_n + 12 g_n h_n^2 q_n + 2 f_n p_n^3 + 24 g_n h_n p_n^2 + 14 h_n^3 p_n,$

 $\begin{aligned} q_{n+1} &= g_n^4 + 12g_n^3h_n + 12g_n^3p_n + 48g_n^2h_n^2 + 4g_n^3q_n + 84g_n^2h_np_n + 72g_nh_n^3 + 24g_n^2h_nq_n + \\ 30g_n^2p_n^2 &+ 156g_nh_n^2p_n + 30h_n^4 + 12g_n^2p_nq_n + 36g_nh_n^2q_n + 84g_nh_np_n^2 + 60h_n^3p_n + \\ 24g_nh_np_nq_n + 8h_n^3q_n + 8g_np_n^3 + 24h_n^2p_n^2. \end{aligned}$

There are always $729 = 3^6$ terms in these equations.

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Relative edge betweenness centrality

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Abstract

We introduce a new edge centrality measure - relative edge betweenness $\gamma(uv) = b(uv)/\sqrt{c(u)c(v)}$, where b(uv) is the standard edge betweenness and c(u) is the adjusted vertex betweenness. In this alternative definition, the importance of an edge is normalized with respect to the importance of its end-vertices. This gives a better presentation of the "local" importance of an edge, i.e. its importance in the near neighborhood. We present sharp upper and lower bounds on this invariant together with the characterization of graphs attaining these bounds. In addition, we discuss the bounds for various interesting graph families, and state several open problems.

Keywords: Centrality measures, betweenness centrality, social networks.

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1 Introduction

One of the fundamental problems in network analysis is to determine the importance (or the *centrality*) of a particular vertex or an edge in a network. Since the 1950's many centrality indices have evolved, each with specific application and based on a different concept of what makes a vertex or an edge central to a network. One of the most common measures of the importance of an edge is its betweenness, i.e. the number of shortest paths passing through that edge (normalized in the case where multiple shortest paths between some vertices occur). More precisely, *betweenness of an edge e, b(e)*, is given by

$$b(e) = \sum_{\{k,l\} \in \binom{V}{2}} \frac{\sigma_{k,l}(e)}{\sigma_{k,l}},$$

where $\sigma_{k,l}$ denotes the number of shortest paths between vertices k and l, and $\sigma_{k,l}(e)$ denotes the number of shortest paths connecting k and l that pass through the edge e. Caporossi at. al [1] defined *adjusted vertex betweenness* of a vertex u, c(u), as the sum of the betweennesses of all edges incident to the vertex u, i.e.

$$c\left(u\right) = \sum_{v \in N(u)} b\left(uv\right),$$

where N(u) is the set of neighbors of the vertex u. In the original definition given by Freeman [2], *betweenness of a vertex* u, b(u), was defined as the number of the shortest paths that contain the vertex u as an interior vertex. It can be shown that it holds

$$c(u) = 2b(u) + n - 1.$$

Some centrality indices, e.g., degree centrality, reflect local properties of the underlying graph, while others, like betweenness centrality, give information about the global network structure, as they are based on shortest path computation and counting [7]. In [3] extremal graphs with respect to vertex betweenness for certain graph families were considered. Some recent applications of betweenness centrality include analyzing social and protein interaction networks [6, 4, 5] and traffic flow optimization [8, 9].

Note that betweenness of an edge measures only importance of a link to the entire network, and that link of the highest betweenness may be completely unimportant to some vertex such that no shortest (or even reasonably short) path from that vertex passes through this link. Hence, on the level of individuals the same link can be observed in completely different way. If we observe a social network, the existence of an edge depends on the level of importance attributed to this edge by its adjacent vertices. These vertices (actors) are the ones that create, sustain and destroy this edge (relationship). Namely, they decide how much they want to invest in their friendship. Obviously, edges with high betweenness should be valuable to both vertices considering that many information circulate through such edges.

In this paper, we are interested in measuring the relative importance of an edge to its end-vertices. To clarify the notion of the relative importance, one can use also analogy with a business venture. It is important to partners in this venture if the size of a deal is large comparing to the sizes of the companies involved. While a thousand dollars deal might be extremely important to (say) individual building contractor, it is a very small job to a large corporation. Hence, in order to estimate the value of the edge to its end vertices, one needs to normalize it using their adjusted betweennesses. We define the *relative betweenness* as

$$\gamma(uv) = \frac{b(uv)}{\sqrt{c(u)c(v)}}.$$
(1.1)

Note that we use the geometric mean between c(u) and c(v). The reason why we use the geometric mean and not the arithmetic is that the geometric mean is much lower than the arithmetic mean when there is a large difference between c(u) and c(v), say $c(u) \ll c(v)$. Hence in this case, $\gamma(uv)$ is significantly larger compared to the usage of the arithmetic mean. This corresponds to the relationship between persons with large difference in the influence. We may assume that this relationship is of great value to the actor u and hence he will put significant effort in sustaining this relationship. Therefore, we give to such edge high relative betweenness.

The aim of this paper is to measure how weak can be the weakest link and how strong may be the strongest link in the (social) network. In other words, we are interested in finding extremal values for relative edge betweenness and in analyzing distribution of relative betweenness values on edges of graphs. In Section 2 we give sharp upper and lower bound for relative betweenness in the case of general graphs, and characterize graphs for which these bounds are attained. In Section 3 the bounds for various graphs classes are discussed. We conclude the paper by stating some open problems.

2 Bounds for general graphs

Let B_n be the graph obtained from the complete bipartite graph $K_{2,n-2}$ by adding the edge that connects two vertices in the part of cardinality 2, see Fig. 1. Let this edge be denoted as e^* .



Figure 1: Graph B_n and the edge e^* .

Theorem 2.1. Let uv be an edge of a connected graph G with $n \ge 3$ vertices. Then,

$$\gamma(uv) \ge \frac{2}{n^2 - 3n + 4}.$$
(2.1)

Moreover, equality holds if and only if G is isomorphic to B_n and uv corresponds to e^* .

Proof. Let us denote by $\alpha(u)$ the sum of all edge betweennesses of edges incident to u (but not to v), and by $\alpha(v)$ the sum of all edge betweennesses of edges incident to v (but not to u). In other words, $\alpha(u) = c(u) - b(uv)$ and $\alpha(v) = c(v) - b(uv)$. Note that $\alpha(u) + \alpha(v)$ consists of three types of contributions:

- (a) those from shortest paths not having neither u nor v as an end-vertex. They contribute in total at most $2\binom{n-2}{2} = n^2 5n + 6$.
- (b) those from the shortest path with an end-vertex u, but not v. They contribute all together at most n-2.
- (c) those from the shortest path with an end-vertex v, but not u. They contribute all together at most n-2.

By (a)-(c), it holds $\alpha(u) + \alpha(v) \le n^2 - 3n + 2$. Note that $c(u) + c(v) = \alpha(u) + \alpha(v) + 2b(uv)$. Now, as $b(uv) \ge 1$, we have

$$\gamma(uv) = \frac{b(uv)}{\sqrt{c(u)c(v)}} \ge \frac{2b(uv)}{c(u) + c(v)} = \frac{2b(uv)}{\alpha(u) + \alpha(v) + 2b(uv)}$$

$$\ge \frac{2b(uv)}{n^2 - 3n + 2 + 2b(uv)} \ge \frac{2}{n^2 - 3n + 4},$$
(2.2)

which establishes inequality (2.1). Note that equality in (2.1) holds if and only c(u) = c(v), b(uv) = 1 and $\alpha(u) + \alpha(v) = n^2 - 3n + 2$. The latter implies that the numbers given in (a), (b) and (c) are in fact the exact values of contributions to $\alpha(u) + \alpha(v)$ of the paths described in (a), (b) and (c), respectively.

To assure that the shortest paths having neither u nor v as an end-vertex contribute exactly $n^2 - 5n + 6$, the contribution has to be 2 for each pair of vertices from $V(G) \setminus \{u, v\}$. But this is not the case if there exists an edge xy for $x, y \in V(G) \setminus \{u, v\}$. Since G is connected we have $V(G) \setminus \{u, v\} = N(u) \cup N(v)$. Moreover, since b(uv) = 1, every vertex from $N(u) \cup N(v)$ is adjacent to both u and v. We infer that if for an edge uv of a graph G equality holds in (2.1), then G is isomorphic to B_n and uv corresponds to e^* . \Box

Now we establish the upper bound for $\gamma(uv)$. To prove its sharpness we will consider graphs containing an edge with certain properties. An edge uv of a graph is called a *handle* if u is a pendant vertex and the set $N(v) \setminus \{u\}$ induces a clique. We will denote the edge uv by h^* , see Fig. 2. Note that the path P_n contains two handles.

Theorem 2.2. Let uv be an edge of a connected graph G with $n \ge 3$ vertices. Then,

$$\gamma(uv) \le \sqrt{\frac{n-1}{3n-5}}.$$

Moreover, equality holds if and only if G contains a handle.

Proof. Let us introduce the following notation:

(a) p_u (resp. p_v) denotes the contribution to c(u) (resp. c(v)) of all shortest paths for which both end-vertices are different from u and v, and which do not pass through the edge uv;



Figure 2: A handle h^* in a graph.

- (b) p_{uv} is the contribution to b(uv) of all the shortest paths for which both end-vertices are different from u and v;
- (c) q_{uv} (resp. q_{vu}) is the contribution to b(uv) of all paths that start in u (resp. v) and pass through the edge uv, but do not finish in v (u, respectively).

Note that $q_{uv} + q_{vu} \le n-2$ and $c(u) = p_u + 2p_{uv} + 2q_{vu} + n-1$. In c(u), the second and the third summand appear with factor 2 since each contributing path passes through the edge uv and another edge incident with u, and the last summand corresponds to all paths that start in u. Analogously, $c(v) = p_v + 2p_{uv} + 2q_{uv} + n - 1$. Further, $b(uv) = p_{uv} + q_{uv} + q_{vu} + 1$. Hence,

$$\gamma(uv) = \frac{b(uv)}{\sqrt{c(u)c(v)}} \le \frac{p_{uv} + q_{uv} + q_{vu} + 1}{\sqrt{(2p_{uv} + 2q_{vu} + n - 1)(2p_{uv} + 2q_{uv} + n - 1)}}.$$
 (2.3)

We need to prove that

$$\frac{p_{uv} + q_{uv} + q_{vu} + 1}{\sqrt{(2p_{uv} + 2q_{vu} + n - 1)(2p_{uv} + 2q_{uv} + n - 1)}} \le \sqrt{\frac{n - 1}{3n - 5}}$$

This is equivalent to

$$(p_{uv} + q_{uv} + q_{vu} + 1)^2 (3n - 5) - (2p_{uv} + 2q_{vu} + n - 1)(2p_{uv} + 2q_{uv} + n - 1)(n - 1) \le 0,$$

which is further equivalent to

$$(-1-n)p_{uv}^{2} + (-2+4n-2n^{2}+(6-2n)(n-2-q_{uv}-q_{vu}))p_{uv} + ((q_{uv}+q_{vu}+1)^{2}(3n-5) - (2q_{vu}+n-1)(2q_{uv}+n-1)(n-1)) \le 0.$$
(2.4)

It is obvious that $-n-1 \le 0$, $-2+4n-2n^2 < 0$, $6-2n \le 0$ and $n-2-q_{uv}-q_{vu} \ge 0$. Hence, it is sufficient to prove that

$$(q_{uv} + q_{vu} + 1)^2 (3n - 5) - (2q_{vu} + n - 1)(2q_{uv} + n - 1)(n - 1) \le 0.$$
 (2.5)

Without loss of generality (because of the symmetry of the last equation), we may assume that $q_{uv} \ge q_{vu}$. Let us denote $s = q_{uv} + q_{vu}$ and $d = q_{uv} - q_{vu}$. Obviously, $0 \le d \le s \le n-2$. Inequality (2.5) reduces to

$$(s+1)^2(3n-5) - (s-d+n-1)(s+d+n-1)(n-1) \le 0,$$

and further to

$$(s+1)^2(3n-5) - \left((s+n-1)^2 - d^2\right)(n-1) \le 0.$$

Since $0 \le d \le s$, it is sufficient to prove that:

$$(s+1)^2(3n-5) - \left((s+n-1)^2 - s^2\right)(n-1) \le 0.$$
(2.6)

On the left-hand side we have a quadratic function in s,

$$f(s) = s^{2}(3n-5) + (-2n^{2} + 10n - 12)s - n^{3} + 3n^{2} - 4,$$
(2.7)

with quadratic coefficient 3n - 5 > 0 and roots n - 2 and $\frac{-n^2 + n + 2}{3n - 5}$. Hence, in order to prove (2.6), it is sufficient to show that $\frac{-n^2 + n + 2}{3n - 5} \leq 0$. A simple check shows that the numerator is negative and the denominator is positive. This completes the proof that $\gamma(uv) \leq \sqrt{\frac{n-1}{3n-5}}$.

Let $h^* = uv$ be an edge in a graph L_n such that d(u) = 1 and $N(v) \setminus \{u\}$ induces a clique. Then clearly $p_u = p_v = p_{uv} = q_{vu} = 0$ and $q_{uv} = n - 2$, hence the upper bound for γ is attained, i.e. $\gamma(h^*) = \sqrt{\frac{n-1}{3n-5}}$.

To prove the converse, assume G is a connected graph of order at least 3 with an edge uv such that $\gamma(uv) = \sqrt{\frac{n-1}{3n-5}}$. This implies equality in (2.3) and (2.4). From equality in (2.3) follows $p_u = p_v = 0$, and form equality in (2.4) we obtain that $p_{uv} = 0$ and that equality holds in (2.5). The latter is equivalent to the fact that $(s + 1)^2(3n - 5) - ((s + n - 1)^2 - d^2)(n - 1) = 0$. As a consequence (since $0 \le d \le s$) we have also equality in (2.6). Now, it follows that s and d coincide, and hence $s = q_{uv}$ and $q_{vu} = 0$. Equality in (2.6) implies also that s is a (positive) root of the quadratic function in (2.7), so $s = n - 2 = q_{uv}$.

To summarize, for $uv \in E(G)$ we have $p_u = p_v = p_{uv} = q_{vu} = 0$ and $q_{uv} = n - 2$. From this, observe that there is no vertex $w \in V(G) \setminus \{u, v\}$ such that $uw \in E(G)$ and $vw \notin E(G)$, otherwise we obtain a contradiction with $q_{vu} = 0$. The fact that $q_{uv} = n - 2$ implies that every shortest path from u to any other vertex in $V(G) \setminus \{u, v\}$ passes through the edge uv. Thus v is the only neighbor of u. Since G is connected and of order at least 3, $N(v) \setminus \{u\}$ is nonempty and induces a clique, otherwise we obtain a contradiction with $p_v = 0$. Thus, we infer that uv is a handle in G.

Corollary 2.3. For any edge e of a graph with $n \ge 3$ vertices, it holds that

$$\frac{2}{n^2-3n+4} \leq \gamma(e) \leq \sqrt{\frac{n-1}{3n-5}} \,.$$

3 Bounds for some graph classes

In this section, the bounds of Corollary 2.3 for various graph classes are considered.

Graphs with higher connectivity. The graphs containing handles, for which the upper bound in Corollary 2.3 is attained, belong to the class of graphs with bridges. Thus, one might wonder whether this bound can be improved if we forbid them. But it turns out that even in the case of k-connected graphs the leading term in upper bound remains essentially $\frac{1}{\sqrt{3}}$. To illustrate this, consider the graph $C_{n,k}$, constructed as follows: take a complete graph on n - k vertices, $k \ge 2$, n > 2k, choose k of its vertices, make a copy of each chosen vertex and join it with the original one, and finally add edges so that copied vertices induce a clique (see Fig. 3 where general situation is presented on the left, while the right graph is isomorphic to $C_{10,3}$). Let v be one of k chosen vertices and u its copy in the above construction of $C_{n,k}$. Then we have b(uv) = n - k, c(u) = n + k - 2, c(v) = 3n - 3k - 2, and thus $\gamma(uv) = \frac{n-k}{\sqrt{(n+k-2)(3n-3k-2)}}$.



Figure 3: A k-connected graph $C_{n,k}$ (left) and the graph $C_{10,3}$ (right).

In what follows, we discuss the bounds of the above corollary in a various interesting graph classes.

Bipartite graphs. The upper bound in Corollary 3.2 is clearly attained also when restricted to two-mode data networks (bipartite graphs). We now give an example of a bipartite graph and an edge of it that achieves asymptotically the lower bound $\Theta(n^{-2})$.

Proposition 3.1. There exist bipartite graphs on n vertices containing an edge e with $\gamma(e) \in \Theta(n^{-2})$.

Proof. To prove the claim consider the graph G from Fig. 4 constructed in the following way. Take eight independent sets A_0, A_1, \ldots, A_7 , each of size k, connect each vertex of A_i with each vertex of A_{i+1} , index being taken modulo 8. Finally, take two new adjacent vertices a_0 and a_1 , and connect each vertex of A_i with $a_i \pmod{2}$, for $i = 0, \ldots, 7$. Now, we will show that

$$b(a_0a_1) \in \Theta(1)$$
 and $c(a_0), c(a_1) \in \Theta(n^2)$,

which immediately implies that $\gamma(a_0 a_1) \in \Theta(1/n^2)$.

First, we evaluate $b(a_0a_1)$. Consider the contribution to $b(a_0a_1)$ of shortest paths that contain a_0a_1 according to their length. The edge a_0a_1 is the only path of length 1 that

contains a_0a_1 , and it contributes 1 to $b(a_0a_1)$. There are 8k paths of length 2 containing a_0a_1 and each of them contributes 1/(2k+1) to $b(a_0a_1)$. Notice that there are $8k^2$ paths of length 3 that contain a_0a_1 , and each of them contributes $1/(k^2 + 4k + 1)$ to $b(a_0a_1)$. Observe that no shortest path of length 4 or more contains a_0a_1 as the diameter of this graph is 3. Summing up all together, we obtain that $b(a_0a_1)$ is slightly less than 13.

Now, we evaluate $c(a_0)$. Note that any shortest path from a vertex in A_0 to a vertex in A_4 is of length 2 and it contributes 2 to $c(a_0)$. As these paths are k^2 , it follows that $c(a_0) \in \Theta(k^2) = \Theta(n^2)$. Similarly, we evaluate $c(a_1)$.



Figure 4: A bipartite graph from the proof of Proposition 3.1.

Trees. As the trees are bipartite graphs the same upper bound holds but regarding the lower bound we get slightly different result.

Theorem 3.2. For any edge e of a tree with $n \ge 3$ vertices, it holds that

$$\frac{1}{\sqrt{n-1}} \le \gamma(e) \le \sqrt{\frac{n-1}{3n-5}},\tag{3.1}$$

and the lower bound is attained at an edge of the *n*-star unless n = 4 and *e* is the middle edge of a 4-path, in which case $\gamma(e) = \frac{4}{7}$.

Proof. Obviously, the upper bound holds by Corollary 2.3, and is attained at any edge incident to a leaf and to a vertex of degree 2, e.g. such an edge is an end-edge of a path on *n*-vertices.

Now, we argue the lower bound. In its proof we use the following notation: for an edge $f = w_1 w_2$, as T - f has two components, we name them by $T_f(w_1)$ and $T_f(w_2)$, where the first one contains w_1 and the second contains w_2 .

Let T be a tree and e = xy its edge with minimum γ . Suppose $T_e(x)$ has a vertices, and $T_e(y)$ has b vertices; hence n = a + b.

We claim that x is of degree a. Suppose to the contrary that it is of degree strictly less than a. Then there is a leaf u of T that belongs to $T_e(x)$ and is not adjacent to x. Let f = xv be the edge the removal of which from T, separates x and u. Then u belongs to the component $T_f(v)$, and let this component have s vertices. As u and v belong to $T_f(v)$, we have $s \ge 2$.

Let T^* be the tree obtained from T by first removing u from T and then reattaching it to x. Notice that

$$c_{T^*}(x) - c_T(x) = (s-1)(n-s+1) + 1 \cdot (n-1) - s(n-s) = 2s - 2 > 0.$$

So, we have $c_T(x) < c_{T^*}(x)$. Notice that $b_T(e) = b_{T^*}(e) = ab$, and $c_T(y) = c_{T^*}(y)$. Thus, $\gamma_{T^*}(e) < \gamma_T(e)$, which is a contradiction. This establishes the claim.

Similarly we prove that y is of degree b, and hence T is a double star. Now, notice that

$$\gamma(e) = \frac{ab}{\sqrt{ab + (a-1)(n-1)}\sqrt{ab + (b-1)(n-1)}}$$

We want to prove that

$$\gamma(e) \ge \frac{1}{\sqrt{n-1}}$$

(unless the exceptional case) and this is equivalent to

$$(n-1)a^{2}b^{2} \ge (ab + (a-1)(n-1))(ab + (b-1)(n-1)).$$

As n = a + b, this equality can be rewritten into

$$((ab - a - b)(a + b - 2) - 1)(a - 1)(b - 1) \ge 0.$$
(3.2)

Notice that this inequality does not hold only if a = b = 2, but then G is a 4-path and e is its middle edge, which is the exceptional case. In all other cases, it is easy to see that (3.2) holds. Also notice that equation holds in (3.2) if a = 1 or b = 1 but in that case G is a star.

In the classes of graphs with girth 3 and 4 the lower bound of γ is asymptotically $\Theta(n^{-2})$, for the trees which are class of graphs of girth infinity, it is $\Theta(1/\sqrt{n})$. We expect that at girth 5 the following change happens.

Conjecture 3.3. In graphs G on $n \ge 3$ vertices and with girth ≥ 5 it holds $\gamma(e) \in \Omega(n^{-1})$ for every edge e.

Regarding the lower bound for trees we wonder if some finite girth may occur.

Problem 3.4. Is there any finite number g such that for graphs G with girth at least g, every edge e has $\gamma(e) \in \Omega(1/\sqrt{n})$?

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Characterization of graphs with exactly two non-negative eigenvalues

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Abstract

In this paper we characterize all graphs with exactly two non-negative eigenvalues. As a consequence we obtain all graphs G such that $\lambda_3(G) < 0$, where $\lambda_3(G)$ is the third largest eigenvalue of G.

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1 Introduction

Throughout this paper all graphs are simple, that is finite and undirected without loops and multiple edges. Let G be a graph with vertex set $\{v_1, \ldots, v_n\}$. The adjacency matrix of G, $A(G) = [a_{ij}]$, is an $n \times n$ matrix such that $a_{ij} = 1$ if v_i and v_j are adjacent, and $a_{ij} = 0$, otherwise. Thus A(G) is a symmetric matrix with zeros on the diagonal and all the eigenvalues of A(G) are real. By the eigenvalues of G we mean those of its adjacency matrix. We denote the eigenvalues of G by $\lambda_1(G) \ge \cdots \ge \lambda_n(G)$. By the spectrum of G that is denoted by Spec(G), we mean the multiset of eigenvalues of G. The characteristic polynomial of G, $det(\lambda I - A(G))$, is denoted by $P(G, \lambda)$. Studying the eigenvalues of graphs, the roots of characteristic polynomials of graphs, has always been of great interest to researchers, for instance see [1, 2, 3, 4, 5, 6, 7, 8, 9, 10] and the references therein.

It is well known that $\lambda_1(G) + \cdots + \lambda_n(G) = 0$ and $\lambda_1^2(G) + \cdots + \lambda_n^2(G) = 2m$, where m is the number of edges of G. Thus if G has at least one edge, then G has at least one positive eigenvalue. One of the attractive problems is the characterization of graphs with a

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few non-zero eigenvalues. In [5] all bipartite graphs with at most six non-zero eigenvalues have been characterized. The another interesting problem is the characterization of graphs with a few positive eigenvalues. In [10] Smith characterized all graphs with exactly one positive eigenvalue. In fact, a graph has exactly one positive eigenvalue if and only if its non-isolated vertices form a complete multipartite graph. In [9] Petrović has studied the characterization of graphs with exactly two non-negative eigenvalues. In this paper with a different proof we state a new characterization of all graphs G with exactly two non-negative eigenvalues. In other words we find the graphs G with $\lambda_1(G) \ge 0$, $\lambda_2(G) \ge 0$ and $\lambda_3(G) < 0$.

For a graph G, V(G) and E(G) denote the vertex set and the edge set of G, respectively; \overline{G} denotes the complement of G. The *order* of G denotes the number of vertices of G. The *closed neighborhood* of a vertex v of G which is denoted by N[v], is the set $\{u \in V(G) : uv \in E(G)\} \cup \{v\}$. For every vertex $v \in V(G)$, the *degree* of v is the number of edges incident with v and is denoted by $deg_G(v)$ (for simplicity we use deg(v) instead of $deg_G(v)$). By $\delta(G)$ we mean the minimum degree of vertices of G. A set $S \subseteq V(G)$ is an *independent set* if there is no edge between the vertices of S. The *independence number* of G, $\alpha(G)$, is the maximum cardinality of an independent set of G. For two graphs G and Hwith disjoint vertex sets, G + H denotes the graph with the vertex set $V(G) \cup V(H)$ and the edge set $E(G) \cup E(H)$, i.e. the disjoint union of two graphs G and H. In particular, nG denotes the disjoint union of n copies of G. The complete product (join) $G \vee H$ of graphs G and H is the graph obtained from G + H by joining every vertex of G with every vertex of H. For positive integers n_1, \ldots, n_ℓ , K_{n_1,\ldots,n_ℓ} denotes the complete multipartite graph with ℓ parts of sizes n_1, \ldots, n_ℓ . Let K_n , $nK_1 = \overline{K_n}$, C_n and P_n be the complete graph, the null graph, the cycle and the path on n vertices, respectively.

2 The structure of graphs with exactly two positive eigenvalues

In this section we obtain a characterization of graphs that have exactly two positive eigenvalues. We need the Interlacing Theorem.

Theorem 2.1. ([4, Theorem 9.1.1]) Let G be a graph of order n and H be an induced subgraph of G with order m. Suppose that $\lambda_1(G) \ge \cdots \ge \lambda_n(G)$ and $\lambda_1(H) \ge \cdots \ge \lambda_m(H)$ are the eigenvalues of G and H, respectively. Then for every $i, 1 \le i \le m$, $\lambda_i(G) \ge \lambda_i(H) \ge \lambda_{n-m+i}(G)$.

Theorem 2.2. ([10], see also [3, Theorem 6.7]) A graph has exactly one positive eigenvalue if and only if its non-isolated vertices form a complete multipartite graph.

First we characterize all graphs with exactly one non-negative eigenvalue.

Theorem 2.3. Let G be a graph of order $n \ge 2$ with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. Then $\lambda_2 < 0$ if and only if $G \cong K_n$.

Proof. If $G \cong K_n$ and $n \ge 2$, then $\lambda_2 = -1$. Now suppose that $\lambda_2 < 0$. We show that $G \cong K_n$. Suppose that $G \not\cong K_n$. Thus $2K_1$ is an induced subgraph of G. So by Interlacing Theorem 2.1, $\lambda_2 \ge \lambda_2(2K_1) = 0$, a contradiction. Hence $G \cong K_n$.

Lemma 2.4. Let G be a graph of order $n \ge 3$ with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. Suppose that $\lambda_1 \ge 0$, $\lambda_2 \ge 0$ and $\lambda_3 < 0$. Then the following hold:

- 1. If G is disconnected, then $G \cong K_r + K_{n-r}$, for some positive integer r, where $r \leq n-1$.
- 2. If G is connected and $\lambda_2 = 0$, then $G \cong K_n \setminus e$ for an edge e of K_n .

Proof. 1. Let G be disconnected. Assume that G_1, \ldots, G_k are the connected components of G, where $k \ge 2$. Since $\lambda_1(G_1) \ge 0, \ldots, \lambda_1(G_k) \ge 0$ are k eigenvalues of G and $\lambda_3 < 0$ we obtain that k = 2. In other words G has exactly two connected components. Thus $G = G_1 + G_2$. We prove that G_1 and G_2 are complete graphs. First we show that G_1 is a complete graph. If $G_1 \cong K_1$, there is nothing to prove. Assume that $|V(G_1)| \ge 2$ (equivalently $G_1 \ncong K_1$). We claim that $\lambda_2(G_1) < 0$. By contradiction suppose that $\lambda_2(G_1) \ge 0$. Since $\lambda_1(G_1) \ge 0$, $\lambda_2(G_1) \ge 0$ and $\lambda_1(G_2) \ge 0$ are three eigenvalues of G we obtain that $\lambda_3 \ge 0$, a contradiction (since $\lambda_3 < 0$). Hence the claim is proved. In other words $\lambda_2(G_1) < 0$. So by Theorem 2.3, G_1 is a complete graph. Similarly we obtain that G_2 is a complete graph. Hence G is a disjoint union of two complete graphs.

2. Suppose that G is connected and $\lambda_2 = 0$. Since $\lambda_3 < 0$, $G \not\cong nK_1$. Thus $\lambda_1 > 0$. Hence G has exactly one positive eigenvalue. By Theorem 2.2 there are some positive integers t and $n_1 \ge \cdots \ge n_t \ge 1$, so that $n_1 + \cdots + n_t = n$ and $G \cong K_{n_1,\ldots,n_t}$. If t = 1, then $G \cong nK_1$, a contradiction (since G is connected). Thus $t \ge 2$. If $n_1 = 1$, then $G \cong K_n$ and so $\lambda_2 = -1$, a contradiction. Therefore $n_1 \ge 2$. If $n_2 \ge 2$, then C_4 is an induced subgraph of G. Using Interlacing Theorem 2.1 we get $\lambda_3 \ge \lambda_3(C_4) = 0$, a contradiction. Thus $n_2 = \cdots = n_t = 1$. Now if $n_1 \ge 3$, then $K_{1,3}$ is an induced subgraph of G. Similarly by Interlacing Theorem 2.1 we obtain $\lambda_3 \ge \lambda_3(K_{1,3}) = 0$, a contradiction. So $n_1 = 2$. Thus $G \cong K_{2,1,\ldots,1}$. In other words $G \cong K_n \setminus e$, for an edge e of K_n . We note that

$$Spec(K_n \setminus e) = \{\frac{n-3+\sqrt{n^2+2n-7}}{2}, 0, \underbrace{-1, \dots, -1}_{n-3}, \frac{n-3-\sqrt{n^2+2n-7}}{2}\}.$$

The proof is complete.

In [2] all graphs G with $\lambda_1 > 0$, $\lambda_2 \le 0$ and $\lambda_3 < 0$ have been characterized.

Remark 2.5. Let n_1, \ldots, n_t be some positive integers and $G = K_{n_1,\ldots,n_t}$. Similar to the proof of the second part of Lemma 2.4 by Interlacing Theorem 2.1 one can see that $\lambda_2(G) < 0$ if and only if $n_1 = \cdots = n_t = 1$. On the other hand by Theorem 2.2, $\lambda_2(K_{n_1,\ldots,n_t}) \leq 0$. Thus $\lambda_2(K_{n_1,\ldots,n_t}) = 0$ if and only if $n_k > 1$ for some k. In other words, the second largest eigenvalue of any complete multipartite graph except complete graph is zero.

Remark 2.6. Let G be a graph of order $n \ge 3$ with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. Assume that G has exactly two non-negative eigenvalues. In other words, $\lambda_1 \ge 0$, $\lambda_2 \ge 0$ and $\lambda_3 < 0$. Since $\lambda_3 < 0$, $G \not\cong nK_1$. Thus $\lambda_1 > 0$. Hence $\lambda_1 > 0$, $\lambda_2 \ge 0$ and $\lambda_3 < 0$. If G is disconnected, then by the first part of Lemma 2.4, $G \cong K_r + K_{n-r}$ for some positive integer $r \le n - 1$. If G is connected and $\lambda_2 = 0$, then by the second part of Lemma 2.4, $G \cong K_n \setminus e$, where e is an edge of K_n . Thus to characterize all graphs with exactly two non-negative eigenvalues it remains to find connected graphs G such that $\lambda_1(G) > 0$, $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$. In sequel we find this characterization.

Definition 2.7. A graph G is called *semi-complete* if G is a disjoint union of two complete graphs or is obtained by adding some new edges to disjoint union of two complete graphs (see Figure 1).



Figure 1: The graphs H_1 , H_2 and H_3 are semi-complete that are obtained from $K_3 + K_4$.

Now we prove one of the main results of this section.

Lemma 2.8. Let G be a connected graph of order $n \ge 3$ and with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. If $\lambda_2 > 0$ and $\lambda_3 < 0$, then for every vertex $v \in V(G)$ with degree $\delta(G)$ we have $N[v] \cong K_{\delta(G)+1}$ and $G \setminus N[v] \cong K_{n-\delta(G)-1}$. In particular, G is semi-complete.

Proof. Let $\lambda_2 > 0$ and $\lambda_3 < 0$. Since $\lambda_2 > 0$, G is not complete graph. Therefore $\alpha(G) \ge 2$. If $\alpha(G) \ge 3$, then $3K_1$ is an induced subgraph of G. Thus by Interlacing Theorem 2.1, $\lambda_3(G) \ge \lambda_3(3K_1) = 0$, a contradiction. Therefore $\alpha(G) = 2$. Thus for every vertex $u \in V(G)$, $G \setminus N[u]$ is a complete graph. In fact, $G \setminus N[u] \cong K_{n-deg(u)-1}$.

Let v_0 be a vertex of G with degree $\delta(G)$, that is v_0 has the minimum degree among all vertices of G. Since $G \not\cong K_n$, $deg(v_0) \leq n-2$. Since $G \setminus N[v_0]$ is a complete graph, to complete the proof it is sufficient to show that the induced subgraph on the set $N[v_0]$ is a complete graph, that is every two vertices of $N[v_0]$ are adjacent. This also shows that G is obtained by adding some edges to the complete graphs $N[v_0]$ and $G \setminus N[v_0]$ and so G is semi-complete.

Now we show that $N[v_0]$ is a complete graph. By contradiction, suppose that w and z are two non-adjacent vertices of $N[v_0]$. Let a be an arbitrary vertex of $V(G) \setminus N[v_0]$. The induced subgraph on $\{v_0, w, z, a\}$ in G is one of the graphs, A_1, A_2, A_3 or A_4 (see Figure 2). Since $\lambda_3(A_1) = \lambda_3(A_4) = 0$ and $\lambda_3 < 0$, Interlacing Theorem 2.1 shows that



Figure 2: The subgraphs A_1, A_2, A_3 and A_4 .

the induced subgraph on $\{v_0, w, z, a\}$ is A_2 or A_3 . In other words any vertex of $G \setminus N[v_0]$

has exactly one neighbor in $\{w, z\}$. Without losing the generality assume that a is adjacent to w. Now we show that every vertex of $G \setminus N[v_0]$ is adjacent to w. By contradiction suppose that $b \neq a$ is a vertex of $G \setminus N[v_0]$ such that b is adjacent to z. Since $G \setminus N[v_0]$ is complete and $a, b \in V(G) \setminus N[v_0]$, the vertices a and b are adjacent. Thus the induced subgraph on $\{v_0, w, z, a, b\}$ is isomorphic to the cycle C_5 . Since $\lambda_3(C_5) \simeq .618 > 0$, by Interlacing Theorem 2.1, we have $\lambda_3 > 0$, a contradiction. This contradiction shows that all vertices of $G \setminus N[v_0]$ are adjacent only to w. This implies that $deg(z) \leq deg(v_0) - 1$, a contradiction, since v_0 has minimum degree. This contradiction completes the proof. \Box

Claim 2.9. Let G be a connected graph of order $n \ge 3$ and with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$ such that $\lambda_2 > 0$ and $\lambda_3 < 0$. Let $X = N[v_0]$ and $Y = G \setminus N[v_0]$, where v_0 is a vertex of G with degree $\delta(G)$. Then for every two vertices a and b in X (also for a and b in Y) $N[a] \subseteq N[b]$ or $N[b] \subseteq N[a]$.

Proof. Let a and b be two vertices of X. We show that $N[a] \subseteq N[b]$ or $N[b] \subseteq N[a]$. First note that by Lemma 2.8, X is a complete graph. This implies that $N[a] \cap X = N[b] \cap X = X$. Now by contradiction suppose that there are some vertices c and d in Y such that $c \in N[a] \setminus N[b]$ and $d \in N[b] \setminus N[a]$. Thus the induced subgraph on $\{a, b, c, d\}$ is isomorphic to C_4 . Using Interlacing Theorem 2.1 we get $\lambda_3 \ge \lambda_3(C_4) = 0$, a contradiction (since $\lambda_3 < 0$). Thus the result follows. Similarly one can prove that for any two vertices v and w in Y, $N[v] \subseteq N[w]$ or $N[w] \subseteq N[v]$.

As an example we find an infinite family of connected graphs with positive second largest eigenvalue and negative third largest eigenvalue.

Corollary 2.10. Let $n \ge 4$ be an integer. Let K(n,t) be the graph obtained by deleting t edges incident to one vertex of K_n , where $2 \le t \le n-2$. Then $\lambda_2(K(n,t)) > 0$ and $\lambda_3(K(n,t)) < 0$.

Proof. Let $\lambda_1 \geq \cdots \geq \lambda_n$ be the eigenvalues of K(n,t). Since K_{n-1} is an induced subgraph of K(n,t), by Interlacing Theorem 2.1, $\lambda_1 \geq n-2 \geq \lambda_2 \geq -1 \geq \lambda_3$. Thus $\lambda_3 < 0$. On the other, since K(n,t) is not a complete multipartite, by Theorem 2.2, $\lambda_2 > 0$.

Definition 2.11. A graph G is called *quasi-reduced* if for every two vertices u and v of G, $N[u] \neq N[v]$.

As an example of quasi-reduced graphs, we define the graphs G_n that have important role for characterizing graphs with $\lambda_2 > 0$ and $\lambda_3 < 0$.

Definition 2.12. For every integer $n \ge 2$, let G_n be the graph of order n such that G_n is obtained from disjoint complete graphs $K_{\lceil \frac{n}{2} \rceil}$ and $K_{\lfloor \frac{n}{2} \rfloor}$ as following: Let $V(K_{\lceil \frac{n}{2} \rceil}) = \{v_1, \ldots, v_{\lceil \frac{n}{2} \rceil}\}$ and $V(K_{\lfloor \frac{n}{2} \rfloor}) = \{w_1, \ldots, w_{\lfloor \frac{n}{2} \rfloor}\}$. Then add some new edges to $K_{\lceil \frac{n}{2} \rceil} + K_{\lfloor \frac{n}{2} \rfloor}$ such that the following hold:

(i) $N[v_1] \subset \cdots \subset N[v_{\lceil \frac{n}{2} \rceil}]$ and $N[w_1] \subset \cdots \subset N[w_{\lceil \frac{n}{2} \rceil}]$.

(ii)
$$\left| N[v_i] \cap V(K_{\lfloor \frac{n}{2} \rfloor}) \right| = i - 1 \text{ for } i = 1, \dots, \lceil \frac{n}{2} \rceil.$$

(iii)
$$|N[w_j] \cap V(K_{\lceil \frac{n}{2} \rceil})| = \begin{cases} j-1, & \text{if } n \text{ is even;} \\ j, & \text{if } n \text{ is odd} \end{cases}$$
 for $j = 1, \dots, \lfloor \frac{n}{2} \rfloor$.

In Figure 3, the graphs G_2, G_3, G_4, G_5 and G_6 have been shown. In addition in Figure 4 one can see the complement of G_7, \ldots, G_{12} . We note that $G_{2k} = B_{2k}(1, \ldots, 1; 1, \ldots, 1)$ and $G_{2k+1} = B_{2k+1}(1, \ldots, 1; 1, \ldots, 1; 1)$, where B_{2k} and B_{2k+1} are the graphs that have been defined in [9].

Remark 2.13. For every $n \ge 2$, G_n is semi-complete and quasi-reduced. In addition if $n \ge 3$, then G_n is connected. We note that for every $n \ge 3$, G_n is an induced subgraph of G_{n+1} . In fact if n is even, then $G_{n+1} \cong K_1 \lor G_n$ and if n is odd, then G_{n+1} is obtained from G_n by adding a new vertex w such that w is adjacent to any vertex of $\{w_1, \ldots, w_{\lfloor \frac{n}{2} \rfloor}\} = V(K_{\lfloor \frac{n}{2} \rfloor})$, where $K_{\lfloor \frac{n}{2} \rfloor}$ is one of the parts of G_n (see Definition 2.12).

Remark 2.14. We note that for every $n \ge 2$, the group of all automorphisms of the graph G_n , $Aut(G_n)$, has exactly two elements.



Figure 3: The graphs G_2, G_3, G_4, G_5 and G_6 are semi-complete and quasi-reduced.

The next result shows that there is only one connected quasi-reduced graph with $\lambda_2 > 0$ and $\lambda_3 < 0$.

Lemma 2.15. Let G be a connected graph of order $n \ge 3$. If G is quasi-reduced and $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$, then $G \cong G_n$.

Proof. Assume that $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$. Since G is connected, by Lemma 2.8, G is semi-complete. Let $\delta(G) = t$ and v'_1 be a vertex of G with degree t. By Lemma 2.8, $N[v'_1] \cong K_{t+1}$ and $G \setminus N[v'_1] \cong K_{n-t-1}$. In fact G is obtained from the disjoint complete graphs K_{t+1} and K_{n-t-1} by adding some new edges (see the proof of Lemma 2.8). Let $V(K_{t+1}) = \{v'_1, v'_2, \ldots, v'_{t+1}\}$ and $V(K_{n-t-1}) = \{w'_1, \ldots, w'_{n-t-1}\}$. By Claim 2.9, for every two vertices v'_i and v'_j in K_{t+1} , $N[v'_i] \subseteq N[v'_j]$ or $N[v'_j] \subseteq N[v'_i]$. Also for every two vertices w'_i and w'_j in K_{n-t-1} , $N[w'_i] \subseteq N[w'_j]$ or $N[w'_j] \subseteq N[w'_i]$. So without losing the generality assume that $N[v'_1] \subseteq \cdots \subseteq N[v'_{t+1}]$ and $N[w'_1] \subseteq \cdots \subseteq N[w'_{n-t-1}]$ (note that $N[v'_1] = V(K_{t+1})$ and for every $1 \leq i \leq t+1$, $N[v'_1] \subseteq N[v'_i]$). Now suppose that G is quasi-reduced. Therefore we find that

$$0 = |N[v_1'] \cap V(K_{n-t-1})| < \dots < |N[v_{t+1}'] \cap V(K_{n-t-1})| \le n-t-1,$$
(2.1)

and

$$0 \le |N[w_1'] \cap V(K_{t+1})| < \dots < |N[w_{n-t-1}'] \cap V(K_{t+1})| \le t.$$
(2.2)



Figure 4: The complement graphs of G_7 , G_8 , G_9 , G_{10} , G_{11} and G_{12} .

Since $|N[v'_1] \cap V(K_{n-t-1})|, \ldots, |N[v'_{t+1}] \cap V(K_{n-t-1})|$ are t+1 distinct integers between 0 and n-t-1, the Equation (2.1) shows that $t \le n-t-1$. Similarly, the Equation (2.2) implies that $n-t-2 \le t$. Hence $n-2 \le 2t \le n-1$. So $t = \lceil \frac{n}{2} \rceil - 1$.

If n is even, then the Equation (2.2) shows that $|N[w'_j] \cap V(K_{t+1})| = j - 1$, for $j = 1, \ldots, n - t - 1$. So w'_1 has no neighbor in K_{t+1} . Thus for any $1 \le i \le t + 1$, $|N[v'_i] \cap V(K_{n-t-1})| \le n - t - 2$. Using Equation (2.1) we conclude that $|N[v'_i] \cap V(K_{n-t-1})| = i - 1$, for $i = 1, \ldots, t + 1$. Hence $G \cong G_n$.

Similarly, for odd n we obtain that $|N[v'_i] \cap V(K_{n-t-1})| = i - 1$, for $i = 1, \ldots, t + 1$. Thus v'_{t+1} is adjacent to every vertex of $V(K_{n-t-1})$. Hence $1 \leq |N[w'_1] \cap V(K_{t+1})|$. Using inequality (2.2) we find that $|N[w'_j] \cap V(K_{t+1})| = j$, for $j = 1, \ldots, n - t - 1$. Thus $G \cong G_n$.

Lemma 2.16. Let G_n be the semi-complete and quasi-reduced graph as mentioned above. Then $\lambda_2(G_n) > 0$ and $\lambda_3(G_n) < 0$ if and only if $4 \le n \le 12$.

Proof. One can see that $\lambda_2(G_3) = 0$ and for every $4 \le n \le 12$, $\lambda_2(G_n) > 0$ and $\lambda_3(G_n) < 0$. Now assume that $n \ge 13$. Since $\lambda_3(G_{13}) = 0$ and G_{13} is an induced subgraph of G_n (by Remark 2.13), by Interlacing Theorem 2.1 we find that $\lambda_3(G_n) \ge \lambda_3(G_{13}) = 0$. This completes the proof.

Definition 2.17. Let G be a graph with vertex set $\{v_1, \ldots, v_n\}$. By $G[K_{t_1}, \ldots, K_{t_n}]$ we mean the graph obtained by replacing the vertex v_j by the complete graph K_{t_j} for

 $1 \le j \le n$, where every vertex of K_{t_i} is adjacent to every vertex of K_{t_j} if and only if v_i is adjacent to v_j (in G). For example $K_2[K_p, K_q] \cong K_{p+q}$ and $\overline{K_2}[K_p, K_q] \cong K_p + K_q$.

Now we prove one of the main results of the paper.

Theorem 2.18. Let G be a connected graph of order $n \ge 3$. If $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$, then there exist some positive integers s and t_1, \ldots, t_s so that $3 \le s \le 12$ and $t_1 + \cdots + t_s = n$ and $G \cong G_s[K_{t_1}, \ldots, K_{t_s}]$.

Proof. Suppose that $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$. By Lemma 2.8, G is semi-complete. If G is quasi-reduced, then by Lemma 2.15, $G \cong G_n \cong G_n[K_1, \ldots, K_1]$. So $\lambda_2(G_n) = \lambda_2(G) > 0$ and $\lambda_3(G_n) = \lambda_3(G) < 0$. Hence by Lemma 2.16, $4 \le n \le 12$.

Now assume that G is not quasi-reduced. Thus there exists a connected induced subgraph of G, say H, such that H is quasi-reduced and $G = H[K_{t_1}, \ldots, K_{t_s}]$, where s is the order of H and t_1, \ldots, t_s are some positive integers. Thus $t_1 + \cdots + t_s = n$. If $H \cong K_s$, then $G \cong K_n$, a contradiction (since $\lambda_2(K_n) = -1 < 0$ while $\lambda_2(G) > 0$). Thus H is not a complete graph. On the other hand H is a connected graph of order s. Thus $s \ge 3$. Since H is obtained from G by removing some vertices and G is semi-complete, H is also semi-complete. Suppose that C_4 is an induced subgraph of H. Since H is an induced subgraph of G, by Interlacing Theorem 2.1 we conclude that $\lambda_3(G) \ge \lambda_3(H) \ge \lambda_3(C_4) = 0$, a contradiction. Thus H has no induced cycle C_4 .

Now we show that $H \cong G_s$. Since H is semi-complete, H is obtained from the disjoint union of two complete graphs, say K_p and K_q , for some positive integers p and q. Let $X = K_p$ and $Y = K_q$. We claim that for every two vertices $a, b \in V(X)$, $N[a] \subseteq N[b]$ or $N[b] \subseteq N[a]$. By contradiction assume that $N[a] \notin N[b]$ and $N[b] \notin N[a]$. Thus there are two vertices c and d such that $c \in N[a] \setminus N[b]$ and $d \in N[b] \setminus N[a]$. Since $V(X) \subseteq N[a] \cap N[b]$, we find that c and d are two vertices of Y. Now we remark that the induced subgraph on the vertices a, b, c, d is isomorphic to C_4 . It is a contradiction, since H has no induced cycle C_4 . So the claim holds. Similarly for every two vertices $z, w \in V(Y), N[z] \subseteq N[w]$ or $N[w] \subseteq N[z]$. On the other hand H is quasi-reduced, thus similar to the proof of Lemma 2.15 one can see that $H \cong G_s$.

If $s \ge 13$, then by Remark 2.13, G_{13} is an induced subgraph of H and so is an induced subgraph of G. Thus by Interlacing Theorem 2.1, $\lambda_3(G) \ge \lambda_3(G_{13}) = 0$, a contradiction, since $\lambda_3(G) < 0$. Hence $s \le 12$. The proof is complete.

We end this section by characterization the graphs with $\lambda_3 < 0$. We note that if G is a graph with $\lambda_3(G) < 0$, then G is not the null graph. Thus $\lambda_1(G) > 0$. Using Remark 2.5, the second part of Lemma 2.4 and Theorems 2.2, 2.3 and 2.18 we obtain this characterization.

Theorem 2.19. Let G be a graph with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. Assume that $\lambda_3 < 0$. Then the following hold:

- 1. If $\lambda_1 > 0$ and $\lambda_2 > 0$, then $G \cong K_p + K_q$ for some integers $p, q \ge 2$ or there exist some positive integers s and t_1, \ldots, t_s so that $3 \le s \le 12$ and $t_1 + \cdots + t_s = n$ and $G \cong G_s[K_{t_1}, \ldots, K_{t_s}]$.
- 2. If $\lambda_1 > 0$ and $\lambda_2 = 0$, then $G \cong K_1 + K_{n-1}$ or $G \cong K_n \setminus e$, where e is an edge of K_n .
- 3. If $\lambda_1 > 0$ and $\lambda_2 < 0$, then $G \cong K_n$.

Since $K_n \setminus e \cong G_3[K_1, K_1, K_{n-2}]$ and $K_p + K_q \cong \overline{K_2}[K_p, K_q]$, we can rewrite Theorem 2.19 as following:

Theorem 2.20. Let G be a graph. If $\lambda_3(G) < 0$, then $G \cong K_n$ or there exist some positive integers s and t_1, \ldots, t_s such that $2 \leq s \leq 12$ and $t_1 + \cdots + t_s = n$ and $G \cong G_s[K_{t_1}, \ldots, K_{t_s}]$.

In the next section we investigate the converse of Theorem 2.20. In other words we obtain all values of t_1, \ldots, t_s (for $2 \le s \le 12$) such that $\lambda_3(G_s[K_{t_1}, \ldots, K_{t_s}]) < 0$. We need the following important result for computing the characteristic polynomial of $G_s[K_{t_1}, \ldots, K_{t_s}]$, the polynomial $P(G_n[K_{t_1}, \ldots, K_{t_n}], \lambda)$.

Theorem 2.21. [7] Let $n \ge 2$. Suppose that $\{v_1, \ldots, v_n\}$ is the vertex set of G_n and $A = [a_{ij}]$ is the adjacency matrix of G_n with respect to $\{v_1, \ldots, v_n\}$ ($a_{ij} = 1$ if and only if v_i and v_j are adjacent and $a_{ij} = 0$, otherwise). Let t_1, \ldots, t_n be some positive integers and $M = [m_{ij}]$ be a $n \times n$ matrix, where

$$m_{ij} := \begin{cases} t_i - 1, & \text{if } i = j; \\ a_{ij}t_j, & \text{if } i \neq j. \end{cases}$$

Then

$$P(G_n[K_{t_1},\ldots,K_{t_n}],\lambda) = (\lambda+1)^{t_1+\cdots+t_n-n} g(\lambda),$$

where $g(\lambda) = det(\lambda I - M)$. In addition, the multiplicity of -1 as an eigenvalue of $G_n[K_{t_1}, \ldots, K_{t_n}]$ is equal to $t_1 + \cdots + t_n - n$.

3 The list of all connected graphs with $\lambda_2 > 0$ and $\lambda_3 < 0$

In this section we investigate the converse of Theorem 2.20. We use Petrović's notation [9] that is very similar to the notation of Definition 2.17. We note that in Definition 2.17, the graph $G[H_1, \ldots, H_n]$ is dependent to the labeling of the vertices of G while in the next definition first we fix a labeling for the vertices of G_n (see Definition 2.12), and then use the operation of Definition 2.17. For instance we consider the labeling v_1, \ldots, v_s and w_1, \ldots, w_s for the vertices of G_{2s} and then apply the operation of Definition 2.17.

Definition 3.1. Let $s \ge 1$ be an integer and n_1, \ldots, n_{2s+1} be some positive integers. Let $B_{2s}(n_1, \ldots, n_s; n_{s+1}, \ldots, n_{2s})$ denote the graph obtained from G_{2s} by replacing the vertices v_1 by K_{n_1}, v_2 by K_{n_2}, \ldots , and v_s by K_{n_s} and w_1 by $K_{n_{s+1}}, w_2$ by $K_{n_{s+2}}, \ldots$, and w_s by $K_{n_{2s}}$ (see Definition 2.12). In other words

$$B_{2s}(n_1,\ldots,n_s;n_{s+1},\ldots,n_{2s})=G_{2s}[K_{n_1},\ldots,K_{n_{2s}}],$$

where the ordering of the vertices of G_{2s} is $V(G_{2s}) = \{v_1, \ldots, v_s, w_1, \ldots, w_s\}$.

Similarly, by $B_{2s+1}(n_1, ..., n_s; n_{s+1}, ..., n_{2s}; n_{2s+1})$ we mean

 $B_{2s+1}(n_1,\ldots,n_s;n_{s+1},\ldots,n_{2s};n_{2s+1}) = G_{2s+1}[K_{n_1},\ldots,K_{n_{2s+1}}],$

where the ordering of the vertices of G_{2s+1} is $V(G_{2s+1}) = \{v_1, ..., v_s, w_1, ..., w_s, v_{s+1}\}$, (see Figure 5).

Remark 3.2. For every positive integers s and n_1, \ldots, n_{2s+1} , one can easily see that

$$B_{2s}(n_1,\ldots,n_s;n_{s+1},\ldots,n_{2s}) \cong B_{2s}(n_{s+1},\ldots,n_{2s};n_1,\ldots,n_s),$$

and

$$B_{2s+1}(n_1,\ldots,n_s;n_{s+1},\ldots,n_{2s};n_{2s+1}) \cong B_{2s+1}(n_{s+1},\ldots,n_{2s};n_1,\ldots,n_s;n_{2s+1}).$$

For avoiding the repeating, using the dictionary ordering on (n_1, \ldots, n_s) and $(n_{s+1}, \ldots, n_{2s})$ we just cite one of the graphs $B_{2s}(n_1, \ldots, n_s; n_{s+1}, \ldots, n_{2s})$ or $B_{2s}(n_{s+1}, \ldots, n_{2s}; n_1, \ldots, n_s)$ in our characterization. Similarly for the graphs $B_{2s+1}(n_1, \ldots, n_s; n_{s+1}, \ldots, n_{2s}; n_{2s+1})$ and $B_{2s+1}(n_{s+1}, \ldots, n_{2s}; n_1, \ldots, n_s; n_{2s+1})$ we only consider one of them. For example since by dictionary ordering $(4, 3, 2) \ge (4, 3, 1)$ we use $B_6(4, 3, 2; 4, 3, 1)$ instead of $B_6(4, 3, 1; 4, 3, 2)$. As another example we use $B_7(5, 3, 2; 5, 2, 4; 8)$ instead of $B_7(5, 2, 4; 5, 3, 2; 8)$, since $(5, 3, 2) \ge (5, 2, 4)$.



Figure 5: The graphs $B_3(2; 2; 4)$ and $B_4(1, 2; 4, 2)$.

The following theorem is the main result of [9].

Theorem 3.3. [9] Graph G has the property $\lambda_3 < 0$ if and only if G is an induced subgraph of one of the following graphs:

- 1. $B_4(3,2;2,r)$,
- 2. $B_5(1,r;2,3;1)$,
- 3. $B_5(r, 1; 2, 3; 1)$,
- 4. $B_5(3,2;2,1;r)$,
- 5. $B_5(r, 2; 1, 2; 2)$,
- 6. $B_6(r, 1, s; 1, 2, 2)$,
- 7. $B_6(2, 1, r; 2, 1, s)$,
- 8. $B_6(1, 2, 2; 1, r, 1)$,
- 9. $B_6(2,2,1;1,1,r)$,
- 10. $B_7(2, 1, 1; 2, 1, 1; r)$,

- 11. $B_7(r, 1, 2; 1, s, 1; 1)$,
- 12. $B_7(r, 1, 1; 1, 1, 2; 1)$,
- 13. $B_7(2, 2, 1; 1, r, 1; s)$,
- 14. $B_8(r, 1, 1, s; 1, 1, t, 1)$,
- 15. $B_9(1, r, 1, 1; 1, s, 1, 1; t)$,

where r, s and t are some positive integers or G is an induced subgraph of one of the 323 graphs with 12 vertices belonging respectively to the classes B_4 (10 graphs), B_5 (25 graphs), B_6 (69 graphs), B_7 (74 graphs), B_8 (80 graphs), B_9 (40 graphs), B_{10} (20 graphs), B_{11} (4 graphs) and B_{12} (1 graph).

Now we give a nicer characterization for graphs with $\lambda_3 < 0$. Note that the Petrović's result shows that any graph with exactly two non-negative eigenvalues is an induced subgraph of one the graphs described by Theorem 3.3. Since finding the structure of induced subgraphs of a graph is complicated, it is better to find the exact structure of all graphs with $\lambda_3 < 0$. In sequel we find this structure. To find our characterization, first we note that by Theorem 2.20 every graph with exactly two non-negative eigenvalues is isomorphic to $G_s[K_{t_1},\ldots,K_{t_s}]$ for some positive integers t_1,\ldots,t_s , where $2 \leq s \leq 12$. In this section we find all values of t_1, \ldots, t_s such that $G_s[K_{t_1}, \ldots, K_{t_s}]$ has exactly two non-negative eigenvalues. In other words we solve the converse of Theorem 2.20. We note that by Remark 2.6 it suffices to find all connected graphs with $\lambda_1 > 0, \lambda_2 > 0$ and $\lambda_3 < 0$. In other words we find all connected graphs $G_s[K_{t_1}, \ldots, K_{t_s}]$ such that $3 \le s \le 12$ and $\lambda_1 > 0$, $\lambda_2 > 0$ and $\lambda_3 < 0$. We obtain these graphs in ten theorems (for every $s, 3 \le s \le 12$, we consider a theorem). First we prove the case s = 3. Since the cases $s = 4, \ldots, s = 9$ similarly are proved, we just prove the case s = 6. In addition the proofs of the cases s = 10, 11, 12 are similar and we only prove the case s = 10. Our proofs are based on three theorems, Theorem 2.21 for computing the characteristic polynomials of $G_s[K_{t_1}, \ldots, K_{t_s}]$, Descartes' Sign Rule for polynomials and Interlacing Theorem 2.1. Since $G_s[K_{t_1}, \ldots, K_{t_s}] = B_s(t_1, \ldots, t_s)$, in sequel we use $B_s(t_1, \ldots, t_s)$ instead of $G_s[K_{t_1},\ldots,K_{t_s}]$.

Theorem 3.4. Let $G = B_3(a; b; c)$, where a, b, c are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if $ab \neq 1$.

Proof. Let $g(\lambda) = P(B_3(a; b; c), \lambda)$. By Theorem 2.21 we obtain that

$$g(\lambda) = (\lambda + 1)^{a+b+c-3} f(\lambda), \qquad (3.1)$$

where

$$f(\lambda) = \lambda^3 - (a+b+c-3)\lambda^2 + (ab-2a-2b-2c+3)\lambda + ac(b-1) + (a-1)(b+c-1).$$

If ab = 1, that is a = b = 1, then $g(\lambda) = \lambda(\lambda + 1)^{c-1}(\lambda^2 - (c-1)\lambda - 2c)$. This shows that $\lambda_1(G) > 0$ and $\lambda_2(G) = 0$. Now suppose that $ab \ge 2$. Let $z_1 \ge z_2 \ge z_3$ be all roots of f. Hence $f(\lambda) = (\lambda - z_1)(\lambda - z_2)(\lambda - z_3)$. Therefore $z_1 + z_2 + z_3 = a + b + c - 3 > 0$ and $z_1 z_2 z_3 = -f(0) = -(ac(b-1) + (a-1)(b+c-1)) < 0$. These equalities show that $z_1 > 0$, $z_2 > 0$ and $z_3 < 0$. On the other hand by the Equation (3.1), the eigenvalues

of $B_3(a; b; c)$ are $z_1, z_2, z_3, -1, \ldots, -1$ (the multiplicity of -1 is a + b + c - 3). Hence $\lambda_1(G) = z_1 > 0, \lambda_2(G) = z_2 > 0$ and $\lambda_3(G) = max\{z_3, -1\} < 0$. The proof is complete.

Theorem 3.5. Let $G = B_4(a_1, a_2; a_3, a_4)$, where a_1, a_2, a_3, a_4 are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following graphs:

- 1. $B_4(a, b; 1, d)$, $B_4(a, x; y, 1)$, $B_4(a, 1; c, 1)$, $B_4(a, 1; w, x)$,
- 2. $B_4(a, 1; x, d), B_4(w, b; x, 1), B_4(w, x; y, d), B_4(x, b; y, d),$
- 3. 25 specific graphs: 5 graphs of order 10, 10 graphs of order 11, and 10 graphs of order 12,

where a, b, c, d, x, y, w are some positive integers such that $x \leq 2, y \leq 2$ and $w \leq 3$.

Theorem 3.6. Let $G = B_5(a_1, a_2; a_3, a_4; a_5)$, where a_1, a_2, a_3, a_4, a_5 are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following graphs:

- 1. $B_5(a, w; 1, 1; 1), B_5(a, x; 1, d; 1), B_5(a, x; 1, y; z), B_5(a, x; 1, 1; e),$
- 2. $B_5(a, 1; c, 1; e), B_5(a, 1; x, w; 1), B_5(a, 1; x, y; e), B_5(a, 1; 1, d; e),$
- 3. $B_5(w, x; y, 1; e), B_5(x, b; 1, 1; 1), B_5(x, w; 1, d; 1), B_5(x, w; 1, 1; e),$
- 4. $B_5(1,b;1,d;1), B_5(1,b;1,x;y), B_5(1,x;1,y;e),$
- 5. 63 specific graphs: 13 graphs of order 10, 25 graphs of order 11, and 25 graphs of order 12,

where a, b, c, d, e, x, y, z, w are some positive integers such that $x \leq 2$, $y \leq 2$, $z \leq 2$ and $w \leq 3$.

Theorem 3.7. Let $G = B_6(a_1, a_2, a_3; a_4, a_5, a_6)$, where a_1, \ldots, a_6 are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following graphs:

- 1. $B_6(a, x, c; 1, 1, 1), B_6(a, 1, c; 1, e, 1), B_6(a, 1, c; 1, x, y), B_6(a, 1, c; 1, 1, f),$
- 2. $B_6(a, 1, 1; x, e, 1), B_6(x, b, 1; y, 1, 1), B_6(x, y, 1; 1, e, 1),$
- 3. $B_6(x, y, 1; 1, 1, f), B_6(x, 1, c; y, 1, f), B_6(1, b, x; 1, 1, 1),$
- 4. $B_6(1, b, 1; 1, e, 1), B_6(1, b, 1; 1, x, y), B_6(1, x, y; 1, 1, f),$
- 5. 145 specific graphs: 22 graphs of order 10, 54 graphs of order 11, and 69 graphs of order 12,

where a, b, c, d, e, f, x, y are some positive integers such that $x \leq 2$ and $y \leq 2$.

Proof. Let Ω_6 be the set of all 13 above types of graphs. In other words,

$$\Omega_6 = \Big\{ B_6(a, x, c; 1, 1, 1), B_6(a, 1, c; 1, e, 1), \dots, B_6(1, b, 1; 1, x, y), B_6(1, x, y; 1, 1, f) \Big\},\$$

where a, b, c, d, e, f are arbitrary positive integers and $x, y \in \{1, 2\}$. First we prove that every graph of Ω_6 has positive second largest eigenvalue and negative third largest eigenvalue. For instance we show that for any positive integers a, c and $f, \lambda_2(B_6(a, 1, c; 1, 1, f)) > 0$ and $\lambda_3(B_6(a, 1, c; 1, 1, f)) < 0$. The others are proved similarly.

First we note that G_6 is an induced subgraph of $B_6(a, 1, c; 1, 1, f)$. Thus by Interlacing Theorem 2.1, $\lambda_2(B_6(a, 1, c; 1, 1, f)) \ge \lambda_2(G_6) > 0$. On the other hand, if $m = \max\{a, c, f\}$, then $B_6(a, 1, c; 1, 1, f)$ is an induced subgraph of $B_6(m, 1, m; 1, 1, m)$. So by Interlacing Theorem 2.1, $\lambda_3(B_6(a, 1, c; 1, 1, f)) \le \lambda_3(B_6(m, 1, m; 1, 1, m))$. Thus to show that the inequality $\lambda_3(B_6(a, 1, c; 1, 1, f)) < 0$, it is sufficient to prove that $\lambda_3(B_6(m, 1, m; 1, 1, m)) < 0$. Now we show that for every positive integer m, $\lambda_3(B_6(m, 1, m; 1, 1, m)) < 0$.

Let M and m be two positive integers. If $M \ge m$, then by Interlacing Theorem 2.1, $\lambda_3(B_6(M, 1, M; 1, 1, M)) \ge \lambda_3(B_6(m, 1, m; 1, 1, m))$. This shows that if for $m \ge 12$, $\lambda_3(B_6(m, 1, m; 1, 1, m)) < 0$, then for all m, $\lambda_3(B_6(m, 1, m; 1, 1, m)) < 0$. Hence suppose that $m \ge 12$. By Theorem 2.21 we can obtain the characteristic polynomial of $B_6(m, 1, m; 1, 1, m)$. Let $\Phi_m(\lambda) = P(B_6(m, 1, m; 1, 1, m), \lambda)$. By Theorem 2.21

$$\Phi_m(\lambda) = (\lambda + 1)^{3m-3} \Psi_m(\lambda), \tag{3.2}$$

where

$$\Psi_m(\lambda) = 3m + (6m^2 + 7m - 1)\lambda + (2m^3 + 12m^2 - m - 3)\lambda^2 + (m^3 + 7m^2 - 14m - 2)\lambda^3 + (m^2 - 12m + 2)\lambda^4 + (3 - 3m)\lambda^5 + \lambda^6.$$

Since $m \geq 12$, all coefficients of $\Psi_m(\lambda)$ are positive except the coefficient of λ^5 . In fact the coefficient of λ^5 is negative. Now by *Descartes' Sign Rule* we conclude that the number of positive roots of $\Psi_m(\lambda)$ is 0 or 2 and the number of negative roots is 0 or 2 or 4. Since $\Psi_m(0) = 3m \neq 0$, every root of $\Psi_m(\lambda)$ is non-zero. On the other hand by Equation (3.2) the roots of $\Psi_m(\lambda)$ with many numbers -1 are the eigenvalues of $B_6(m, 1, m; 1, 1, m)$. Hence every root of $\Psi_m(\lambda)$ is real. Since $B_6(1, 1, 1; 1, 1, 1) \cong G_6$ is an induced subgraph of $B_6(m, 1, m; 1, 1, m)$, by Interlacing Theorem 2.1 and Lemma 2.16 we find that $\lambda_1(B_6(m, 1, m; 1, 1, m)) \geq \lambda_1(G_6) > 0$ and $\lambda_2(B_6(m, 1, m; 1, 1, m)) \geq \lambda_2(G_6) > 0$. Therefore by Equation (3.2), $\lambda_1(B_6(m, 1, m; 1, 1, m))$ and $\lambda_2(B_6(m, 1, m; 1, 1, m))$ are two roots of $\Psi_m(\lambda)$. Hence $\Psi_m(\lambda)$ has exactly two positive roots. Since the degree of $\Psi_m(\lambda)$ is six and $\Psi_m(\lambda)$ has exactly two positive roots and $\Psi_m(0) \neq 0$, the number of negative roots of $\Psi_m(\lambda)$ is four. Therefore by Equation (3.2), $B_6(m, 1, m; 1, 1, m)$ has exactly two positive eigenvalues and 3m + 1 negative eigenvalues. This shows that $\lambda_3(B_6(m, 1, m; 1, 1, m)) < 0$. Now we prove the necessity.

Claim 1. Let $H = B_6(a', b', c'; d', e', f')$ be a graph with at least 19 vertices, that is $a' + \dots + f' \ge 19$. If $H \notin \Omega_6$, then one of the graphs $H_1 = B_6(a' - 1, b', c'; d', e', f')$ or $H_2 = B_6(a', b' - 1, c'; d', e', f')$ or $H_3 = B_6(a', b', c' - 1; d', e', f')$ or $H_4 = B_6(a', b', c'; d', e', f')$ or $H_5 = B_6(a', b', c'; d', e' - 1, f')$ or $B_6(a', b', c'; d', e', f' - 1)$ is not in Ω_6 . Note that these graphs are all induced subgraphs of H of order |V(H)| - 1.

Proof of Claim 1. Suppose that $H \notin \Omega_6$. By contradiction assume that all graphs H_1, \ldots, H_6 are in Ω_6 . Now we consider H_1 . If $H_1 = B_6(a, x, c; 1, 1, 1)$ for some positive integers a, c and $x \leq 2$, then $H \in \Omega_6$, a contradiction. If $H_1 = B_6(a, 1, c; 1, e, 1)$, for some positive integers a, c and e, then $H \in \Omega_6$, a contradiction. Similarly one can see that $H_1 \neq B_6(a, 1, c; 1, x, y), B_6(a, 1, c; 1, 1, f), B_6(a, 1, 1; x, e, 1)$. So $H_1 = B_6(x, b, 1; y, 1, 1)$ or $B_6(x, y, 1; 1, e, 1)$ or $B_6(x, y, 1; 1, 1, f)$ or $B_6(x, 1, c; y, 1, f)$ or $B_6(1, b, 1; 1, e, 1)$ or $B_6(1, b, 1; 1, x, y)$ or $B_6(1, x, y; 1, 1, f)$, for some positive integers b, c, e, f and $x, y \leq 2$. Since $x \leq 2$, we find that $a' - 1 \leq 2$. Thus $a' \leq 3$. Similarly if $H_2, \ldots, H_6 \in \Omega_6$, we obtain that $b', \ldots, f' \leq 3$. Therefore $a' + \cdots + f' \leq 18$, a contradiction. Thus the claim is proved.

Claim 2. Let $K = B_6(a'', b'', c''; d'', e'', f'')$ be a graph with at least 13 vertices. If $K \notin \Omega_6$, then $\lambda_3(K) \ge 0$.

Proof of Claim 2. Assume that $K \notin \Omega_6$. We prove the claim by induction on n = |V(K)|. By computer one can check the validity for $n = 13, \ldots, 18$. Hence let $n \ge 19$. By Claim 1, K has an induced subgraph, say L, of order n - 1 such that $L \notin \Omega_6$. Since $n - 1 \ge 18$, by the induction hypothesis $\lambda_3(L) \ge 0$. Thus by Interlacing Theorem 2.1, $\lambda_3(K) \ge \lambda_3(L) \ge 0$. Thus the claim is proved.

Now let $W = B_6(a''', b''', c'''; a''', e''', f''')$ be a graph of order n. Assume that $\lambda_2(W) > 0$ and $\lambda_3(W) < 0$. If $W \notin \Omega_6$, then by Claim 2, $n \leq 12$. By computer we find that there are only 145 graphs with this property. More precisely there are 22 graphs of order 10, 54 graphs of order 11 and 69 graphs of order 12 such that they are not in Ω_6 while their second eigenvalues are positive and third eigenvalues are negative. The proof is complete.

Theorem 3.8. Let $G = B_7(a_1, a_2, a_3; a_4, a_5, a_6; a_7)$, where a_1, \ldots, a_7 are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following graphs:

- 1. $B_7(a, 1, x; 1, e, 1; 1), B_7(a, 1, 1; 1, e, 1; g), B_7(a, 1, 1; 1, 1, x; 1),$
- 2. $B_7(x, y, 1; 1, e, 1; g), B_7(x, 1, 1; y, 1, 1; g), B_7(1, b, x; 1, 1, 1; g),$
- 3. $B_7(1, b, 1; 1, e, 1; g), B_7(1, 1, c; 1, 1, f; 1),$
- 4. 143 specific graphs: 18 graphs of order 10, 52 graphs of order 11, and 73 graphs of order 12,

where a, b, c, d, e, f, g, x, y are some positive integers such that $x \leq 2$ and $y \leq 2$.

Theorem 3.9. Let $G = B_8(a_1, a_2, a_3, a_4; a_5, a_6, a_7, a_8)$, where a_1, \ldots, a_8 are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following graphs:

- 1. $B_8(a, 1, 1, d; 1, 1, g, 1), B_8(1, b, 1, 1; 1, f, 1, 1),$
- 2. 134 specific graphs: 12 graphs of order 10, 42 graphs of order 11, and 80 graphs of order 12,

where a, b, d, f, g are some positive integers.

Theorem 3.10. Let $G = B_9(a_1, a_2, a_3, a_4; a_5, a_6, a_7, a_8; a_9)$, where a_1, \ldots, a_9 are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following graphs:

- 1. $B_9(1, b, 1, 1; 1, f, 1, 1; k)$,
- 2. 59 specific graphs: 3 graphs of order 10, 17 graphs of order 11, and 39 graphs of order 12,

where b, f, k are some positive integers.

Remark 3.11. The complete list of the mentioned 25 graphs in Theorem 3.5, 63 graphs in Theorem 3.6, 145 graphs in Theorem 3.7, 143 graphs in Theorem 3.8, 134 graphs in Theorem 3.9 and 59 graphs in Theorem 3.10 can be obtained from the author upon request.

Theorem 3.12. Let $G = B_{10}(a_1, a_2, a_3, a_4, a_5; a_6, a_7, a_8, a_9, a_{10})$, where a_1, \ldots, a_{10} are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following 26 graphs:

I. $B_{10}(1, 1, 1, 1, 1; 1, 1, 1, 1)$,

2. $B_{10}(1,1,1,1,2;1,1,1,1), B_{10}(1,1,1,2,1;1,1,1,1),$

3. $B_{10}(1,1,2,1,1;1,1,1,1), B_{10}(1,2,1,1,1;1,1,1,1),$

4. $B_{10}(2,1,1,1,1;1,1,1,1,1)$,

- 5. $B_{10}(1,1,1,1,3;1,1,1,1), B_{10}(1,1,1,2,1;1,1,1,1,2),$
- 6. $B_{10}(1,1,1,2,1;1,1,1,2,1), B_{10}(1,1,1,2,2;1,1,1,1,1),$
- 7. $B_{10}(1,1,1,3,1;1,1,1,1)$, $B_{10}(1,1,2,1,1;1,1,1,1,2)$,

8. $B_{10}(1,1,2,2,1;1,1,1,1), B_{10}(1,1,3,1,1;1,1,1,1),$

- 9. $B_{10}(1,2,1,1,1;1,1,2,1,1), B_{10}(1,2,1,1,1;1,2,1,1,1),$
- 10. $B_{10}(1,2,1,1,2;1,1,1,1), B_{10}(1,2,2,1,1;1,1,1,1),$
- 11. $B_{10}(1,3,1,1,1;1,1,1,1), B_{10}(2,1,1,1,1;1,1,1,2,1),$
- 12. $B_{10}(2,1,1,1,1;1,1,2,1,1), B_{10}(2,1,1,1,1;2,1,1,1),$
- 13. $B_{10}(2,1,1,1,2;1,1,1,1), B_{10}(2,1,1,2,1;1,1,1,1),$

14.
$$B_{10}(2,2,1,1,1;1,1,1,1), B_{10}(3,1,1,1,1;1,1,1,1).$$

Proof. One can see that all of the above graphs have positive second largest eigenvalue and negative third largest eigenvalue. Now we prove the necessity. Let $G = B_{10}(a_1, \ldots, a_5; a_6, \ldots, a_{10})$ such that $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$. We show that for $i = 1, \ldots, 10, a_i \leq 3$. For example by contradiction suppose that $a_1 \geq 4$. Thus $H = B_{10}(4, 1, 1, 1, 1; 1, 1, 1, 1)$ is an induced subgraph of G. So by Interlacing Theorem 2.1, $\lambda_3(G) \geq \lambda_3(H)$. On the other hand $\lambda_3(H) > 0$, a contradiction. Similarly we obtain $a_2, \ldots, a_{10} \leq 3$. Also one can

see that at most one of the numbers a_1, \ldots, a_{10} is 3. For example if $a_1 = 3$ and $a_2 = 3$, then $K = B_{10}(3, 3, 1, 1, 1; 1, 1, 1, 1, 1)$ is an induced subgraph of G. So by Interlacing Theorem 2.1, $\lambda_3(G) \ge \lambda_3(K)$ while $\lambda_3(K) > 0$, a contradiction. Since $a_1, \ldots, a_{10} \le 3$ and at most one of them is $3, a_1 + \cdots + a_{10} \le 21$. Thus the order of G is at most 21. Now by computer one can check the result.

Theorem 3.13. Let $G = B_{11}(a_1, a_2, a_3, a_4, a_5; a_6, a_7, a_8, a_9, a_{10}; a_{11})$, where a_1, \ldots, a_{11} are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if G is isomorphic to one of the following 5 graphs:

- *I.* $B_{11}(1, 1, 1, 1, 1; 1, 1, 1, 1; 1)$,
- 2. $B_{11}(1, 1, 1, 1, 1; 1, 1, 1, 1; 2)$, $B_{11}(1, 1, 1, 1, 2; 1, 1, 1, 1; 1)$,
- 3. $B_{11}(1,2,1,1,1;1,1,1,1;1), B_{11}(1,1,2,1,1;1,1,1,1,1;1).$

Theorem 3.14. Let $G = B_{12}(a_1, a_2, a_3, a_4, a_5, a_6; a_7, a_8, a_9, a_{10}, a_{11}, a_{12})$, where a_1, \ldots, a_{12} are some positive integers. Then $\lambda_2(G) > 0$ and $\lambda_3(G) < 0$ if and only if $G \cong B_{12}(1, 1, 1, 1, 1, 1; 1, 1, 1, 1)$.

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A classification of the Veldkamp lines of the near hexagon $L_3 imes \mathrm{GQ}(2,2)$

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Abstract

Using a standard technique sometimes (inaccurately) known as Burnside's Lemma, it is shown that the Veldkamp space of the near hexagon $L_3 \times GQ(2, 2)$ features 156 different types of lines. We also give an explicit description of each type of a line by listing the types of the three geometric hyperplanes it consists of and describing the properties of its core set, that is the subset of points of $L_3 \times GQ(2, 2)$ shared by the three geometric hyperplanes in question.

Keywords: Near hexagons, Geometric hyperplanes, Veldkamp spaces. Math. Subj. Class.: 51Exx, 81R99

1 Introduction

Brouwer *et al.* [1] proved that there are eleven isomorphism types of slim dense near hexagons. Of these eleven, the near hexagons of sizes 27, 45 and 81 are the most promising for physical applications. This paper is devoted to a study of the second of these three examples and its Veldkamp space. The first of the three examples was described in our paper [4], and we plan to study the third case in a future work. The 45 point space we study here is the product $L_3 \times GQ(2, 2)$, where L_3 is the line containing three points and GQ(2, 2) is the generalized quadrangle of order two.

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2 Near polygons, quads, geometric hyperplanes and Veldkamp spaces

In this section we gather all the basic notions and well-established theoretical results that will be needed in the sequel.

A near polygon (see, e. g., [3] and references therein) is a connected partial linear space $S = (P, L, I), I \subset P \times L$, with the property that given a point x and a line L, there always exists a unique point on L nearest to x. (Here distances are measured in the point graph, or collinearity graph of the geometry.) If the maximal distance between two points of S is equal to d, then the near polygon is called a near 2d-gon. A near 0-gon is a point and a near 2-gon is a line; the class of near quadrangles coincides with the class of generalized quadrangles.

A nonempty set X of points in a near polygon S = (P, L, I) is called a subspace if every line meeting X in at least two points is completely contained in X. A subspace X is called geodetically closed if every point on a shortest path between two points of X is contained in X. Given a subspace X, one can define a sub-geometry S_X of S by considering only those points and lines of S that are completely contained in X. If X is geodetically closed, then S_X clearly is a sub-near-polygon of S. If a geodetically closed sub-near-polygon S_X is a non-degenerate generalized quadrangle, then X (and often also S_X) is called a *quad*.

A near polygon is said to have order (s,t) if every line is incident with precisely s + 1 points and if every point is on precisely t + 1 lines. If s = t, then the near polygon is said to have order s. A near polygon is called *dense* if every line is incident with at least three points and if every two points at distance two have at least two common neighbours. A near polygon is called *slim* if every line is incident with precisely three points. It is well known (see, e. g., [6]) that there are, up to isomorphism, three slim non-degenerate generalized quadrangles. The (3×3) -grid is the unique generalized quadrangle of order (2, 1), GQ(2, 1). The unique generalized quadrangle of order 2, GQ(2, 2), is the generalized quadrangle of the points and lines of PG(3, 2) that are totally isotropic with respect to a given symplectic form. The points and lines lying on a given nonsingular elliptic quadric of PG(5, 2) define the unique generalized quadrangle of order (2, 4), GQ(2, 4). Any *slim dense* near polygon contains quads, which are necessarily isomorphic to either GQ(2, 1), GQ(2, 2) or GQ(2, 4).

Next, a *geometric hyperplane* of a partial linear space is a proper subspace meeting each line (necessarily in a unique point or the whole line). The set of points at non-maximal distance from a given point x of a dense near polygon S is a hyperplane of S, usually called the singular hyperplane (or perp-set) with deepest point x. Given a hyperplane H (or any subset of points C) of S, one defines the *order* of any of its points as the number of lines through the point that are fully contained in $H(\mathcal{C})$; a point of $H(\mathcal{C})$ is called *deep* if all the lines passing through it are fully contained in $H(\mathcal{C})$. If H is a hyperplane of a dense near polygon S and if Q is a quad of S, then precisely one of the following possibilities occurs: (1) $Q \subseteq H$; (2) $Q \cap H = x^{\perp} \cap Q$ for some point x of Q; (3) $Q \cap H$ is a sub-quadrangle of Q; and (4) $Q \cap H$ is an ovoid of Q. If case (1), case (2), case (3), or case (4) occurs, then Q is called, respectively, *deep*, *singular*, *sub-quadrangular*, or *ovoidal* with respect to H. If S is slim and H_1 and H_2 are its two distinct hyperplanes, then the complement of symmetric difference of H_1 and H_2 , $\overline{H_1 \Delta H_2}$, is again a hyperplane; this means that the totality of hyperplanes of a slim near polygon form a vector space over the Galois field with two elements, \mathbb{F}_2 . In what follows, we shall put $\overline{H_1 \Delta H_2} \equiv H_1 \oplus H_2$ and call it the (Veldkamp) sum of the two hyperplanes.

Finally, we shall introduce the notion of the Veldkamp space, $\mathcal{V}(\Gamma)$, of a point-line incidence geometry $\Gamma(P, L)$ [2]. Here, $\mathcal{V}(\Gamma)$ is the space in which (i) a point is a geometric hyperplane of Γ and (ii) a line is the collection H'H'' of all geometric hyperplanes H of Γ such that $H' \cap H'' = H' \cap H = H'' \cap H$ or H = H', H'', where H' and H'' are distinct points of $\mathcal{V}(\Gamma)$. Following [10, 8], we adopt also here the definition of Veldkamp space given by Buekenhout and Cohen [2] instead of that of Shult [11], as the latter is much too restrictive by requiring any three distinct hyperplanes H', H'' and H''' of Γ to satisfy the following two conditions: i) H' is not properly contained in H'' and ii) $H' \cap H'' \subseteq H'''$ implies $H' \subset H'''$ or $H' \cap H'' = H' \cap H'''$. The two definitions differ in the crucial fact that whereas the Veldkamp space in the sense of Shult is *always* a linear space, that of Buekenhout and Cohen needs not be so; in other words, Shult's Veldkamp lines are always of the form $\{H \in \mathcal{V}(\Gamma) \mid H \supseteq H' \cap H''\}$ for certain geometric hyperplanes H' and H''.

3 The near hexagon $L_3 \times GQ(2,2)$

The near hexagon $L_3 \times GQ(2, 2)$ has recently [9] caught an attention of theoretical physicists due to the fact that its main constituent, the generalized quadrangle GQ(2, 2), reproduces the commutation relations of the 15 elements of the two-qubit Pauli group (see, e. g., [7]), with each of its ten embedded copies of GQ(2, 1) playing, remarkably, the role of the so-called *Mermin magic square* [5] — the smallest configuration of two-qubit observables furnishing a very important proof of contextuality of quantum mechanics. A well-known construction of GQ(2, 2) identifies the points with two-element subsets of $\{1, 2, 3, 4, 5, 6\}$, with two points being collinear if and only if they are equal or disjoint. The natural action of S_6 on this set of size 6 induces automorphisms of GQ(2, 2). In fact, when considered in this way, S_6 turns out to be the full automorphism group.

It is known that every geometric hyperplane of a slim dense near polygon arises from its universal embedding. It can be shown from this that, equipped with the operation of Veldkamp sum, the Veldkamp space $V_{GQ(2,2)}$ is isomorphic to PG(4, 2), the projective space obtained from a 5-dimensional space over \mathbb{F}_2 (see also [10]). It follows that GQ(2, 2) has $2^5 - 1 = 31$ geometric hyperplanes, which turn out to be of three types:

- (i) 15 perp-sets, with 7 points each;
- (ii) 10 grids (copies of GQ(2, 1)), with 9 points each;
- (iii) 6 ovoids, with 5 points each.

In other words, there are three orbits of geometric hyperplanes under the action of S_6 . Identifying the points of GQ(2, 2) with two-element subsets of the set $\{1, 2, 3, 4, 5, 6\}$ as described earlier, we find that an example of an ovoid is the set

$$e_1 := \{\{1,2\},\{1,3\},\{1,4\},\{1,5\},\{1,6\}\}.$$

The other ovoids, e_2, e_3, \ldots, e_6 are obtained from e_1 by acting by the transposition (1, i) for $i = 2, 3, \ldots, 6$ respectively.

The Veldkamp sum $e_i + e_j$ (for $1 \le i < j \le 6$) is the perp-set of the point $\{i, j\}$. If we have

$$\{1, 2, 3, 4, 5, 6\} = \{i, j, k, l, m, n\}$$

in some order, then the sum $e_i + e_j + e_k$ is the grid whose elements are the nine points

$$\{\{a, b\} : a \in \{i, j, k\} \text{ and } b \in \{l, m, n\}\}.$$

It follows that the six ovoids are a spanning set for $V_{GQ(2,2)}$. Since each point of GQ(2,2) lies in precisely two ovoids, it follows that we have the relation

$$e_1 + e_2 + e_3 + e_4 + e_5 + e_6 = 0,$$

where 0 denotes the subset of GQ(2, 2) consisting of all 15 points. Since we have an isomorphism $V_{GQ(2,2)} \cong PG(4, 2)$, it follows by a counting argument that this is the only nontrivial dependence relation between the e_i , and thus that the ovoids e_1, \ldots, e_5 form a basis for $V_{GQ(2,2)}$.

The points of the near hexagon $L_3 \times GQ(2, 2)$ are simply the 45 ordered pairs (p, q) where p is a point of L_3 and q is a point of GQ(2, 2). We call a collection of 15 points (p, q) sharing the same value of p a *layer* of the near hexagon. A layer is an example of a quad in the sense of §2. We imagine that the points of L_3 are arranged vertically, and we will sometimes use terms like "the top quad" to refer to one of the layers of the near hexagon.

Two points (p_1, q_1) and (p_2, q_2) of $L_3 \times GQ(2, 2)$ are collinear if either

- (i) $p_1 = p_2$ and q_1 is collinear to q_2 , or
- (ii) p_1 is collinear to p_2 and $q_1 = q_2$.

The lines of $L_3 \times GQ(2, 2)$ are of two types. The *type-one* lines are the 15 lines of the form $\{(p,q) : p \in L_3\}$ for a fixed point $q \in GQ(2, 2)$. The *type-two* lines are the 45 lines of the form $\{(p,q) : q \in L\}$ for a fixed $p \in L_3$ and some line L of GQ(2, 2).

The near hexagon $L_3 \times GQ(2, 2)$ has a number of obvious automorphisms. One type of automorphism involves permuting the three GQ(2, 2)-quads, but making no other changes. The subgroup of all such automorphisms is isomorphic to S_3 . Another type of automorphism involves acting diagonally on the three GQ(2, 2)-quads by S_6 , the automorphism group of GQ(2, 2). This action commutes with the action of S_3 just mentioned, and produces a group of automorphisms isomorphic to $S_6 \times S_3$. It turns out that this is the full automorphism group, as shown by Brouwer *et al.* [1].

From now on, let us denote the Veldkamp space of $L_3 \times GQ(2, 2)$ by V. Some features of V are close to obvious, which stems from Sec. 2. One of these is that the intersection of one of the three GQ(2, 2)-quads with a point of V (regarded as a subset of the 45 points) can take one of two forms. Either the GQ(2, 2)-quad is completely filled in (i. e., it is deep), or takes the form of one of the geometric hyperplanes of GQ(2, 2) (i. e., it is singular, sub-quadrangular or ovoidal). Furthermore, the Veldkamp sum of any two of the layers (regarded as subsets of GQ(2, 2) under some obvious identification) must be equal to the third layer. It follows from this that V contains $2^{10} - 1 = 1023$ points.

The above discussion shows that, as an $S_6 \times S_3$ -module over \mathbb{F}_2 , V is isomorphic to $M \otimes N$, where M is the 5-dimensional module for S_6 described earlier, and N is the S_3 -module obtained by quotienting the 3-dimensional permutation module $\{f_1, f_2, f_3\}$ for S_3 by the submodule spanned by $f_1 + f_2 + f_3$. The set $\{f_1, f_2\}$ then form a basis for N, and the set

$$\{e_i \otimes f_j : 1 \le i \le 5, \ 1 \le j \le 2\}$$

forms a basis for V. We will write this basis for short as $\{e_1, \ldots, e_{10}\}$, where for $1 \le i \le 5$, e_i denotes $e_i \otimes f_1$, and for $6 \le i \le 10$, e_i denotes $e_{i-5} \otimes f_2$.

4 The classification of hyperplanes

The geometric hyperplanes of $L_3 \times GQ(2, 2)$ were classified in [9]. Up to automorphisms, there are eight types of them, denoted by H_1 to H_8 and described in detail in [9, Table 2]. We now explain how these eight types can be reconstructed using the results in the previous section.

The description of the hyperplanes of GQ(2, 2) above can be used to identify each hyperplane with one of the 31 nontrivial set partitions of a 6-element into two pieces. If *S* and *T* are disjoint nonempty sets for which

$$S \cup T = \{1, 2, 3, 4, 5, 6\},\$$

then we identify the pair $\{S, T\}$ with the hyperplane

$$\sum_{i \in S} e_i = \sum_{j \in T} e_j.$$

If $|S| \ge |T|$, we associate the partition (|S|, |T|) of the number 6 to the set partition $\{S, T\}$. Under these identifications, the partitions of 6 given by (5, 1), (4, 2) and (3, 3) correspond, via set partitions, to ovoids, perp sets and grids, respectively.

The Veldkamp sum operation on $V_{GQ(2,2)}$ described in the previous section may now be defined purely in terms of sets: the Veldkamp sum of the two set partitions $\{A|B\}$ and $\{C|D\}$ is given by

$$\{(A \cap C) \cup (B \cap D) | (A \cap D) \cup (B \cap C)\}.$$

This identification extends to a set-theoretic description of the hyperplanes of $L_3 \times$ GQ(2, 2). The hyperplanes of this larger space may be put into bijection with ordered quadruples of pairwise disjoint sets (A, B, C, D) such that (a) no three of the sets are empty and (b) the union of the four sets is $\{1, 2, 3, 4, 5, 6\}$. Such a quadruple corresponds to the hyperplane given by the ordered triple of partitions

$$(\{A \cup B | C \cup D\}, \{A \cup C | B \cup D\}, \{A \cup D | B \cup C\}).$$

Here, the leftmost component of the ordered triple describes the hyperplane of GQ(2, 2) appearing in the uppermost GQ(2, 2)-quad of $L_3 \times GQ(2, 2)$, and so on. For example, if the sets *C* and *D* are empty, the top GQ(2, 2)-quad will be deep and the other two will be identical to each other, being either singular, sub-quadrangular or ovoidal.

The correspondence between the ordered quadruples and the hyperplanes is four-toone, because the quadruples (A, B, C, D), (B, A, D, C), (C, D, A, B) and (D, C, B, A)all index the same hyperplane. It follows that acting by an element of the Klein four-group V_4 on an ordered quadruple leaves the corresponding hyperplane invariant. The group $S_6 \times S_4$ acts on the quadruples, where S_6 acts diagonally on each of the set partitions A, B, C and D, and S_4 acts by place permutation. This induces an action of $S_6 \times S_4$ on the hyperplanes of $L_3 \times \text{GQ}(2, 2)$, and since the action of $V_4 \leq S_4$ is trivial, this in turn induces an action of $S_6 \times (S_4/V_4) \cong S_6 \times S_3$ on the hyperplanes, thus recovering the full automorphism group of $L_3 \times \text{GQ}(2, 2)$ in which S_3 acts by permuting the GQ(2, 2)-quads.

This approach yields another way to deduce that the number of hyperplanes of $L_3 \times$ GQ(2, 2) is $2^{10} - 1$, as follows. There are 4^6 possible quadruples of pairwise disjoint sets (A, B, C, D) whose union is $\{1, 2, 3, 4, 5, 6\}$, and four of these quadruples have three

Name	Partition	Orbit size	Stabilizer	Order
H_1	(3,3)	30	$(S_3 \wr \mathbb{Z}_2) \times S_2$	144
H_2	(4, 2)	45	$S_4 \times S_2 \times S_2$	96
H_3	(5,1)	18	$S_5 \times S_2$	240
H_4	(2, 2, 1, 1)	270	$S_2 \times S_2 \times S_2 \times S_2$	16
H_5	(2, 2, 2)	90	$S_2 \times S_2 \times S_2 \times S_3$	48
H_6	(3, 1, 1, 1)	120	$S_3 imes S_3$	36
H_7	(3, 2, 1)	360	$S_3 imes S_2$	12
H_8	(4, 1, 1)	90	$S_4 imes S_2$	48

Table 1: A classification of geometric hyperplanes of $L_3 \times GQ(2, 2)$.

empty components. Since the correspondence between quadruples and hyperplanes is fourto-one, the number of hyperplanes is $(4^6 - 4)/4$.

The correspondence described above induces a natural correspondence between $S_6 \times S_4$ -orbits (or $S_6 \times S_3$ -orbits) of hyperplanes on the one hand, and partitions of 6 into two, three or four parts on the other. There are eight such partitions; they are shown in Table 1, together with their orbit sizes, stabilizers isomorphism types, stabilizer orders, and their name in the $H_1 - H_8$ notation of [9, Table 2].

5 Counting and classifying different types of Veldkamp lines

The orbits of lines in the Veldkamp space V may be enumerated using a standard technique sometimes (inaccurately) known as Burnside's Lemma, which proves the following.

Let G be a finite group acting on a finite set X with t orbits, and for each $g \in G$, let X^g denote the number of elements of X fixed by g. Then we have $t = \frac{1}{|G|} \sum_{g \in G} |X^g|$.

Furthermore, if C is a set of conjugacy class representatives of G, then we have

$$t = \frac{1}{|G|} \sum_{g \in \mathcal{C}} |\mathcal{C}| |X^g|.$$

Using this technique, we can recover known results about orbits of lines under the action of the automorphism group S_6 of GQ(2, 2): there are 3 orbits of hyperplanes (Veld-kamp points) and 5 orbits of Veldkamp lines. We can also recover the result the Veldkamp space V has 8 orbits of hyperplanes under the automorphism group $S_6 \times S_3$.

The same idea can be adapted to count the orbits of Veldkamp lines of V. The counting argument is more complicated than for the case of Veldkamp points, because it is possible for a line to be fixed by a group element g without the three individual points being fixed. There are three possibilities to consider, which we denote by (1), (2) and (3) in Table 2.

- (1) Every point of the Veldkamp line is fixed by g. Such lines lie entirely within the fixed point space of g. Each number in the Fix(1) column is the number of lines in a projective space PG(d(g) 1, 2), for a suitable integer d(g) depending on the conjugacy class of g.
- (2) One point of the Veldkamp line is fixed by g, and the other two are exchanged. To enumerate such lines, we take one point x outside the fixed point space of g. The

other two points are the point g(x), and the point collinear with both of them (which is fixed by g). We then divide by 2 to correct for the overcount.

Writing d(g) as above, it follows in each case that the entry in the Fix(2) column of g is given by

$$\frac{1}{2} \left(2^{d(g^2)} - 2^{d(g)} \right).$$

(3) The element g rotates the three points of the Veldkamp line in a 3-cycle. Each entry in the Fix(3) column is a number of the form (4^k - 1)/3, and the enumeration of these cases is the most complicated. An ordered Veldkamp line can be thought of as a sequence of 30 binary digits. Typically, some even number, 2k, of these bits can be chosen arbitrarily, provided that not all of them are zero, and then the rest of the structure is forced. It is then necessary to divide by 3 to correct for an overcount, by identifying an ordered Veldkamp line with each of its cyclic shifts.

We identify the group $S_6 \times S_3$ in the obvious way with the subgroup of S_9 fixing setwise each of the subsets $\{1, 2, 3, 4, 5, 6\}$ and $\{7, 8, 9\}$. Since there are 11 partitions of 6 and 3 partitions of 3, it follows that $S_6 \times S_3$ has 33 conjugacy classes, and it is straightforward to find conjugacy class representatives. Table 2 shows the calculation for the Veldkamp lines of $L_3 \times GQ(2, 2)$. The grand total of

$$673920 = |S_6 \times S_3| \times 156 = 720 \times 6 \times 156$$

proves that there are 156 orbits of Veldkamp lines of the near hexagon.

All 156 types are then listed in Table 3. Here, each type is characterized by its composition (columns 9 to 16) and the properties of the core C of the line, that is the set of points that are common to all the three geometric hyperplanes of a line of the given type. In particular, for each type (column 1) we list the number of points (column 2) and lines (column 3) of the core as well as the distribution of the orders of its points. The last three columns show the intersection of C with each of the three GQ(2, 2)-quads. Here, 'g-perp' stands for a perp-set in a certain GQ(2, 1) located in the particular GQ(2, 2), and 'unitr/tritr' abbreviates a unicentric/tricentric triad. If two or more types happen to possess the same string of parameters, the distinction between them is given by an explanatory remark/footnote.

Conjugacy class	Fix(1)	Fix(2)	Fix(3)	Size of class	Product
id	174251	0	0	1	174251
(12)	10795	384	0	15	167685
(12)(34)	651	480	0	45	50895
(12)(34)(56)	651	480	0	15	16965
(123)	651	0	5	40	26240
(123)(456)	1	0	85	40	3440
(1234)	35	24	0	90	5310
(1234)(56)	35	24	0	90	5310
(123)(45)	35	24	5	120	7680
(12345)	1	0	0	144	144
(123456)	1	0	5	120	720
(78)	155	496	0	3	1953
(12)(78)	155	496	0	45	29295
(12)(34)(78)	155	496	0	135	87885
(12)(34)(56)(78)	155	496	0	45	29295
(123)(78)	7	28	1	120	4320
(123)(456)(78)	0	1	5	120	720
(1234)(78)	7	28	0	270	9450
(1234)(56)(78)	7	28	0	270	9450
(123)(45)(78)	7	28	1	360	12960
(12345)(78)	0	1	0	432	432
(123456)(78)	0	1	5	360	2160
(789)	0	0	341	2	682
(12)(789)	0	0	85	30	2550
(12)(34)(789)	0	0	21	90	1890
(12)(34)(56)(789)	0	0	21	30	630
(123)(789)	1	0	85	80	6880
(123)(456)(789)	35	0	21	80	4480
(1234)(789)	0	0	5	180	900
(1234)(56)(789)	0	0	5	180	900
(123)(45)(789)	1	0	21	240	5280
(12345)(789)	0	0	1	288	288
(123456)(789)	1	6	5	240	2880
					673920

Table 2: Orbits of Veldkamp lines of $L_3 \times GQ(2, 2)$.

			#	of Po	oints o	of Ord	ler	Composition										
Тр	Pt	Ln	0	1	2	3	4	H_1 H_2 H_3 H_4 H_5 H_6 H_7 H_8								1st	2nd	3rd
1	27	27	0	0	0	27	0	3	-	-	_	_	-	-	-	grid	grid	grid
2	25	24	0	0	10	10	5	2	1	-	-	-	-	-	-	full	g-perp	g-perp
3	23	19	0	0	12	11	0	2	-	-	1	-	-	-	-	grid	g-perp	grid
4	21	20	0	0	6	12	3	-	3	-	-	-	-	-	-	full	line	line
5	21	18	0	6	0	12	3	1	1	1	-	-	-	-	-	full	unitr	unitr
6	21	18	0	6	0	12	3	-	3	-	-	-	-	-	-	full	tritr	tritr
7	21	16	0	2	12	6	1	1	1	-	1	-	-	-	-	perp	grid	g-perp
8	21	16	0	0	18	0	3	-	3	-	-	-	-	-	-	perp	perp	perp
9	19	15	0	0	12	7	0	1	-	-	2	-	-	-	-	grid	g-perp	g-perp
10	19	13	0	4	10	5	0	1	-	-	2	-	-	-	-	grid	g-perp	g-perp
11	19	12	0	6	9	4	0	1	1	-	-	-	-	1	-	perp	grid	unitr
12	17	16	0	2	0	14	1	-		2	-	-	-	-	-	full	point	point
13	17	12	0	2	12	2		-		-	2	-	-	-	-	perp	g-perp	g-perp
14	17	12	0	2		4	0	-	1	-	2	-	-	-	-	grid	line	g-perp
15	17	10	0	8	6	2	1	1	-	-		1	-	-	-	g-perp	g-perp	perp
16	17	10	1	4	10	2	0	1	-	-	1	-	-		-	grid	unitr	g-perp
1/	17	10	0	8	10	0	2	-	2	-	-	1	-	-	-	perp	line	perp
18	17	10	1	4	10	2	0	-	1	-	2	_	-	-	-	grid	tritr	g-perp
19	17	10	2	8	6	2	1	-	1	-	2	-	-	1	-	perp	g-perp	g-perp
20	17	9	2	0	0	1	0	1	-	1	1	_	1	1	-	ovoid	unitr a porp	grid g porp
21	17	9	0	0	6	2	0	1	2	_	1	_	1	-	-	perp	g-perp	g-perp
22	17	11	0		12	2	0		- 2		2		1			g porp	a porp	g porp
23	15	0	0	6	6	3	0	1		_	5		_	2		g-perp	g-perp	g-perp
25	15	9	0	6	6	3	0	-	_	_	3	_	_		_	g-perp1	g-nern	g-nern
26	15	9	0	6	6	3	0	_	_	_	3	_	_	_	_	g-perp ¹	g-perp	g-nern
27	15	8	2	4	7	2	Ő	_	1	_	1	_	_	1	_	grid	tritr	unitr
28	15	8	2	3	9	1	Ő	_	1	_	1	_	_	1	_	line	grid	unitr
29	15	8	2	4	7	2	0	_	_	1	2	_	_	_	_	grid	unitr	unitr
30	15	8	0	6	9	0	0	_	_	-	3	_	_	-	-	g-perp	g-perp	g-perp
31	15	7	1	8	5	1	0	1	-	_	_	_	1	1	-	perp	g-perp	unitr
32	15	7	4	2	8	1	0	1	-	-	-	-	-	2	-	unitr	grid	unitr
33	15	7	1	8	5	1	0	-	1	-	1	-	-	1	-	perp	unitr	g-perp
34	15	7	0	9	6	0	0	-	-	-	3	-	-	-	-	g-perp	g-perp	g-perp
35	15	6	2	10	1	2	0	1	-	-	-	1	-	1	-	perp	unitr	g-perp
36	15	6	3	6	6	0	0	1	-	-	-	-	-	2	-	ovoid	g-perp	g-perp
37	15	6	2	9	3	1	0	-	1	1	-	-	-	1	-	ovoid	unitr	perp
38	15	5	0	15	0	0	0	-	-	3	-	-	-	-	-	ovoid	ovoid	ovoid
39	13	8	0	4	8	0	1	-	1	-	-	2	-	-	-	perp	line	line
40	13	8	0	3	9	1	0	-	1	-	-	-	-	2	-	line	grid	point
41	13	8	0	4	7	2	0	-	-	-	2	1	-	-	-	line	g-perp	g-perp
42	13	1	2	2	8	1	0	-	-	1	1	-	-		-	grid	unitr	point
43	13	6	0	9	3	1	0	-		-	-	-	2	-	-	perp	tritr	tritr
44	13	6	0	9	3		0	-	1	-	-	-	2	-	-	perp	ine	trite
43	13	6	4	10	2	1	0	-	1	-	-	_	-		-	point	gria	uttr
40	13	6	0	10	2	1	0	_	1	_	-	_	-	$\begin{vmatrix} 2\\ 2 \end{vmatrix}$	-	perp	g-perp	point
4/	13	6	1	9	5	1	0	_	1	_	2	_	1	²	-	perp tritr	a porp	a porp
40	13	6	0	8	5	0	0				$\frac{2}{2}$	_	1			line	g-perp	g-perp
50	13	6	1	6	6	0	0				2		1	1	1.	g_perp	g-perp	g-perp
50	15	0	1	0	0	U	U	_		_	- 4	_	_	1		s-berb	g-perp	unnu

Table 3: The types of Veldkamp lines of $L_3 \times GQ(2, 2)$.

Table 3: (Continued.)

											<i>a</i>							
Tn	Dt	In	# 0	f Poir	$\frac{1}{2}$	f Or	der	H.	H.	H_{r}	Comp	ositior		H_	H.	1 et	2nd	3rd
<u> </u>	12		0	1	2	5	4	111	112	113	114	115	116	117	118	150	2110	510
52	13	5	2	0	$\begin{vmatrix} 2\\ 2 \end{vmatrix}$	1		-	1	1	1	1		-	-	perp	unitr	unitr
52	13	5	2	8	$\begin{vmatrix} 2\\ 2 \end{vmatrix}$	1		-	-	1	2	1	1	-	-	tritr	a pern	a perp
54	13	5	0	11	$\left \begin{array}{c} 2\\ 2 \end{array} \right $	0					2	1				line	g-perp	g-perp
55	13	5	2	7	4	0	0		_	_	2	_	1	_	_	tritr	g-perp	g-perp
56	13	5	2	8	2	1	0	_	_	_	2	_		1	_	g-perp	g-perp	unitr
57	13	5	2	7	4	0	0	_	_	_	2	_	_	1	_	unitr	g-perp	g-perp
58	13	4	4	8	0	0	1	1	_	_	_	1	_	_	1	perp	unitr	unitr
59	13	4	4	8	0	0	1	-	1	1	-	-	-	-	1	perp	ovoid	point
60	13	4	4	8	0	0	1	-	1	_	1	-	-	-	1	perp	unitr	unitr
61	13	4	4	8	0	0	1	-	1	_	-	2	-	-	-	perp	tritr	tritr
62	13	4	4	7	1	1	0	-	1	-	-	-	2	-	-	tritr	tritr	perp
63	13	4	4	7	1	1	0	-	1	-	-	-	-	2	-	line	g-perp	ovoid
64	13	4	4	7	1	1	0	-	1	-	-	-	-	2	-	perp	unitr	unitr
65	13	4	4	6	3	0	0	-	1	-	-	-	-	2	-	tritr	g-perp	ovoid
66	13	4	4	8	0	0	1	-	-	1	1	1	-	-	-	perp	unitr	unitr
67	13	3	6	6	0	1	0	1	-	-	-	-	1	-	1	perp	unitr	unitr
68	13	3	6	6	0	1	0	1	-	-	-	-	-	1	1	ovoid	g-perp	unitr
69	11	6	2	0	9	0	0	-	-	1	-	-	-	2	-	grid	point	point
70	11	5	0	7	4	0	0	-	-	-	1	-	-	2	-	g-perp	g-perp	point
71		4	2	7				-	-	1	-		-		-	perp	unitr	point
72		4	2					-	-	-	1		-		-	line	g-perp	unitr
73		4	2	0	3	0		-	-	-	1	1	1	1	-	line	unitr	g-perp
74		4	2	0	2	0		-	-	-	1	-		1	-	unitr 1:	uritr	g-perp
76	11	4	2	6	3	0		-	-	_	1	-	1	2	-	a perp ²	unitr	g-perp
70	11		2	6	3	0					1			$\frac{2}{2}$		g-perp ²	unitr	unitr
78	11	4	1	8	2	0		_		_	1	_		2	_	noint	g-nern	g-nern
79	11	3	4	6	l õ	1		_	1	_	<u> </u>	_	_	1	1	nern	noint	unitr
80	11	3	4	6	0	1	0	_		1	_	_	1	1	_	nern	unitr	point
81	11	3	2	9	0	0	0	_	_	1	_	_	_	2	_	unitr	unitr	ovoid
82	11	3	4	6	0	1	0	-	_	_	2	_	_	_	1	unitr	g-perp	unitr
83	11	3	4	6	0	1	0	-	-	_	1	1	-	1	-	tritr	unitr	g-perp
84	11	3	4	5	2	0	0	-	-	_	1	-	1	1	-	tritr	g-perp	unitr
85	11	3	3	7	1	0	0	-	-	-	1	-	1	1	-	line	g-perp	unitr
86	11	3	4	6	0	1	0	-	-	-	1	-	-	2	-	unitr ³	g-perp	unitr
87	11	3	4	6	0	1	0	-	-	-	1	-	-	2	-	unitr ³	g-perp	unitr
88	11	3	4	5	2	0	0	-	-	-	1	-	-	2	-	g-perp ⁴	unitr	unitr
89	11	3	4	5	2	0	0	-	-	-	1	-	-	2	-	g-perp ⁴	unitr	unitr
90	11	2	6	4	1	0	0	-	1	-	-	-	-	1	1	line	unitr	ovoid
91	11	2	6	4	1	0	0	-	-	-	2	-	-	-	1	unitr	g-perp	unitr
92	11	2	6	4	1	0	0	-	-	-	1	1	-	1	-	tritr	unitr	g-perp
93		2	6	4		0		-	-	-	1	-	1	1	-	tritr	g-perp	unitr
94		2	6					-	-	-	1	-	-	2	-	g-perp	unitr	unitr
95			8	3		0		-	-	2	-	-	-	-	1	ovoid	point	ovoid
96			8	5		0		-	-	1	-	-	-	2	-	unitr	unitr	ovoid
9/			11			0		1	1	-	-	-	-	1	2	unitr tritr	unitr	ovoia
90	0	6	11	0	0	0	0	-	1		-	2	-	1	1	line	line	line
1 22	1 2	0	0		1			-	1.	-	-	5	-	-		inite .	· · .	· · ·

Table 3: (Continued.)

			#	of P	oint	s of (Order				Comp	ositior	1					
Тр	Pt	Ln	0	1	2	3	4	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8	1st	2nd	3rd
101	9	3	2	6	0	1	0	-	-	1	-	-	1	-	1	perp	point	point
102	9	3	2	6	0	1	0	-	-	-	1	-	-	1	1	point	g-perp	unitr
103	9	3	0	9	0	0	0	-	-	-	-	3	-	-	-	line	line	line
104	9	3	2	5	2	0	0	-	-	-	-	2	1	-	-	line	tritr	line
105	9	3	0	9	0	0	0	-	-	-	-	1	2	-	-	line	line	line
106	9	3	2	5	2	0	0	-	-	-	-	1	-	2	-	tritr	g-perp	point
107	9	3	1	7	1	0	0	-	-	-	-	1	-	2		point	g-perp	line
108	9	3	0	9	0	0	0	-	-	-	-	-	3	-		tritr	tritr	tritr
109	9	3	1	7	1	0	0	-	-	-	-	-	1	2		point	g-perp	line
110	9	3	0	9	0	0	0	-	-	-	-	-	-	3		unitr	unitr	unitr
111	9	2	4	4	1	0	0	-	-	-	1	-	1	-	1	line	unitr	unitr
112	9	2	4	4	1	0	0	-	-	-	1	-	-	1	1	g-perp	point	unitr
113	9	2	4	4	1	0	0	-	-	-	-	1	-	2	-	line	unitr ⁵	unitr
114	9	2	4	4	1	0	0	-	-	-	-	1	-	2	-	line	unitr ⁵	unitr
115	9	2	4	4	1	0	0	-	-	-	-	1	2	-	-	tritr	tritr	line
116	9	2	3	6	0	0	0	-	-	-	-	-	3	-	-	line	line	tritr
117	9	2	4	4	1	0	0	-	-	-	-	-	1	2	-	tritr	g-perp	point
118	9	2	3	6	0	0	0	-	-	-	-	-	1	2	-	tritr	unitr	unitr
119	9	2	4	4	1	0	0	-	-	-	-	-	-	3	-	point ⁶	g-perp	unitr
120	9	2	4	4	1	0	0	-	-	-	-	-	-	3	-	point ⁶	g-perp	unitr
121	9	1	6	3	0	0	0	-	-	-	1	1	-	-	1	unitr	line	unitr
122	9	1	6	3	0	0	0	-	-	-	-	3	-	-	-	tritr	tritr	line
123	9	1	6	3	0	0	0	-	-	-	-	1	2	-	-	line	tritr	tritr
124	9	1	6	3	0	0	0	-	-	-	-	1	-	2	-	line	unitr	unitr
125	9	1	6	3	0	0	0	-	-	-	-	-	3	-	-	tritr	tritr	tritr
126	9	1	6	3	0	0	0	-	-	-	-	-	1	2	-	line	unitr	unitr
127	9	1	6	3	0	0	0	-	-	-	-	-	1	2	-	tritr	unitr	unitr
128	9	1	6	3	0	0	0	-	-	-	-	-	-	3	-	unitr	unitr	unitr
129	9	0	9	0	0	0	0	-	1	-	-	-	-	-	2	tritr	point	ovoid
130	9	0	9	0	0	0	0	-	-	1	-	-	-	1	1	ovoid	unitr	point
131	9	0	9	0	0	0	0	-	-	-	1	1	-	-	1	tritr	unitr	unitr
132	9	0	9	0	0	0	0	-	-	-	1	-	1	-	1	tritr	unitr	unitr
133	9	0	9	0	0	0	0	-	-	-	1	-	-	1	1	unitr'	unitr	unitr
134	9	0	9	0	0	0	0	-	-	-	1	-	-	1	1	unitr	unitr	unitr
135	9	0	9	0	0	0	0	-	-	-	-	2	1	-	-	tritr	tritr	tritr
136	9	0	9	0	0	0	0	-	-	-	-	1	-	2	-	tritr	unitr	unitr
137	9	0	9	0	0	0	0	-	-	-	-	-	1	2	-	tritr	unitr	unitr
138	9	0	9	0	0	0	0	-	-	-	-	-	-	3	-	unitr	unitr	unitr
139	7	2	2	4	1	0	0	-	-	-	-	1	-	1	1	point	unitr	line
140	7	2	2	4	1	0	0	-	-	-	-	-	-	2	1	point	g-perp	point
141	7	1	4	3	0	0	0	-	-	1	-	-	-	-	2	ovoid	point	point
142	7	1	4	3	0	0	0	-	-	-	-	-	1		1	line	unitr	point
143	7	1	4	3	0	0	0	-	-	-	-	-	-	2	1	unitr ⁸	unitr	point
144	7	1	4	3	0	0	0	-	-	-	-	-	-	2	1	point	unitr ⁸	unitr
145	7	0	7	0	0	0		-	-	-	1	-	-	-	2	unitr	unitr	point
146	7	0	7	0	0	0	0	-	-	-	-	1	-	1	1	tritr	point	unitr
147	7	0	7	0	0	0	0	-	-	-	-	-	1		1	tritr	point ⁹	unitr
148	7	0	7	0	0	0	0	-	-	-	-	-	1	1	1	tritr	point9	unitr
149	7	0	7	0	0	0	0	-	-	-	-	-	-	2	1	point ¹⁰	unitr	unitr
150	7	0	7	0	0	0	0	-	-	-	-	-	-	2	1	point ¹⁰	unitr ¹¹	unitr

Table 3: (Continued.)

			#	of P	oint	s of (Order				Comp							
Тр	Pt	Ln	0	1	2	3	4	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8	1st	2nd	3rd
151	7	0	7	0	0	0	0	-	-	-	-	-	-	2	1	point10	unitr ¹¹	unitr
152	5	1	2	3	0	0	0	-	-	-	-	1	-	-	2	line	point	point
153	5	0	5	0	0	0	0	-	-	-	-	-	1	-	2	tritr	point	point
154	5	0	5	0	0	0	0	-	-	-	-	-	-	1	2	unitr	point	point
155	3	1	0	3	0	0	0	-	-	-	-	-	-	-	3	point	point	point
156	3	0	3	0	0	0	0	-	-	-	-	-	-	-	3	point	point	point

Explanatory remarks:

¹Two (25) or no two (26) of the g-perps are such that their centers are joined by a type-one line.

 2 The center of the g-perp does (77) or does not (76) lie on the type-one line passing through the center of one of the two unicentric triads.

 3 The centers of the two unicentric triads are (86) or are not (87) joined by a type-one line.

⁴One line (88) or no line (89) of the g-perp is incident with the type-one line passing through the center of one of the two unicentric triads.

 5 The five type-one lines through the points of the two triads do (114) or do not (113) cut a doily-quad in an ovoid.

⁶One line (120) or no line (119) of type-two through the point is incident with the type-one line through the center of the g-perp.

⁷One (133) or none (134) of the unicentric triads is such that the type-one lines through two of its points pass through the centers of the other two triads.

 8 The centers of the two unicentric triads are (143) or are not (144) joined by a type-one line.

⁹The point does (147) or does not (148) lie on the type-one line passing through a center of the tricentric triad.

¹⁰The point does (149) or does not (150 and 151) lie on the type-one line passing through the center of one of the two unicentric triads.

¹¹The centers of the two unicentric triads do (150) or do not (151) belong to the same grid-quad.

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Search for the end of a path in the *d*-dimensional grid and in other graphs

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Abstract

We consider the worst-case query complexity of some variants of certain **PPAD**complete search problems. Suppose we are given a graph G and a vertex $s \in V(G)$. We denote the directed graph obtained from G by directing all edges in both directions by G'. D is a directed subgraph of G' which is unknown to us, except that it consists of vertex-disjoint directed paths and cycles and one of the paths originates in s. Our goal is to find an endvertex of a path by using as few queries as possible. A query specifies a vertex $v \in V(G)$, and the answer is the set of the edges of D incident to v, together with their directions.

We also show lower bounds for the special case when D consists of a single path. Our proofs use the theory of graph separators. Finally, we consider the case when the graph G is a grid graph. In this case, using the connection with separators, we give asymptotically tight bounds as a function of the size of the grid, if the dimension of the grid is considered as fixed. In order to do this, we prove a separator theorem about grid graphs, which is interesting on its own right.

Keywords: Separator, graph, search, grid. Math. Subj. Class.: 90B40, 05C85

1 Introduction

This paper deals with the following search problem. We are given a simple, undirected, connected graph G and a vertex $s \in V(G)$. We denote the directed graph obtained from G by directing all edges in both directions by G'. Let D be a directed subgraph of G', which is the vertex-disjoint union of a directed path starting at s and possibly some other directed paths and cycles. D is unknown to us, and our goal is to identify an endvertex of a directed path. We may *query* a vertex v, and as an answer, we learn the edges of D incident to v together with their directions. In particular, if the answer is only one incoming edge, then we know that v is an endvertex. We analyze the minimum number of queries that are necessary in the worst case.

We give lower bounds in the more restrictive model where we know D is one directed path. Note that if instead of looking for an endvertex, we look for an ending or a starting vertex of a path (different from s), then this model still gives a lower bound for this easier problem. In Section 4 we mention some additional models.

Denote by h(G) the minimum number of queries needed to find an endvertex in the worst case for any $s \in G$. If we know that D is one directed path, denote this quantity by $h_P(G)$.

Biseparators and multiseparators. To state some of our results we need to define separators of graphs. This notion can be defined in two different ways and both definitions are widely used. Here we distinguish between the two definitions.

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Definition 1.1.

- 1. Given a graph G = (V, E), a subset $S \subseteq V$ is called an α -biseparator of G if $V \setminus S$ can be divided into two parts, A and B, such that there are no edges between A and B, and both have cardinality at most $\alpha |V|$.
- 2. Given a graph G = (V, E), a subset $S \subseteq V$ is called an α -multiseparator of G if every connected component of $V \setminus S$ has cardinality at most $\alpha |V|$.

Note that A or B in the definition of a biseparator can be empty: we do not require $V \setminus S$ to be disconnected. Small biseparators make sense only for $\alpha \ge 1/2$.

Given these definitions, when we write *separator*, it can mean either a biseparator or a multiseparator, as in many cases it makes no difference. In the literature, the notation f(n)-separator can also be found, where f(n) is an upper bound on the cardinality of S in terms of the number n of vertices. In this paper it is more straightforward to fix α and then look for the smallest α -separator. Therefore, we let $s_{\alpha}^{\text{bi}}(G)$ be the minimum cardinality of an α -biseparator in G and $s_{\alpha}^{m}(G)$ be the minimum cardinality of an α -multiseparator in G.

It follows from the definitions that every α -biseparator is an α -multiseparator, and thus $s_{\alpha}^{\rm bi}(G) \geq s_{\alpha}^m(G)$. In many cases they are of the same order of magnitude. In particular, if we have a bound $s_{\alpha}^m(G) \leq O(n^c)$ for a class of graphs which is closed under taking subgraphs for some c < 1 and for *some arbitrary* $\alpha < 1$, we get the same asymptotic bound on $s_{1/2}^{\rm bi}(G)$, by iteratively separating one of the components. However, there are cases when multiseparators are much smaller than biseparators. For example, if G consists of three disjoint cliques of equal size, all connected to a degree-three vertex, then $s_{1/2}^m(G) = 1$ but $s_{1/2}^{\rm bi}(G) = \lceil n/6 \rceil$. For any tree, $s_{1/2}^m(G) = 1$ but it is not hard to show that for a complete ternary tree, $s_{1/2}^{\rm bi}(G) = \Theta(\log n)$, see Appendix A. Finally, if we consider a class of graphs closed under taking subgraphs, by repeatedly refining the separation, then it is obvious that $s_{\alpha}^m(G)$ and $s_{\alpha'}^m(G)$ have the same order of magnitude for any two constants α and α' .

Results. Our main result establishes a connection between the biseparators and the search complexity for general graphs.

Theorem 1.2. For any connected graph G with at least 2 vertices, we have $s_{1/2}^{bi}(G) \le h_P(G) \le h(G)$.

We can prove an upper bound of the same order of magnitude, if every subgraph has small multiseparators. Note that when bounding h(G), $s^{bi}(G)$, the larger of the separators, gives the lower bound and $s^m(G)$, the smaller one, gives the almost matching upper bound, which implies that indeed for a large class of graphs $s^{bi}(G)$ and $s^m(G)$ have the same order of magnitude.

Theorem 1.3. Let $0 < \alpha, \beta < 1$ be constants, let f be a monotone function, and let G be a graph such that any subgraph H of G has an α -multiseparator of size at most f(|V(H)|). If $f(\alpha x) \leq \beta f(x)$ for all x > 0, then

$$h_P(G) \le h(G) \le \frac{f(|V(G)|)}{1-\beta}.$$

The condition on f could be interpreted as having "at least polynomial growth". The condition is fulfilled by the function $f(x) = \text{const} \cdot x^c$ if and only if $c \ge \log_{\alpha} \beta$. To put it differently, if α and c > 0 are given, the theorem applies with $\beta := \alpha^c$.

We also study the search problem for the special case of grid graphs.

Definition 1.4. Let d be a positive integer and (n_1, \ldots, n_d) a sequence of positive integers. The d-dimensional grid graph of side length (n_1, \ldots, n_d) , denoted by $G_d(n_1, \ldots, n_d)$, has vertex set $X_i \{0, 1, 2, \ldots, n_i - 1\}$, and there is an edge between two vertices if and only if they differ in exactly one coordinate and the difference is 1. If $n_1 = n_2 = \cdots = n_d$, then we simply write $G_d(n)$.

We estimate the search complexity of grid graphs as follows.

Theorem 1.5. $\Omega(n^{d-1}/\sqrt{d}) \le h_P(G_d(n)) \le h(G_d(n)) \le O(n^{d-1}).$

As a tool, we will prove a bound on the cardinality of separators of grid graphs, using classic results from the theory of vertex isoperimetric problems and cube slicing.

Theorem 1.6. The smallest 1/2-biseparator of the grid graph $G_d(n)$ has cardinality

$$s^{\mathrm{bi}}(G_d(n)) = \Theta(n^{d-1}/\sqrt{d}).$$

We note that when considering grid graphs, one could also study the related problem that the path starting at s is monotone, i.e., if u and v are on the path and $u \le v$ (according to the usual partial order of the vectors), then the edge between u and v (if it exists) is directed towards v. In this case the needed number of queries reduces dramatically. Indeed, the trivial algorithm which follows the path uses at most dn queries. In two dimensions we could improve slightly this upper bound, yet there is a more significant improvement by Xiaoming Sun (personal communication), who proved that 8n/5 queries are enough in two dimensions. From below, at least n - 2 queries are needed regardless of d [7, Lemma 6]. This problem resembles the pyramid-path search problem (but it is not exactly the same), where also a lower bound of n is proved for the two-dimensional case [5].

Motivation. Hirsch, Papadimitriou and Vavasis [7] have proved worst-case lower bounds for finding Brouwer fixed points for algorithms using only function evaluation. They showed a lower bound that is exponential in the dimension, disproving the conjecture that Scarf's algorithm is polynomial. In our language, they have (implicitly) proved that $h(G_d(n)) = \Omega(n^{d-2}/d^2)$ [7, Lemma 16]. Our Theorem 1.5 is an improvement of their result, although we do not use the continuous setting but rather focus only on the discretization of the problem.

Later, Papadimitriou [10] considered similar complexity search problems in great detail and defined corresponding complexity classes **PPA**, **PPAD**, etc. In his model, an exponential-size graph is given by a *succinct* representation, i.e., by the description of a Turing-machine T. The vertices of the graph correspond to binary sequences of length nand if we input such a sequence to T, it outputs all the neighbors of the corresponding vertex in polynomial time (thus the degrees are bounded by a polynomial). Therefore, in his model, instead of considering query cost, one can work with the classical running time of the algorithm that gets T as input. If the algorithm uses T as a black box, we get back the query-cost model. Papadimitriou considered the problem when the maximum degree of the graph is 2, i.e., it consists of vertex disjoint paths and cycles and we are also given, as part of the input, a degree-one vertex, *s*, and our goal is to output another degree-one vertex. This search problem is denoted by LEAF, and the complexity class **PPA** is defined such that LEAF is complete for **PPA**. (**PPA** stands for "Polynomial Parity Argument".)

Papadimitriou introduced another variant, where the underlying graph is directed (T outputs both the in- and out-neighbors of its input in this case), the in- and out-degree of every vertex is at most one, and we are given a starting vertex s with in-degree zero and out-degree one. Therefore, the resulting digraph is the vertex-disjoint union of a directed path starting at s and possibly some other directed paths and cycles, exactly like in the problem that we study. Here our goal can be either to output an in-degree one, out-degree zero vertex (called LEAFDS problem) or an in-degree plus out-degree equals one vertex (called LEAFD problem), which means the end of a path, just like in the problem we study. Thus, the query-cost of LEAFD is exactly $h(K_{2n})$.

The complexity classes for which the problems LEAFDS and LEAFD are complete are denoted, respectively, by **PPADS** and **PPAD**. It is easy to see that **PPAD** is contained in both **PPA** and **PPADS**, while an oracle separation is known for the two latter classes [2]. Nowadays **PPAD** enjoys huge popularity, as several problems, among them finding an ϵ -approximate Nash-equilibrium, turned out to be **PPAD**-complete. This is why this paper focuses on h(G), the query-cost version of **PPAD**, though most of our results would also hold for the other variants.

An extensive list of **PPAD**-complete problems can be found on Wikipedia.

2 Upper bounds

Claim 2.1. Suppose that the connected components of $G \setminus S$ are Y_1, \ldots, Y_k . If every vertex of S has been queried, we know a Y_i which contains an endvertex (or that an endvertex is in S, hence already identified).

Proof. The answers clearly show how many times we enter and leave S from each component Y_i . If we enter a component Y_i more times than we leave it, then Y_i must contain an endvertex. If there is no such component, the component containing s must contain an endvertex.

This simple observation is crucial for our upper bounds and it does not hold if the answers would contain only the edges leaving the queried vertex.

Proof of Theorem 1.3. Let us choose an α -multiseparator S_1 with $|S_1| \leq f(|V(G)|)$ which cuts G into parts Y_1, \ldots, Y_k , and query all vertices of S_1 . By Observation 2.1 we know a part Y_j which contains an endvertex. Let G_1 be G restricted to Y_j and choose an α multiseparator S_2 of size at most $f(|V(G_1)|)$, which cuts G_1 into parts Z_1, \ldots, Z_l .

Then $S_1 \cup S_2$ is a separator of G, which cuts it into parts $Y_1, \ldots, Y_{j-1}, Y_{j+1}, \ldots, Y_k$, Z_1, \ldots, Z_l . Thus, by again using Observation 2.1 after asking every vertex of $S_1 \cup S_2$ we know which part Z_i contains an endvertex.

After this we can continue the same way, defining G_2 and asking S_3 , defining G_3 and asking S_4 and so on, until an endvertex is in some S_i . As $|V(G_j)| \leq \alpha |V(G_{j-1})|$ for any j, one can easily see that $|V(G_j)| \leq \alpha^j |V|$. By the assumptions on f, $f(|S_j|) \leq f(|V(G_{j-1})|) \leq f(\alpha^{j-1}|V|) \leq \beta^{j-1}f(|V|)$. Altogether at most $\sum_{j=1}^{\infty} \beta^{j-1}f(|V|) \leq f(|V|)/(1-\beta)$ questions were asked.

A celebrated theorem of Lipton and Tarjan [8] states that planar graphs have 2/3-separators of size at most $\sqrt{8} \cdot \sqrt{|V|}$. Thus we have the following corollary.

Corollary 2.2. If G is planar, then $h(G) = O(\sqrt{|V|})$.

Now, let us look at *d*-dimensional grid graphs. Miller, Teng and Vavasis [9] introduced the so-called overlap graphs for every *d* and proved that every member *G* of the class has separator of size $O(|V(G)|^{(d-1)/d})$. They mention that any subset of the *d*-dimensional infinite grid graph belongs to the class of overlap graphs. The polynomial function $f(x) = cx^{(d-1)/d}$ satisfies the assumption of Theorem 1.3. Since $|V(G_d(n))| = n^d$, this implies that $h(G) = O(n^{d-1})$. Here we show that the multiplicative constant is less than 3.

Theorem 2.3.
$$h(G_d(n)) \le (2 + \frac{1}{2^{d-1}-1})n^{d-1}$$
.

Proof. We follow the proof of Theorem 1.3, but the cuts we use are always axis-aligned hyperplanes, which cut the current part into two smaller grid graphs. More precisely, for any i let $j \equiv i \mod d$, $0 \leq j \leq d-1$; now S_i is a hyperplane perpendicular to the j^{th} coordinate axis, and it cuts G_{i-1} into two parts of size at most $|V(G_{i-1})|/2$. One can easily see that this is possible and $|S_{i+1}| \leq |S_i|/2$, except if j = 0, in which case $|S_{i+1}| \leq |S_i|$. This means that there are at most

$$n^{d-1}(1+1/2+1/4+\ldots+1/2^{d-1})(1+1/2^{d-1}+1/2^{2(d-1)}+\ldots)$$

$$\leq n^{d-1}(2-1/2^{d-1})\frac{1}{1-1/2^{d-1}} = n^{d-1}\left(2+\frac{1}{2^{d-1}-1}\right)$$

queries.

3 Lower bounds

Before proving Theorem 1.6 which claims that any 1/2-separator in the grid graph $G_d(n)$ has cardinality $\Omega(n^{d-1}/\sqrt{d})$, we present a slightly weaker result, as it has a short proof not using results from the theory of isoperimetric problems.

Claim 3.1. Any α -multiseparator in the grid graph $G_d(n)$ has cardinality at least $(1 - \alpha)n^{d-1}/d$ for $\alpha \ge 1/2$.

Proof. We use induction on d. The claim is trivial for d = 1. Let us denote by S an α -multiseparator.

Let us choose an arbitrary axis, and denote by \mathcal{L} the n^{d-1} parallel lines in the grid which go in that direction. Let $\mathcal{L}' \subset \mathcal{L}$ be the set of those lines which intersect S. Note that every other element of \mathcal{L} contains vertices only from one component of $G \setminus S$. If $|\mathcal{L}'| \geq (1-\alpha)n^{d-1}/d$, then we are done. Hence we can suppose $|\mathcal{L}'| < (1-\alpha)n^{d-1}/d$.

Elements of \mathcal{L}' cover less than $(1-\alpha)n^d/d$ points, hence for any component C of $G \setminus S$, the other components together contain at least $((1-\alpha)d - (1-\alpha))n^d/d$ vertices, which are not covered by elements of \mathcal{L}' . This means that there are at least $(1-\alpha)(d-1)n^{d-1}/d$ elements of \mathcal{L} which contain only vertices not in C. Now consider a hyperplane in the grid, orthogonal to the direction of the lines of \mathcal{L} , and denote by \mathcal{H} the vertices of $G_d(n)$ that belong to the hyperplane. Clearly, \mathcal{H} contains at least $(1-\alpha)(d-1)n^{d-1}/d$ elements not in C, hence $S \cap \mathcal{H}$ is an α' -multiseparator of \mathcal{H} (with $\alpha' := 1 - (1-\alpha)(d-1)/d$) and so we can apply induction on each of these (d-1)-dimensional hyperplanes.

By induction, there are at least $(1-\alpha)(d-1)n^{d-2}/d(d-1)$ elements of S in every such hyperplane, which gives at least $n(1-\alpha)n^{d-2}/d = (1-\alpha)n^{d-1}/d$ elements in total. \Box
Before proving the stronger version of this result, we need to introduce some notations and results.

Let A be an arbitrary set of vertices. The set of vertices that are not in A, but are connected to some vertex of A is called the *boundary* of A, denoted by ∂A . Following the notations of Bollobás and Leader [3], we define an order on the vertices, the simplicial order, by setting x < y if $\sum x_i < \sum y_i$, or $\sum x_i = \sum y_i$ and for some j we have $x_j > y_j$ and $x_i = y_i$ for all i < j. This coincides with the lexicographic order according to the vector $(\sum x_i, -x_1, -x_2, \dots, -x_n)$.

Theorem 3.2 (Bollobás and Leader [3]). In $G_d(n)$, among sets of vertices of a given size, the initial segment of the simplicial order has the smallest boundary.

The special case n = 2, i.e., the hypercube, was previously treated by Harper [6], while the unbounded case of $n = \infty$ was solved by Wang and Wang [13]. We note that in the paper of Bollobás and Leader the definition of boundary is different: they also include Ain ∂A .

We will also need some results about the volume of slices of a cube, i.e., intersections of the cube with specific hyperplanes. For a contemporary approach to this area we refer to [14]. In the next theorem $H^d(t)$ denotes the following set in the *d*-dimensional unit cube $I^d: H^d(t) = \{x \in I^d \mid \sum x_i = t\}$; Vol_i denotes the *i*-dimensional volume of some set of dimension *i*.

Theorem 3.3 ([11, 14]).
$$\lim_{d\to\infty} \operatorname{Vol}_{d-1}(H^d(d/2 + s\sqrt{d})) = \sqrt{\frac{6}{\pi}}e^{-6s^2}$$
, for each fixed s.

Let L_k denote the k-th layer of $G_d(n)$: the set of all vertices in $G_d(n)$ whose coordinates sum to k. The layer range from 0 to (n-1)d. We define the size of the "middle-most" layers $Z_{n,d}$ by

$$Z_{n,d} := \begin{cases} |L_{((n-1)d-1)/2}| = |L_{((n-1)d+1)/2}|, & \text{for } (n-1)d \text{ odd,} \\ \min\{|L_{(n-1)d/2-1}|, |L_{(n-1)d/2}|, |L_{(n-1)d/2+1}|\}, & \text{for } (n-1)d \text{ even.} \end{cases}$$

$$Z_{n,d}^{\max} := \begin{cases} |L_{((n-1)d-1)/2}| = |L_{((n-1)d+1)/2}| = Z_{n,d}, & \text{for } (n-1)d \text{ odd,} \\ |L_{(n-1)d/2}|, & \text{for } (n-1)d \text{ even.} \end{cases}$$

In the even case, we actually know that the middle level $L_{(n-1)d/2}$ is the largest of the three levels in the definition of $Z_{n,d}$, as the levels decrease symmetrically in size from the middle to the ends [4]. From discretizing the above theorem, one can obtain the following bound on $Z_{n,d}$. Its proof can be found in Appendix B.

Corollary 3.4. For every d, there exists a constant C_d such that

$$Z_{n,d} = C_d / \sqrt{d} \cdot n^{d-1} \pm O(n^{d-2}) \text{ and}$$

$$Z_{n,d}^{\max} = C_d / \sqrt{d} \cdot n^{d-1} \pm O(n^{d-2}).$$

 $C_d \to \sqrt{6/\pi} \text{ as } d \to \infty.$

Now we are ready to prove Theorem 1.6.

Proof of Theorem 1.6. We start with the lower bound. Let us denote by S a 1/2-biseparator which separates the vertex set A and B (such that $V = A \cup B \cup S$). If $|S| \ge Z_{n,d}$ we are

done. Thus we suppose that $|S| < Z_{n,d}$. Denote by A' the vertex set of size |A| which is an initial segment of the simplicial order. By Theorem 3.2 we know that $|S| \ge |\partial A| \ge |\partial A'|$.

By the definition of the simplicial order, $\partial A'$ is contained in the union of two successive layers k and k + 1: $\partial A' = P_1 \cup P_2$, where $P_1 \subseteq L_k$ and $P_2 \subseteq L_{k+1}$. First we claim that k must be very close to the middlemost layer. More precisely, if nd is odd, we can assume $k = \frac{nd-1}{2}$, and if nd is even, we can assume $k = \frac{nd}{2} - 1$ or $k = \frac{nd}{2}$. We treat only the odd case, the even case being similar. First, we show that A' must

We treat only the odd case, the even case being similar. First, we show that A' must reach at least level $k = \frac{nd-1}{2}$. If A' were disjoint from L_k , we would get

$$|A| + |S| = |A'| + |S| < |A'| + Z_{n,d} = |A' \cup L_k| \le n^2/2,$$

since the last set contains only vertices in the lower half of the levels. This contradicts the requirement fact that $A \cup S$ must cover at least half of the vertices. Secondly, if A' would contain vertices of level k+1, it would contain more than the levels $0, 1, \ldots, k$ which make up half of all vertices. This is again a contradiction to the 1/2-biseparator property.

By the definition of $Z_{n,d}$, we have now established that each of the two central layers L_k and L_{k+1} contains at least $Z_{n,d}$ points. To conclude the proof, we show that the separator $\partial A'$ which is contained in the two layers L_k and L_{k+1} must have size at least $Z_{n,d} - O(n^{d-2})$. If a vertex $v = (x_1, \ldots, x_d)$ of L_{k+1} is not in P_2 , then the adjacent vertex $v^$ defined by $v^- = (x_1, \ldots, x_{d-1}, x_d - 1)$ must be in P_1 unless it is not a point of the grid G(n, d) (i.e., $x_d = 0$):

$$(L_{k+1} \setminus P_2)^- \cap G(n,d) \subseteq P_1$$

Since the number of vertices of L_{k+1} for which $x_d = 0$ is $O(n^{d-2})$, we obtain

$$|L_{k+1}| - |P_2| - O(n^{d-2}) \le |P_1|,$$

from which the bound $|\partial A'| = |P_1| + |P_2| \ge Z_{n,d} - O(n^{d-2})$ follows.

For the upper bound, we simply take the central layer $L_{\lfloor (n-1)d/2 \rfloor}$ of size $Z_{n,d}^{\max}$ as a biseparator.

Now we are ready to prove Theorem 1.2, that $s_{1/2}^{\text{bi}}(G) \leq h_P(G)$.

Proof of Theorem 1.2. We will use an adversary argument for the lower bound on the number of queries. The adversary will try to answer the queries in such a way that the discovery of the endvertex by the searcher is delayed as much as possible. The adversary need not choose a path D in advance, but it is required that the answers remain consistent with *some* path.

Let Q denote the vertices that have been queried so far in the search. We will show that the adversary can achieve that after the other end of the path is found, Q becomes a 1/2-biseparator. The adversary maintains a component C of V - Q, see Figure 1. C is the set of vertices which can possibly be the endvertex of the path. (The adversary will follow a greedy strategy of keeping this set as large as possible.) In addition to C, the adversary maintains a path P between s and some vertex $p \in C$, which will be part of the final path and for which $P \cap C = \{p\}$. The remaining components of V - Q are partitioned into two sets $V \setminus (Q \cup C) = A \cup B$ such that both A and B contain at most |V|/2 vertices and there are no edges between A and B. Thus we always have a partition into four disjoint sets $V = Q \cup A \cup B \cup C$. The adversary can reveal all these data to the searcher as free additional information. Initially, C = V, p = s and $Q = A = B = \emptyset$.



Figure 1: A schematic drawing of the situation maintained by the adversary. The queried vertices, Q, are marked by squares.



Figure 2: Updating the set C after a query q

The strategy is the following. If the queried vertex q is in Q, the adversary repeats the previous answer for this vertex. If $q \in P \setminus \{p\}$, the adversary answers by reporting the ingoing and outgoing edge of P at that vertex. If $q \notin C \cup P$, then the answer is that "the path does not pass through this vertex." In these cases, no new information is revealed to the searcher. The vertex p, the set C, and the path P remain unchanged; the only change is that q is moved from $A \cup B$ to Q.

Let us now look at the case $q \in C$. Let $C \setminus \{q\} = D_1 \cup D_2 \cup \cdots \cup D_m$ be the partition of $C \setminus \{q\}$ into $m \ge 1$ connected components. The adversary chooses a largest component D_j , and will answer in such a way that the new set C becomes $C^{\text{new}} = D_j$.

Therefore, if C^{new} contains p, the answer is again "the path does not pass through this vertex," see Figure 2 (a). The current endpoint p and the path P are unchanged. If C^{new} does not contain p (including the case q = p), then choose $p^{\text{new}} \in C^{\text{new}}$ to be a neighbor of q, see Figure 2 (b). As q was a possible endpoint of the path before this step, there is a path P^{new} from p to q which lies in $C \setminus C^{\text{new}}$. The adversary uses P^{new} and the edge qp^{new} to extend the path P to a longer path P^{new} . (This is the only case when the path is updated.) The adversary reports the last arc of P^{new} as the ingoing arc at q and qp^{new} as the outgoing arc.

To maintain the invariant that $|A|, |B| \leq |V|/2$, we go through the components $D_i \neq C^{\text{new}}$ one by one and add them either to A or to B (to eventually obtain A^{new} and B^{new}), whichever is smaller. If, for example, $|A| \leq |B|$, then $|A| + |D_i| \leq |B| + |C^{\text{new}}| \leq |V|/2$ as $A, D_i, B, C^{\text{new}}$ are disjoint subsets of V. Therefore, the invariant is maintained.

The searcher can only identify t, the end of the path, when |C| becomes 1. By assumption, the graph G has at least two vertices and is connected, and therefore $Q \neq \emptyset$. Thus, at this point,

 $\min\{|A|, |B|\} \le |V \setminus (Q \cup C)|/2 \le (|V| - 1 - 1)/2 = |V|/2 - 1.$

We can now add the singleton set $C = \{t\}$ to the smaller of A and B without exceeding the size bound |V|/2. The set Q of queried vertices forms thus a 1/2-biseparator.

Corollary 3.5. $h_P(G_d(n)) = \Omega(n^{d-1}/\sqrt{d}).$

Theorem 1.5 summarizes the above results. The lower and upper bounds are quite close. Specifically, if we consider d as fixed, then the theorem gives exact asymptotics in n for the needed number of queries.

4 Concluding Remarks: Problem Variations

Here we mention three more variants of the problem.

In the first variant, we consider any directed subgraph of G' and a vertex s with larger out-degree than in-degree. In this version there is a vertex with higher in-degree than out-degree, our goal is to find such a vertex. All of our algorithms work in this case, and obviously the same lower bounds hold.

In the second variant, D consists of directed paths and cycles, but we also assume that they cover every vertex. This is a special case of our model, hence the upper bounds hold. However, a lower bound similar to Theorem 1.2 is not plausible, as there are graphs that have only big separators, yet there are only a few valid choices for D. For example if Gcontains a vertex of degree one, different from the source, then this vertex must be the endvertex. But in case of grid graphs we can show that the additional assumption on Ddoes not make the problem much easier.

Denote by $h_U(G)$ the minimum number of queries needed to find an endvertex in the worst-case for any $s \in G$. Now we show how to give a lower bound for $h_U(G_d(n))$. Let us suppose we are given an $r_1 \times r_2 \times r_3 \times \cdots \times r_d$ grid graph G. Then let $G^{4,4}$ denote the $4r_1 \times 4r_2 \times r_3 \times \cdots \times r_d$ grid graph.

Theorem 4.1. Let G be a grid graph. Then $h_P(G) \leq h_U(G^{4,4})$.

The proof of this theorem can be found in Appendix C.

One can easily see that if 4 divides n and G is the $n/4 \times n/4 \times n \times \cdots \times n$ grid graph, then $G_d(n) = G^{4,4}$. We need a lower bound on the size of separators in G. It is easy to see that if we replace every vertex of G by 16 vertices to get $G_d(n)$, an α -separator is replaced by an α -separator, hence the same lower bound of $\Omega(n^{d-1}/\sqrt{d})$, divided by 16, holds for G.

Corollary 4.2.
$$\Omega(n^{d-1}/\sqrt{d}) \le h_U(G_d(n)) \le O(n^{d-1}).$$

In the third variant, D is undirected. Our goal is to find another endvertex and the answer to the query is the at most two incident edges. Obviously, this is a harder problem than the directed variant. Hence our lower bounds hold, and one can easily modify our proofs to get the same upper bounds as well. For example, in Observation 2.1, the endvertex is in the component Y_i which is connected to S by an odd number of edges, counting an extra edge for the component of s.

Finally, a straightforward application of our proofs gives the asymptotics to a question recently asked on MathOverflow [1], which is the following. Given a path P_1 from the bottom-left vertex of an $n \times n$ grid to its top-right vertex, and another path P_2 from its top-left vertex to its bottom-right vertex, how many queries are needed to find a vertex contained in both paths? The proofs of Theorems 1.2 and 2.3 can be adapted to show that $\Theta(n)$ queries are necessary and sufficient.

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A Biseparators for Ternary Trees

We show that a rooted ternary tree with k + 1 complete levels has $s_{1/2}^{\text{bi}}(G) = \Theta(k)$. Any root-to-leaf path is a 1/2-biseparator, establishing the upper bound. Let us turn to the lower bound. A complete ternary tree of height h has $n = (3^{h+1} - 1)/2$ vertices. It is convenient to give each vertex a "weight" of 2. The total weight of the tree becomes $2n = 3^{k+1} - 1$, which is very near to a power of 3. In ternary notation, $2n = (22 \dots 2)_3$ with k twos, and the ideal weight for the halves of the biseparator is $2n/2 = n = (11 \dots 1)_3$.

After removing a separating set, any union of components of the complement can be represented as a sum and difference of subtrees. Here, by a subtree we mean a node together with all its descendants. If the separator has s nodes, we must be able to group the resulting components into a set that has between n/2 - s and n/2 nodes, i.e., weight between n - 2s and n. Each separator node creates at most four new subtrees from which the sum and difference can be formed: its own subtree and the three children subtrees. (These latter ones exist only if the node was not a leaf.) So with s separating nodes, we get 1 + 4s subtrees from which to form the sum and difference. Each tree has a weight of the form $3^h - 1$.

If we take a sum and difference of $L \leq 4s + 1$ subtrees we must fulfill the inequality

$$n-2s \le \sum_{i=1}^{L} (\pm (3^{h_i}-1)) \le n,$$

which implies

$$n - 2s - L \le \sum_{i=1}^{L} (\pm 3^{h_i}) \le n + L$$

and

$$n - 6s - 1 \le \sum_{i=1}^{L} (\pm 3^{h_i}) \le n + 4s + 1.$$

For any number p in the range $n-6s-1 \le p \le n+4s+1$, the ternary representation starts with at least $k-1 - \lceil \log_3(6s+1) \rceil$ ones. On the other hand, one easily sees by induction that a sum and difference of L powers of 3 has at most L ones in its ternary representation. We thus get the relation $4s+1 \ge L \ge k-1 - \lceil \log_3(6s+1) \rceil$, from which $s \ge \Omega(k)$ follows.

B Proof of Corollary 3.4

We show that for any fixed $\delta \ge 0$ (and then by symmetry for every $\delta < 0$ too), whenever $(n-1)d/2 + \delta$ is an integer,

$$|L_{(n-1)d/2+\delta}| = C_d / \sqrt{d} \cdot n^{d-1} \pm O(n^{d-2}).$$

We define $C_d = \operatorname{Vol}_{d-1} H^d(d/2)$, i.e., the volume of the middle slice of the unit hypercube. Setting s = 0 in Theorem 3.3 establishes the convergence of C_d to $\sqrt{6/\pi}$.

The layer L_k , for $k = (n-1)d/2 + \delta$, is a discrete version of a slice of a cube. If we fix the first d-1 coordinates, then there is at most one vertex in L_k that has these first d-1 coordinates. Thus $|L_k| = |L'_k|$, where L'_k is the projection of L_k along the last axis.

To estimate the size of L'_k (and thus of L_k) take first the middle slice $H^d(d/2)$ of the continuous unit cube and project it to the first d-1 coordinates, yielding the polytope $H^d(d/2)'$. As the normal vector of the slice is (1, 1, ..., 1), projecting it to the hyperplane orthogonal to the last axis scales the volume by a factor of $1/\sqrt{d}$:

$$\operatorname{Vol}_{d-1} H^d(d/2)' = \operatorname{Vol}_{d-1} H^d(d/2)/\sqrt{d}.$$

Now let $H^d(d/2)'' = nH^d(d/2)'$, i.e., we blow up $H^d(d/2)'$ by a factor *n*. Let *M* be the set of grid points in this $H^d(d/2)''$. As for fixed d, $H^d(d/2)''$ is a factor-*n* blow up of some fixed (d-1)-dimensional convex polytope, the difference between its volume and the number of grid points in it is $O(n^{d-2})$. (This follows basically from the definition of the volume, for details see e.g., [12, Proposition 4.6.13].) Thus,

$$|M| = n^{d-1} \operatorname{Vol}_{d-1} H^d(d/2)' + O(n^{d-2}) =$$

= $n^{d-1} \operatorname{Vol}_{d-1} H^d(d/2) / \sqrt{d} + O(n^{d-2}) = C_d / \sqrt{d} \cdot n^{d-1} + O(n^{d-2}).$

Now we are left to show that $|L'_k| = |M| + O(n^{d-2})$. For that it is enough to show that $|L'_k \setminus M|$ and $|M \setminus L'_k|$ are $O(n^{d-2})$. For all of these points the sum of the d-1 coordinates is equal to (n-1)d/2 + i (resp. (n-1)d/2 - n + i) for some $0 < i \le \delta$. This is $O(n^{d-2})$ points for every *i*, altogether $2\delta O(n^{d-2}) = O(n^{d-2})$ points, which finishes the proof. \Box

C Proof of Theorem 4.1

Suppose we are given a grid graph G and an Algorithm A which finds t in $G^{4,4}$ in case one path and some cycles cover every vertex. We show an Algorithm B which finds the endvertex in G in case there is only a directed path. We can naturally identify every vertex of G with a 4×4 grid in $G^{4,4}$: the vertex $v = (i_1, \ldots i_d)$ corresponds to the axis-parallel 4×4 rectangle (we call it a block) B(v) having 16 vertices, whose two opposite corners are $(4i_1 - 3, 4i_2 - 3, i_3, \ldots i_d)$ and $(4i_1, 4i_2, i_3, \ldots i_d)$. We call $(4i_1 - 3, 4i_2 - 3, i_3, \ldots i_d)$ and $(4i_1, 4i_2, i_3, \ldots i_d)$ the *even* corners and the two other corners $(4i_1 - 3, 4i_2, i_3, \ldots i_d)$ and $(4i_1, 4i_2 - 3, i_3, \ldots i_d)$ the *odd* corners.

Consider a directed path P in G. We call a system of a directed path and some directed cycles in $G^{4,4}$ good if they cover every vertex and the path goes through exactly those blocks which correspond to the vertices of P, in the same order.

Now we construct good systems. If a vertex $v \in V(G)$ is not on the path, we cover the corresponding block by a cycle. In case of a vertex $v = (i_1, \ldots, i_d)$ on the path in G, the directed path arrives at the corresponding block B(v) in some corner $p_1(v)$, and goes straight to a neighboring corner $p_2(v)$, where it leaves. The remaining vertices form a 4 × 3 rectangle, which can be covered by a cycle. Finally, when v is the very last vertex on the path, we define $p_1(v)$ similarly, and cover the remaining vertices by a path starting in $p_1(v)$.

Our good systems will satisfy an additional property. If, for a vertex $v = (i_1, \ldots i_d)$ of G, the coordinate sum $\sum_{j=3}^d i_j$ is even, then the first vertex $p_1(v)$ of the path in the

corresponding block is an even corner, and the last vertex $p_2(v)$ is an odd corner. In case $\sum_{j=3}^{d} i_j$ is odd, it is the other way round. Note that if it is true for B(s), it has to be true for every other block as well. Indeed, when the path leaves a block at, for example, an odd corner, it either moves in one of the first two dimensions (then it arrives at an even corner, and $\sum_{j=3}^{d} i_j$ does not change), or in another dimension (then it arrives at an odd corner, but the parity of $\sum_{j=3}^{d} i_j$ changes).

Note that these properties do not uniquely determine the system. We will incrementally determine the graph as queries arrive.

Now we are ready to define Algorithm B. At every step we call Algorithm A, and then answer such a way that at the end we get a good system. If Algorithm A would query a vertex v in $G^{4,4}$, Algorithm B queries the corresponding vertex v' in G instead (i.e., the vertex v' with $v \in B(v')$). Using the answer for this query, we choose all the edges incident to vertices of B(v') and answer to Algorithm A according to this. If v' has been asked before, we have already determined the edges in B(v'), and answer accordingly. Suppose that v' has not been queried before. In case the answer is that v' is not on the path, choose an arbitrary cycle covering the vertices of the corresponding block B(v') and answer according to the edges incident to v.

In case the answer gives two arcs uv' and v'w, we have to choose the entering vertex $p_1(v')$ and the exit vertex $p_2(v')$. We will discuss this choice below. This choice will define 5 edges on the path and a cycle of length 12. One edge connects the blocks corresponding to u and v, leaving the last vertex of the path in B(u) and arriving at the first vertex of the path in B(v'), i.e., this edge is $p_2(u)p_1(v')$. Similarly we add the edge $p_2(v')p_1(w)$. We also add the three edges which connect $p_1(v')$ and $p_2(v')$. Finally we cover the remaining 12 vertices with a cycle.

We still have to tell which one of the two possible first vertices we use as $p_1(v')$, and similarly for the possible last vertices. If $p_2(u)$ has already been determined, this fixes the choice of $p_1(v')$ as the vertex adjacent to it. If uv' is parallel to one of the first two axes, this also reduces the choice of the corner $p_1(v')$ to one possibility. Otherwise we pick $p_1(v')$ arbitrarily among the two choices. The exiting vertex $p_2(v')$ is determined analogously.

Even if Algorithm A would know all answers in B(v'), it does not give more information than what Algorithm B knows after asking v'. Algorithm A does not finish before Algorithm B finds the end vertex, thus Algorithm A needs at least as many queries as Algorithm B (on the respective graphs), which finishes the proof.





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A chiral 4-polytope in \mathbb{R}^3

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Abstract

In this paper we describe an infinite chiral 4-polytope in the Euclidean 3-space. This builds on previous work of Bracho, Hubard and the author, where a finite chiral 4-polytope in the Euclidean 4-space is constructed. These two polytopes show that there are finite and infinite chiral polytopes of full rank as defined by McMullen.

Keywords: Chiral 4-polytope, full rank polytope.

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1 Introduction

In this paper we regard *n*-polytopes as combinatorial structures in \mathbb{R}^d constructed from (n-1)-polytopes as building blocks, where 0- and 1-polytopes are points and line segments, respectively.

Regular polytopes are those admitting the highest degree of symmetry in the sense that any two flags are equivalent under the symmetry group. In some way they admit all possible abstract reflections as symmetries.

Nowadays we have plenty of examples of regular polytopes, the most obvious being the convex regular polytopes (see for example [2]) and the tessellations by n-dimensional cubes. Other examples of regular polytopes can be found in [4, 5, 6, 7].

Chiral polytopes have two orbits of flags under the symmetry group with the property that adjacent flags belong to distinct orbits. They admit all abstract rotations as symmetries, but no abstract reflection.

There is very little published work on chiral polytopes on Euclidean spaces. There are no convex chiral polytopes and no chiral tessellations of Euclidean spaces. This illustrates the difficulty to find 'natural' families of chiral polytopes.

In 2005 Schulte classified all chiral polyhedra in \mathbb{R}^3 (see [11] and [12]). They are all infinite; some have finite faces, and some have infinite faces.

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In [5, Theorem 11.2] it was claimed that for any positive integer d there are neither finite chiral d-polytopes in \mathbb{R}^d , nor infinite chiral (d + 1)-polytopes in \mathbb{R}^d .

The first known finite chiral 4-polytope in \mathbb{R}^4 was discovered in [1] in 2014 proving false one half of the claim in [5]. In this paper we describe the first known infinite chiral 4-polytope in \mathbb{R}^3 , proving false the remaining half of the claim.

Definitions and basic results are given in Section 2. In Section 3 we describe the building blocks of the 4-polytope, which is constructed in Section 4. Finally, in Section 5 we discuss the combinatorial symmetry of the 4-polytope.

2 Preliminaries

In this section we recall some concepts and results of the Euclidean space and of polytopes embedded on it.

2.1 Symmetries of the Euclidean space

The rotation group of the octahedron, that we shall denote by $[3, 4]^+$, is one of the finite groups of isometries of \mathbb{R}^3 . It contains 24 elements, out of which six are 4-fold rotations, eight are 3-fold rotations, nine are half-turns, and the remaining one is the identity. In particular, all of its elements preserve orientation (see for example [3] for a more detailed description of this group).

A *lattice* is the orbit of the origin o under a discrete translation group of \mathbb{R}^3 generated by translations with respect to three linearly independent vectors. Up to similarity, there are three lattices that are invariant under the action of the group $[3, 4]^+$ (see [8, Section 6D]).

The *cubic lattice*, denoted by $\Lambda_{(1,0,0)}$, consists of the points of \mathbb{R}^3 with integer coordinates. The translations by the vectors (1,0,0), (0,1,0) and (0,0,1) constitute a basis for the translation group of this lattice.

The *face-centred cubic lattice*, denoted by $\Lambda_{(1,1,0)}$, is generated by the translations by the vectors (1,1,0), (1,0,1) and (0,1,1). It contains the set of points of \mathbb{R}^3 with integer coordinates, whose sum is an even number. The cubic lattice is the union

$$\Lambda_{(1,1,0)} \cup (\Lambda_{(1,1,0)} + (1,0,0))$$

of two isometric copies of the face-centred cubic lattice.

Finally, the *body centred cubic lattice* is the set of points with integer coordinates such that either all of them are even, or all of them are odd. It is generated by the translations by the vectors (1,1,1), (-1,1,1) and (1,-1,1), and it is denoted by $\Lambda_{(1,1,1)}$. The cubic lattice is the union

$$\Lambda_{(1,1,0)} \cup (\Lambda_{(1,1,0)} + (1,0,0)) \cup (\Lambda_{(1,1,0)} + (0,1,0)) \cup (\Lambda_{(1,1,0)} + (0,0,1))$$

of four isometric copies of the body-centred cubic lattice.

The tessellation $\{4, 3, 4\}$ by cubes of \mathbb{R}^3 is the only regular tessellation of the Euclidean space. A *Petrie polygon* of $\{4, 3, 4\}$ is a helix with vertex and edge sets contained in those of $\{4, 3, 4\}$, where every two consecutive edges belong to some square; every three consecutive edges belong to the same cube, but not to the same square; and no four consecutive edges belong to the same cube. The direction vectors of any three consecutive edges of a Petrie polygons of $\{4, 3, 4\}$ are precisely (1, 0, 0), (0, 1, 0) and (0, 0, 1) in some order. These helices have axes with direction vectors (1, 1, 1), (1, 1, -1), (1, -1, 1) and

(-1, 1, 1). Every edge of a Petrie polygon h is a translate of any edge that is 3k steps apart in h (that is, there are 3k - 1 edges between them).

Any two Petrie polygons of $\{4, 3, 4\}$ are isometric. However, any given Petrie polygon is equivalent under orientation preserving isometries (translations, rotations and twists) to only half of the Petrie polygons. We say that a Petrie polygon is a *right helix* if it can be obtained from the helix

 \dots , (1,0,0), (0,0,0), (0,1,0), (0,1,1), (-1,1,1), \dots

by an orientation preserving isometry. The remaining helices are called left helices.

2.2 Polyhedra and 4-polytopes

When studying highly symmetric polytopes we need to move away from convexity to get a richer theory. The definitions below follow the spirit of [4] and subsequent papers.

For us a *polygon* (or 2-*polytope*) in \mathbb{R}^3 is a discrete set of points called *vertices* or 0-*faces* together with a set of line segments called *edges* or 1-*faces* between pairs of vertices, such that the resulting graph is connected and 2-regular. The edges are allowed to intersect in interior points, but there are no vertices in the interior of edges.

A *polyhedron* (or 3-*polytope*) in \mathbb{R}^3 is a set of polygons, called 2-*faces*, with the extra properties that every edge belongs to exactly two polygons, the set of vertices is discrete, the graph determined by the vertices and edges is connected, and the vertex-figures at all vertices are connected. Here the *vertex-figure* at a vertex v is the polygon (or in principle polygons) whose vertices are the neighbours of v, two of which are adjacent if and only if they are the two neighbours of v in a 2-face.

A 4-polytope in \mathbb{R}^3 is a set of polyhedra, called 3-faces with the extra properties that every 2-face belongs to exactly two polyhedra, the set of vertices is discrete, the graph determined by the vertices and edges is connected, and the vertex-figures at all vertices are polyhedra. The vertex-figure at a vertex v in this case consists of the polygons that are the vertex-figures at v in the polyhedra containing it.

Defined as above, polyhedra and 4-polytopes in \mathbb{R}^3 are precisely Euclidean realisations of abstract polyhedra and 4-polytopes as defined in [8, Section 5]. Due to this relationship, we say that two elements of an *n*-polytope are *incident* if one is contained in the other as geometric objects. Vertices, edges, polygons and polyhedra are then regarded as objects of rank 0, 1, 2 and 3, respectively.

The *facets* of an *n*-polytope are its (n - 1)-faces $(n \in \{3, 4\})$. The 1-skeleton of a polyhedron or of a 4-polytope is the graph determined by its sets of vertices and edges. The 2-skeleton of a 4-polytope consists of the sets of vertices, edges and 2-faces.

A *flag* of an *n*-polytope \mathcal{P} is a set of *n* mutually incident elements of \mathcal{P} , one of each rank. That is, a flag of a polygon is a pair of incident vertex and edge, a flag of a polyhedron is a triple of mutually incident vertex, edge and 2-face, and a flag of a 4-polytope contains a vertex, an edge, a polygon and a polyhedron, all incident to the other three.

Given any flag Φ of an *n*-polytope and given $i \in \{0, \ldots, n-1\}$ there exists a unique flag Φ^i that differs from Φ only on the face of rank *i*. The flag Φ^i is known as the *i*-adjacent flag of Φ . We extend recursively this notion and for any word *w* on the elements in $\{0, \ldots, n-1\}$ we define $\Phi^{wi} := (\Phi^w)^i$.

By a symmetry of an *n*-polytope \mathcal{P} we mean an isometry of \mathbb{R}^3 that preserves \mathcal{P} . An *n*-polytope is said to be *regular* whenever its symmetry group acts transitively on the flags

of \mathcal{P} . Clearly, the facets of a regular 4-polytope are regular polyhedra. There are 48 regular polyhedra and 8 regular 4-polytopes in \mathbb{R}^3 ; they were thoroughly studied in [7].

An *n*-polytope is said to be *chiral* whenever its symmetry group induces two orbits on the flags, with adjacent flags in distinct orbits. The term 'chiral' often carries the meaning of being handed, that is, not admitting a mirror symmetry. In our context, where only highly symmetric objects are of interest, chiral polytopes denote the most symmetric polytopes that do not admit a symmetry mapping a flag to an adjacent flag, which is the combinatorial equivalent to mirror symmetry.

There are no finite chiral polyhedra in \mathbb{R}^3 (see for example [11, Theorem 3.1]). Infinite chiral polyhedra were classified in [11] and [12] in six families. One of this polyhedra is described in detail in Section 3.

Regular and chiral *n*-polytopes admit a set of *distinguished abstract rotations* as symmetries. These are isometries S_i that map a given base flag Φ to the flag $\Phi^{i(i-1)}$ for $i \in \{1, \ldots, n-1\}$. Such an isometry needs not be a rotation around an axis in \mathbb{R}^3 . However, the term 'rotation' is in no way inadequate, since their combinatorial impact is similar to that of a rotation on a polygon. S_1 cyclically permutes the vertices and edges of the base 2-face, S_2 cyclically permutes the edges and polygons around the base vertex contained in the base polyhedron, and S_3 cyclically permutes the polygons and polyhedra around the base edge.

The symmetry group of a chiral *n*-polytope is generated by its distinguished abstract rotations. The group generated by all distinguished abstract rotations of a regular *n*-polytope has index at most 2 in the full symmetry group. The tetrahedron $\{3,3\}$ and its Petrial $\{4,3\}_3$ are examples of polyhedra where the subgroups generated by the distinguished abstract rotations have index 2 and 1, respectively.

Conversely, an *n*-polytope whose symmetry group contains all possible distinguished abstract rotations is either regular or chiral, and it is regular if and only if the symmetry group contains an element moving the base vertex but fixing all other elements of the base flag (see [13] for the combinatorial analogue to these claims).

3 The polyhedron $P_1(1,0)$

It is time now to describe the chiral polyhedron $P_1(1,0)$ as a particular case of the general description of the polyhedra $P_1(a, b)$ in [9]. Other description, using the technique known as Wythoff's construction, can be found in [12].

Throughout, \mathcal{T} will denote the cubical tessellation $\{4,3,4\}$ of \mathbb{R}^3 with vertices on \mathbb{Z}^3 , and $\eta : \mathbb{R}^3 \to \Pi$ the orthogonal projection into the plane Π through the origin o with normal vector (1,1,1). It is well known that the image under η of the 1-skeleton of \mathcal{T} is the 1-skeleton of a tessellation \mathcal{T}' by equilateral triangles, and that $\Lambda_{(1,1,1)}\eta$ is the vertex set of a tessellation by equilateral trangles whose edge length is twice as that of $\mathbb{Z}^3\eta$. The preimage under η of any edge of \mathcal{T}' intersects \mathcal{T} in a collection of parallel edges.

Figure 1 shows the tessellation \mathcal{T}' of Π on pale gray and black lines. Assume that the origin *o* projects to the fat vertex and that the coordinate axes project as indicated. That is, assume that one endpoint of the edge to the left of the fat vertex is the projection of (1,0,0), that the black edge at the fat vertex that does not belong to the dotted path ends at the projection of (0,0,1), and that one endpoint of the remaining black edge incident to the fat vertex is the projection of (0,1,0).

Under these assumptions the polyhedron $P_1(1,0)$ can be described as follows. Its ver-



Figure 1: Projection of the 1-skeleton of $P_1(1,0)$

tex set is \mathbb{Z}^3 . The edge set of $P_1(a, b)$ consists of all edges e of \mathcal{T} such that $e\eta$ is a black edge in Figure 1, that is,

- the edge between (x, y, z) and (x + 1, y, z) for every $(x, y, z) \in \Lambda_{(1,1,1)}$ and $(x, y, z) \in \Lambda_{(1,1,1)} + (0, 0, 1)$,
- the edge between (x, y, z) and (x, y + 1, z) for every $(x, y, z) \in \Lambda_{(1,1,1)}$ and $(x, y, z) \in \Lambda_{(1,1,1)} + (1, 0, 0)$,
- the edge between (x, y, z) and (x, y, z + 1) for every $(x, y, z) \in \Lambda_{(1,1,1)}$ and $(x, y, z) \in \Lambda_{(1,1,1)} + (0, 1, 0)$.

Finally, the 2-faces are all Petrie polygons of \mathcal{T} living in this 1-skeleton.

The six edges incident to any given vertex of \mathcal{T} project by η to three gray edges and three black edges. This can be used to show that all vertices of $P_1(a, b)$ have degree 3. Since no two black edges at the same vertex in Figure 1 are collinear, the set of three edges incident to a vertex of $P_1(a, b)$ are translates of the three edges incident to some vertex of the cube \mathcal{C} with vertex set $\{(x, y, z) : x, y, z, \in \{0, 1\}\}$. The precise arrangement of edges at each vertex is explained by the following straightforward lemma.

Lemma 3.1. The three edges incident to any vertex of $P_1(1,0)$ in $\Lambda_{(1,1,1)}$ are translates of the three edges incident to (0,0,0) in the cube C defined as above. Similarly, the three edges incident to any vertex of $P_1(1,0)$ in $\Lambda_{(1,1,1)} + (1,0,0)$ (resp. in $\Lambda_{(1,1,1)} + (0,1,0)$ and $\Lambda_{(1,1,1)} + (0,0,1)$) are translates of the three edges of C incident to (1,0,1) (resp. to (1,1,0) and to (0,1,1)).

The 2-faces of $P_1(1,0)$ are helices over triangles and belong to four parallel classes $\mathcal{H}_1, \mathcal{H}_2, \mathcal{H}_3, \mathcal{H}_4$. Helices in \mathcal{H}_1 project to the triangles with black edges in Figure 1. Every helix in \mathcal{H}_2 projects to Π either in the path with dashed lines or in one of its translates. Helices in \mathcal{H}_3 and \mathcal{H}_4 project to images of helices in \mathcal{H}_2 under rotations by $2\pi/3$ and by $4\pi/3$, respectively.

The axis of every helix in \mathcal{H}_1 has direction vector (1, 1, 1). There is precisely one helix in \mathcal{H}_1 projecting to each triangle in Figure 1. For example, the helix

$$\dots, (-1, 0, -1), (-1, 0, 0), (-1, 1, 0), (0, 1, 0), (0, 1, 1), (0, 2, 1), \dots$$
(3.1)

is the only helix that projects to the triangle with gray interior. All other helices in \mathcal{H}_1 are obtained by translating this helix by integer combinations of (1, 1, -1) and (1, -1, 1).

In contrast, infinitely many helices in \mathcal{H}_2 project to the dotted path. They are the helix

$$\dots, (1, -1, -1), (1, 0, -1), (1, 0, 0), (0, 0, 0), (0, 1, 0), (0, 1, 1), (-1, 1, 1), \dots$$
(3.2)

and its translates by m(1,1,1) for $m \in \mathbb{Z}$. The remaining helices in \mathcal{H}_2 are obtained by translating these helices by m(1,1,-1) for $m \in \mathbb{Z}$. They all have direction vector (-1,1,1).

The parallel classes \mathcal{H}_3 and \mathcal{H}_4 are respectively represented by the helices

$$\dots, (-1, 1, -1), (-1, 1, 0), (0, 1, 0), (0, 0, 0), (0, 0, 1), (1, 0, 1), (1, -1, 1), \dots,$$
(3.3)

$$\dots, (-1, -1, 1), (0, -1, 1), (0, 0, 1), (0, 0, 0), (1, 0, 0), (1, 1, 0), (1, 1, -1), \dots, (3.4)$$

which have the same projection to Π as their translates by m(1, 1, 1) with $m \in \mathbb{Z}$. All other helices in each of these classes are obtained by translating these helices by m(-1, 1, 1) for $m \in \mathbb{Z}$. The axis of every helix in \mathcal{H}_3 (resp. \mathcal{H}_4) has direction vector (1, -1, 1) (resp. (1, 1, -1)).

It should be clear now that every edge in a black-edged triangle in Figure 1 is in the projection of a helix in \mathcal{H}_1 and of a helix in some other parallel class. The horizontal edges in black-edged triangles are the projection of helices in \mathcal{H}_1 and \mathcal{H}_3 ; those edges in black-edged triangles that are translates of the edge in the gray triangle that belongs also to the dotted path are projections of helices in \mathcal{H}_1 and \mathcal{H}_2 ; and the remaining edges in black-edged triangles are projections of helices in \mathcal{H}_1 and \mathcal{H}_2 ; and the remaining edges in black-edged triangles are projections of helices in \mathcal{H}_1 and \mathcal{H}_4 . Similarly, every black edge in Figure 1 that is not in a triangle belongs to the projection of helices in precisely two of the parallel classes \mathcal{H}_2 , \mathcal{H}_3 and \mathcal{H}_4 . From this it is easy to see that every edge of $P_1(1,0)$ belongs precisely to two helices. Furthermore, the parallel classes of the helices containing an edge e are completely determined by whether or not $e\eta$ belongs to a black-edged triangle, together with its direction vector in Figure 1.

In order to discuss the symmetries of $P_1(1,0)$ we take as base flag Φ the one containing the origin o, the edge between o and (0,1,0), and the helix in (3.2). Let S_1 be the screw motion

$$(x, y, z) \mapsto (-y+1, z, -x) \tag{3.5}$$

with axis $\{\frac{1}{3}(1,1,0) + k(-1,1,1) : k \in \mathbb{R}\}$, translation vector $\frac{1}{3}(1,-1,-1)$ and rotation component of $2\pi/3$. Let S_2 be the rotation

$$(x, y, z) \mapsto (z, x, y) \tag{3.6}$$

about the axis $\{k(1,1,1) : k \in \mathbb{R}\}$ by an angle of $2\pi/3$. By applying these isometries to the edges of $P_1(1,0)$ we can see that S_1 and S_2 preserve the 1-skeleton of $P_1(1,0)$. Hence, S_1 and S_2 also preserve the set of 2-faces of $P_1(a, b)$. Furthermore, S_1 cyclically permutes the vertices of the base 2-face and S_2 cyclically permutes the three helices around o. This implies that $P_1(1,0)$ admits symmetries acting like the distinguished abstract rotations and therefore it is either regular or chiral.

The polyhedron $P_1(1,0)$ turns out to be chiral. Indeed, the only isometry T preserving the base edge and base helix, but interchanging the base vertex o with (0,1,0) is the half-turn

$$(x, y, z) \mapsto (z, -y + 1, x)$$

with axis $\{(0, 1/2, 0) + k(1, 0, 1) : k \in \mathbb{R}\}$. However, such a T maps the edge between o and (0, 0, 1) to the edge between (0, 1, 0) and (1, 1, 0), which is not an edge of $P_1(1, 0)$, and hence does not preserve the 1-skeleton of $P_1(1, 0)$.

The base helix of $P_1(1,0)$ is a right helix as explained in Section 2. The symmetries S_1 and S_2 defined above are both orientation preserving. It follows that all helices in $P_1(1,0)$ are right helices.

The symmetry S_1^3 of $P_1(1,0)$ is the translation by the vector (1, -1, -1). The conjugates of this translation by S_2 and S_2^2 are the translations by the vectors (-1, 1, -1) and (-1, -1, 1), respectively. The next proposition follows.

Proposition 3.2. The symmetry group of $P_1(1,0)$ contains the translations by all vectors with endpoints in $\Lambda_{(1,1,1)}$.

Since $P_1(1,0)$ is chiral, it is also helix-transitive, implying the next remark.

Remark 3.3. The orthogonal projections of $P_1(1,0)$ in the directions (1,1,-1), (1,-1,1) and (-1,1,1) of the axes of the helices are all isometric to the projection in the direction (1,1,1) in Figure 1.

It is interesting to note that the set of gray edges in Figure 1 is isometric to the set of black edges, and one can be obtained from the other by a half-turn around the fat point. The polyhedron constructed from the preimages in \mathcal{T} of the gray edges under the projection η is clearly isometric to $P_1(1,0)$ but it contains only left helices. They are precisely the images of the helices of $P_1(1,0)$ under the isometry mapping \bar{x} to $-\bar{x}$ for every $\bar{x} \in \mathbb{R}^3$.

4 The chiral 4-polytope $\mathcal{P}_{\{\infty,3,4\}}$

The polyhedron $P_1(1,0)$ just described is the building block of the chiral 4-polytope $\mathcal{P}_{\{\infty,3,4\}}$. The vertex and edge sets of $\mathcal{P}_{\{\infty,3,4\}}$ are the vertex and edge sets of the cubic tessellation \mathcal{T} . The 2-faces of $\mathcal{P}_{\{\infty,3,4\}}$ are all right Petrie polygons of \mathcal{T} . This set constitutes the regular polygonal complex $\mathcal{K}_7(1,1)$ in [10].

The facets of $\mathcal{P}_{\{\infty,3,4\}}$ are $P_1(1,0)$ and its images under the group $[3,4]^+$ of rotations of the octahedron. Recall that $[3,4]^+$ has 24 elements. Since $P_1(1,0)$ is invariant under three-fold rotations around the line through o with direction vector (1,1,1), there are at most 8 images of $P_1(1,0)$ under $[3,4]^+$.

In fact, $\mathcal{P}_{\{\infty,3,4\}}$ has precisely 8 facets. They are described next. Recall from Section 3 that the three neighbours of o in $P_1(1,0)$ are $e_1 = (1,0,0)$, $e_2 = (0,1,0)$ and $e_3 = (0,0,1)$. This motivates to denote this polyhedron as a facet of $\mathcal{P}_{\{\infty,3,4\}}$ by $F_{(+,+,+)}$. The group $[3,4]^+$ acts transitively on the set of octants of \mathbb{R}^3 and hence $\mathcal{P}_{\{\infty,3,4\}}$ has precisely 8 facets. They are denoted $F_{(a_1,a_2,a_3)}$, where a_i takes the value '+' whenever in that facet e_i is a neighbour of o, and the value '-' otherwise. For example, the orbit of $F_{(+,+,+)}$ under the 4-fold rotation around the z axis mapping (x, y, z) to (y, -x, z) is

$$(F_{(+,+,+)}, F_{(+,-,+)}, F_{(-,-,+)}, F_{(-,+,+)}).$$

In order to better understand the combinatorics of $\mathcal{P}_{\{\infty,3,4\}}$ it is convenient to compute the image of all its facets under the projection η as defined in Section 3. This can be done by directly applying the orientation preserving isometries in $[3,4]^+$ and then η to the edges of $P_1(1,0)$.

Alternatively, we can use the fact that the helices of $P_1(1,0)$ split in four classes \mathcal{H}_1 , \mathcal{H}_2 , \mathcal{H}_3 and \mathcal{H}_4 , consisting of helices with axes having direction vector (1, 1, 1), (-1, 1, 1), (1, -1, 1) and (1, 1, -1), respectively. Every isometry $T \in [3, 4]^+$ permutes the four directions (1, 1, 1), (1, 1, -1), (1, -1, 1) and (-1, 1, 1) of the axes of helices of $P_1(1, 0)$ and



Figure 2: Projections of the eight facets of $\mathcal{P}_{\{\infty,3,4\}}$

so $F_{(+,+,+)}T$ must have a parallel class of helices with axes in the direction of (1,1,1). These helices project orthogonally into triangles on the plane II; furthermore, this triangles must be pointing up, since they are precisely the images of right helices, whereas the left helices project into triangles pointing down. Similarly, the helices in the three remaining parallel classes must project into isometric copies of the dotted path in Figure 1. This information, together with the three neighbours of o on each facet and Remark 3.3, determines the projections of the eight facets of $\mathcal{P}_{\{\infty,3,4\}}$ as in Figure 2, where the fat dot represents the origin o.

We can see that $F_{(+,+,+)}$ and $F_{(-,-,-)}$ are the only facets where *o* does not belong to a helix with axis in the direction of (1, 1, 1). In both instances *o* belongs to helices with axes in the directions of (-1, 1, 1), (1, -1, 1) and (1, 1, -1).

We choose the following seven isometries $T_{(a_1,a_2,a_3)} \in [3,4]^+$ mapping $F_{(+,+,+)}$ to $F_{(a_1,a_2,a_3)}$:

$$\begin{split} T_{(+,-,-)} &: (x,y,z) \mapsto (x,-y,-z), \\ T_{(-,+,-)} &: (x,y,z) \mapsto (-x,y,-z), \\ T_{(-,-,+)} &: (x,y,z) \mapsto (-x,-y,z), \\ T_{(-,+,+)} &: (x,y,z) \mapsto (-z,y,x), \\ T_{(+,-,+)} &: (x,y,z) \mapsto (y,-x,z), \\ T_{(+,+,-)} &: (x,y,z) \mapsto (x,z,-y), \\ T_{(-,-,-)} &: (x,y,z) \mapsto (-x,-y,-z). \end{split}$$

We also denote by H_1 , H_2 , H_3 and H_4 the helices in (3.1), (3.2), (3.3) and (3.4), respectively. Recall that the helices in $F_{(+,+,+)}$ with direction vector (1,1,1) are H_1 and its translates by vectors with endpoints in $\Lambda_{(1,1,1)}$.

The right Petrie polygons of \mathcal{T} with axes in the direction of (1,1,1) are the ones in $F_{(+,+,+)}$ together with their translates by (1,0,0), (0,1,0) and (0,0,1). It can be seen from Figure 2 that the helices in $F_{(+,+,+)}$ with axis in the direction of (1,1,1) are also

helices of $F_{(-,-,-)}$. Furthermore, the helices with axes in the direction of (1,1,1) of $F_{(+,-,-)}$ and of $F_{(+,-,+)}$ are the translates of those in $F_{(+,+,+)}$ by (0,0,1), the helices with axes in the direction of (1,1,1) of $F_{(-,+,-)}$ and of $F_{(+,+,-)}$ are the translates of those in $F_{(+,+,+)}$ by (1,0,0), and the helices with axes in the direction of (1,1,1) of $F_{(-,-,+)}$ and of $F_{(-,+,+)}$ are the translates of those in $F_{(+,+,+)}$ by (0,1,0). This can also be verified by noting that

$$\begin{split} H_1 &= H_1 T_{(-,-,-)} + (-1,1,1), \\ H_1 + (1,-1,1) &= H_2 T_{(+,-,-)} + (0,0,1) = H_2 T_{(+,-,+)} + (0,0,1), \\ H_1 + (1,-1,-1) &= H_3 T_{(-,+,-)} + (1,0,0) = H_3 T_{(+,+,-)} + (1,0,0), \\ H_1 &= H_4 T_{(-,-,+)} + (0,1,0) = H_4 T_{(-,+,+)} + (0,1,0), \end{split}$$

together with the fact that $[3, 4]^+$ permutes the four directions of the axes of the helices of $F_{(+,+,+)}$ and that the set of helices of $F_{(+,+,+)}$ in any of the four directions is invariant by translations by vectors with endpoints in $\Lambda_{(1,1,1)}$. This shows that all right Petrie polygons of \mathcal{T} with axes in the direction of (1, 1, 1) belong to at least two facets of $\mathcal{P}_{\{\infty,3,4\}}$. Recall that the set of helices on $P_1(1,0)$ with axis in the direction of (1,1,1) can be obtained by translating H_1 by vectors with endpoints in $\Lambda_{(1,1,1)}$, and similarly the set of helices of $P_1(1,0)$ with axis in the direction of (1,1,-1) can be obtained by translating H_2 , H_3 or H_4 , respectively, by vectors with endpoints in $\Lambda_{(1,1,-1)}$. This shows that each right Petrie polygon of \mathcal{T} with axis in the direction of (1,1,1) belongs to precesely two facets of $\mathcal{P}_{\{\infty,3,4\}}$. The fact that \mathcal{T} and $\mathcal{P}_{\{\infty,3,4\}}$ are symmetric under $[3,4]^+$ implies the following lemma.

Lemma 4.1. Every helix of $\mathcal{P}_{\{\infty,3,4\}}$ belongs to precisely two facets.

Table 1 indicates the direction vector of the helices that two facets have in common (if any). In the table, (a_1, a_2, a_3) indicates the facet $F_{(a_1, a_2, a_3)}$. In particular one can conclude that the facets $F_{(a_1, a_2, a_3)}$ and $F_{(b_1, b_2, b_3)}$ have a helix in common if (a_1, a_2, a_3) and (b_1, b_2, b_3) coincide either in two coordinates or in none. The entries on the table can be obtained by applying the isometries $T_{(a_1, a_2, a_3)}$ to the helices of $F_{(+, +, +)}$, or by a careful inspection of Figure 2.

Facets	(+, +, +)	(+, +, -)	(+, -, +)	(-, +, +)	(+, -, -)	(-, +, -)	(-, -, +)	(-, -, -)
(+, +, +)	_	(-1, 1, 1)	(1, 1, -1)	(1, -1, 1)	none	none	none	(1, 1, 1)
(+, +, -)	(-1, 1, 1)	—	none	none	(1, -1, 1)	(1, 1, 1)	(1, 1, -1)	none
(+, -, +)	(1, 1, -1)	none	—	none	(1, 1, 1)	(1, -1, 1)	(-1, 1, 1)	none
(-,+,+)	(1, -1, 1)	none	none	_	(-1, 1, 1)	(1, 1, -1)	(1, 1, 1)	none
(+, -, -)	none	(1, -1, 1)	(1, 1, 1)	(-1, 1, 1)	—	none	none	(1, 1, -1)
(-,+,-)	none	(1, 1, 1)	(1, -1, 1)	(1, 1, -1)	none	_	none	(-1, 1, 1)
(-, -, +)	none	(1, 1, -1)	(-1, 1, 1)	(1, 1, 1)	none	none	—	(1, -1, 1)
(-, -, -)	(1, 1, 1)	none	none	none	(1, 1, -1)	(-1, 1, 1)	(1, -1, 1)	_

Table 1: Helices shared by two facets of $\mathcal{P}_{\{\infty,3,4\}}$.

Recall that the vertex-figure at o in $\mathcal{P}_{\{\infty,3,4\}}$ consists of the eight triangles that are the vertex-figures at o of the eight facets of $\mathcal{P}_{\{\infty,3,4\}}$. From the construction it is immediate that the vertex-figure at o in $\mathcal{P}_{\{\infty,3,4\}}$ is an octahedron.

As a consequence of Proposition 3.2, the three neighbours in $F_{(+,+,+)}$ of any vertex vin $\Lambda_{(1,1,1)}$ are v+(1,0,0), v+(0,1,0) and v+(0,0,1). A similar statement can be made for the remaining seven facets of $\mathcal{P}_{\{\infty,3,4\}}$. Indeed, since $F_{(a_1,a_2,a_3)}$ is the image of $F_{(+,+,+)}$ under some isometry in $[3,4]^+$ and $\Lambda_{(1,1,1)}$ is invariant under the entire group $[3,4]^+$, the translations by vectors with endpoints in $\Lambda_{(1,1,1)}$ are symmetries of $F(a_1,a_2,a_3)$. This implies that the vertex-figure at any vertex of $\mathcal{P}_{\{\infty,3,4\}}$ in $\Lambda_{(1,1,1)}$ is an octahedron. This statement is in fact true for any vertex of $\mathcal{P}_{\{\infty,3,4\}}$.

Lemma 4.2. The vertex-figure of any vertex of $\mathcal{P}_{\{\infty,3,4\}}$ is an octahedron.

Proof. Since every facet of $\mathcal{P}_{\{\infty,3,4\}}$ is invariant under translations by vectors with endpoints in $\Lambda_{(1,1,1)}$, we only need to show that the result holds for a representative of each translation class. Since $\Lambda_{(1,0,0)}$ is the disjoint union of four translates of $\Lambda_{(1,1,1)}$, there are only four orbits of vertices of $\mathcal{P}_{\{\infty,3,4\}}$ under the action of the translations by vectors with endpoints in $\Lambda_{(1,1,1)}$. We take o, (1,0,0), (0,1,0) and (0,0,1) as representatives of these orbits.

The previous discussion shows that the result holds for o (and hence for vertices in $\Lambda_{(1,1,1)}$). A close inspection to Figure 2 (or direct verification) shows that the neighbours of the remaining three representatives in facet $F_{(a_1,a_2,a_3)}$ are as in Table 2, where an entry (b_1, b_2, b_3) indicates that v has as neighbour $v + e_i$ when b_i is '+', and $v - e_i$ when b_i is '-'.

	$F_{(+,+,+)}$	$F_{(+,+,-)}$	$F_{(+,-,+)}$	$F_{(-,+,+)}$	$F_{(+,-,-)}$	$F_{(-,+,-)}$	$F_{(-,-,+)}$	$F_{(-,-,-)}$
(1, 0, 0)	(-,+,-)	(-,-,-)	(-, +, +)	(+, -, +)	(-, -, +)	(+, +, +)	(+,-,-)	(+, +, -)
(0, 1, 0)	(-, -, +)	(+, -, +)	(+, +, -)	(-, -, -)	(-, +, -)	(+, -, -)	(+, +, +)	(-, +, +)
(0, 0, 1)	(+, -, -)	(-, +, +)	(-, -, -)	(+, +, -)	(+, +, +)	(-, -, +)	(-, +, -)	(+, -, +)

Table 2: Neighbours of (1, 0, 0), (0, 1, 0) and (0, 0, 1) on the facets of $\mathcal{P}_{\{\infty, 3, 4\}}$.

The entry of Table 2 corresponding to vertex v and facet F indicates the octant determined by the three neighbours of v in F. The vertex-figure of v at F is then a triangle in that octant (determined by the three neighbours of v). All octants appear exactly once on each row, implying that the vertex-figures are all octahedra.

We are now ready for our main result.

Theorem 4.3. The structure $\mathcal{P}_{\{\infty,3,4\}}$ is a chiral 4-polytope in \mathbb{R}^3 .

Proof. We know that $\mathcal{P}_{\{\infty,3,4\}}$ is the set of polyhedra

$$\{P_1(1,0)\alpha : \alpha \in [3,4]^+\},\$$

and that the set of vertices is descrete. We also know that its 1-skeleton coincides with that of the tessellation by cubes, and hence it is connected. Every 2-face belongs to precisely two facets by Lemma 4.1 and all vertex-figures are polyhedra by Lemma 4.2. Hence $\mathcal{P}_{\{\infty,3,4\}}$ is a 4-polytope.

By construction, $\mathcal{P}_{\{\infty,3,4\}}$ is invariant under the rotation S_2 defined in (3.6) and the rotation S_3 given by

$$(x, y, z) \mapsto (z, y, -x),$$

since they just permute the images of $P_1(1,0)$ under $[3,4]^+$. Furthermore, the screw motion S_1 defined in (3.5) also preserves $\mathcal{P}_{\{\infty,3,4\}}$. In fact, by applying S_1 to the edge set of $F_{(a_1,a_2,a_3)}$ for each (a_1,a_2,a_3) we can see that S_1 fixes $F_{(+,+,+)}$ and $F_{(+,+,-)}$, and induces the permutation

$$(F_{(+,-,+)}, F_{(-,-,-)}, F_{(-,+,+)}) \cdot (F_{(+,-,-,)}, F_{(-,-,+)}, F_{(-,+,-)})$$

in the remaining 6 facets of $\mathcal{P}_{\{\infty,3,4\}}$.

These three isometries are the distinguished abstract rotations with respect to the flag Ψ containing o, the edge between o and (0, 1, 0), the helix in (3.2) and the facet $F_{(+,+,+)}$. Indeed, it is not hard to verify that $\Psi S_1 = \Psi^{10}$, $\Psi S_2 = \Psi^{21}$ and $\Psi S_3 = \Psi^{32}$. Hence $\mathcal{P}_{\{\infty,3,4\}}$ is either regular or chiral, and since its facets are chiral, $\mathcal{P}_{\{\infty,3,4\}}$ itself is chiral.

5 Combinatorial symmetry

In the previous section we constructed a 4-polytope that is chiral as a geometric object. In this section we discuss its combinatorial nature. That is, we study $\mathcal{P}_{\{\infty,3,4\}}$ as a partially ordered set with a rank function ranging in $\{0, 1, 2, 3\}$, whose elements are the vertices, edges, polygons and polyhedra of $\mathcal{P}_{\{\infty,3,4\}}$ where two of them are incident if and only if one is contained in the other (see [8] for proper definitions of abstract polytopes).

An *automorphism* of an *n*-polytope is a bijection of its vertices, edges, etc. that preserves the incidence. A polytope is *combinatorially regular* (resp. *combinatorially chiral*) if its automorphism group acts transitively on its flags (resp. if its automorphism group induces two orbits on flags with adjacent flags in distinct orbits). The distinguished abstract rotations of $\mathcal{P}_{\{\infty,3,4\}}$ as a geometric object induce automorphisms as an abstract object.

Due to the connectivity of $\mathcal{P}_{\{\infty,3,4\}}$ and to the uniqueness of *i*-adjacent flags for $i \in \{0, 1, 2, 3\}$, any automorphism of $\mathcal{P}_{\{\infty,3,4\}}$ is completely determined by the image on any flag. As a consequence of this, the group generated by the automorphisms given by the abstract distinguished rotations of $\mathcal{P}_{\{\infty,3,4\}}$ has index at most 2 on the full automorphism group of $\mathcal{P}_{\{\infty,3,4\}}$. Furthermore, $\mathcal{P}_{\{\infty,3,4\}}$ is combinatorially regular if and only if there is an automorphism mapping a flag Φ to its 1-adjacent flag Φ^1 . We next show that this is not the case.

Theorem 5.1. The 4-polytope $\mathcal{P}_{\{\infty,3,4\}}$ is combinatorially chiral.

Proof. We take as base flag $\Psi := \{F_0, F_1, F_2, F_3\}$ where $F_0 = o, F_1$ is the edge between o and $(0, 1, 0), F_2$ is the helix in (3.2), and $F_3 = F_{(+,+,+)}$. We will show that $\mathcal{P}_{\{\infty,3,4\}}$ is abstractly chiral by assuming that there exists an automorphism R_1 mapping Ψ to Ψ^1 , and showing that the image of the vertex (1, -1, 1) under such R_1 is not well defined. In doing so we will abuse notation and use the geometric names and descriptions of the vertices, edges, 2-faces and facets, but the arguments to deduce the action of R_1 will be purely combinatorial (not geometric).

Since R_1 fixes F_2 and o while moving F_1 , it must interchange the neighbours of o in F_2 , namely (1, 0, 0) and (0, 1, 0). The facet F_3 also is fixed by R_1 , and o belongs to three

edges in F_3 . Since R_1 interchages the edge between o and (1,0,0) with F_1 , it must fix the remaining edge, that is, the edge between o and (0,0,1); in particular $(0,0,1)R_1 = (0,0,1)$. This implies that the helices H_3 in (3.3) and H_4 in (3.4) are also interchanged by R_1 , and so R_1 interchanges (1,0,1) with (0,-1,1) and (1,-1,1) with (-1,-1,1).

Now, since R_1 fixes F_3 but interchanges H_3 and H_4 , it must also interchange the facets $F_{(-,+,+)}$ and $F_{(+,-,+)}$ since they are the only facets containing H_3 and H_4 , respectively, other than $F_{(+,+,+)}$. The edge between o and (0,0,1) is contained in precisely the four facets $F_{(+,+,+)}$, $F_{(-,+,+)}$, $F_{(+,-,+)}$ and $F_{(-,-,+)}$. The first of these facets is fixed by R_1 while the second and third are interchanged. Since R_1 fixes the edge between o and (0,0,1), it must also fix the facet $F_{(-,-,+)}$.

Thus R_1 fixes $F_{(-,-,+)}$ and the edge between o and (0, 0, 1). The remaining edges of $F_{(-,-,+)}$ containing o have their other endpoints in (-1, 0, 0) and (0, -1, 0). The edge between o and (-1, 0, 0) is also an edge of $F_{(-,+,+)}$ but not of $F_{(+,-,+)}$, whereas the edge between o and (0, -1, 0) is also an edge of $F_{(+,-,+)}$ but not of $F_{(-,+,+)}$. Therefore R_1 must interchange the edge between o and (-1, 0, 0) with the edge between o and (0, -1, 0). In $F_{(-,-,+)}$ there is only one helix containing these two edges, and so it must be preserved by R_1 . This helix is $H_2T_{(-,-,+)}$ with vertices

$$\dots, (-1, 1, -1), (-1, 0, -1), (-1, 0, 0), (0, 0, 0), (0, -1, 0), (0, -1, 1), (1, -1, 1), \dots$$

and so R_1 must interchange (0, -1, 1) with (-1, 0, -1), and (1, -1, 1) with (-1, 1, -1). But we showed before that $(1, -1, 1)R_1 = (-1, -1, 1)$. This yields the desired contradiction.

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Integral representations for binomial sums of chances of winning

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Abstract

Addona, Wagon and Wilf (Ars Math. Contemp. 4 (1) (2011), 29-62) examined a problem about the winning chances in tossing unbalanced coins. Here we present some integral representations associated with such winning probabilities in a more general setting via using certain Fourier transform method. When our newly introduced parameters (r, d) are set to be (0, 1), one of our results reduces to the main formula in the above reference.

Keywords: Binomial sum, integral representation, probabilistic analysis, unbalanced coin. Math. Subj. Class.: 11B65, 33D45, 42A16, 60C05, 91A60

1 Introduction: How to make it fair and fun?

One of the final two papers published by Herbert S. Wilf (1932-2012) is a joint work with Addona and Wagon entitled "How to lose as little as possible", which investigates an intriguing problem of disadvantaged player Alice competing with Bob [1]:

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Suppose Alice has a coin with probability of heads equal to q (0 < q < 1), Bob has a different coin with probability of heads equal to p (0), and that <math>q < p. They toss their coins independently n times each. The rule says that Alice wins if and only if she gets strictly more heads than Bob does. Clearly, in the above setting Alice's odds of winning are

$$\mathbb{P}(S_n > T_n) = \sum_{j=0}^n \binom{n}{j} p^j (1-p)^{n-j} \sum_{k=j+1}^n \binom{n}{k} q^k (1-q)^{n-k}, \quad (1.1)$$

where the random variable S_n (resp. T_n) stands for the number of heads that Alice gets (resp. Bob gets) after *n* tosses.

For convenience, let

$$f(n) = f(n, p, q) = \mathbb{P}(S_n > T_n). \tag{1.2}$$

In search of the choice of n that maximizes Alice's chances of winning, it is shown in [1] that f(n) is essentially unimodal, and sharp bounds on the turning point N(q, p) are given. Their analysis uses the multivariate form of Zeilbergers algorithm [2]. In particular, one of the main results of [1] that provides a key role in the proof of unimodality and in the derivation of the turning point is the following:

Theorem 1.1. With f(n) defined above,

$$\frac{f(n+1) - f(n)}{((1-p)(1-q))^{n+1}} = (y + \frac{1}{2}(1+xy))\phi_n(xy) - \frac{1}{2}\phi_{n+1}(xy),$$
(1.3)

where x = p/(1-p), y = q/(1-q), $\phi_n(z) = \sum_{j=0}^n {\binom{n}{j}}^2 z^j = (1-z)^n P_n(\frac{1+z}{1-z})$, and $P_n(u)$ is the classical Legendre polynomial:

$$P_n(u) = \frac{1}{\pi} \int_0^{\pi} (u + \sqrt{u^2 - 1} \cos t)^n dt.$$

(Note that $|u| = |\frac{1+xy}{1-xy}| > 1$ for $xy \in (0,1) \cup (1,+\infty)$; the case xy = 1 yields p = 1-q and (1.3) may be verified directly from (1.1) without using the Legendre polynomial.)

Explicitly, the numerator of the left hand side of (1.3), which is the essential part, may be expressed via

$$f(n+1) - f(n) = \frac{1}{\pi} \int_0^\pi \psi^n(t)(q - pq - \sqrt{pq(1-p)(1-q)}\cos t)dt, \qquad (1.4)$$

where $\psi(t) = 1 - p - q + 2pq + 2\sqrt{pq(1-p)(1-q)}\cos t$. In fact, the above expression (1.4) is found by first using the multivariate form of Zeilberger's algorithm and then proved mathematically (with ease once the formula is found). Also, it follows from (1.4) that the probability for Alice to win with *n* tosses is

$$\mathbb{P}(S_n > T_n) = \frac{1}{\pi} \int_0^{\pi} \frac{1 - \psi^n(t)}{1 - \psi(t)} (q - pq - \sqrt{pq(1 - p)(1 - q)} \cos t) dt.$$

To be fair and fun, here in this paper we consider a more general setting. Since Alice has a weaker coin, why should not she toss it for r more times than Bob does? And if

that becomes the fact, maybe we should investigate the chances for Alice to get at least d $(d \ge 1)$ more heads than Bob does.

Now formally, let $S_n \sim Bin(n,q)$ and $T_m \sim Bin(m,p)$. Suppose Alice tosses her $coin n + r \ (r \ge 0)$ times and Bob tosses his *n* times, and that Alice wins iff she gets at least $d \ (d \ge 1)$ more heads than Bob does. Under the new rule, the probability for Alice to win is

$$\mathbb{P}(S_{n+r} \ge T_n + d) = \sum_{j=0}^n \binom{n}{j} p^j (1-p)^{n-j} \sum_{k\ge j+d}^{n+r} \binom{n+r}{k} q^k (1-q)^{n+r-k}$$

For convenience, we let

$$f_{r,d}(n) = f_{r,d}(n, p, q) = \mathbb{P}(S_{n+r} \ge T_n + d).$$
 (1.5)

Apparently, the function f(n) in this setting is $f_{0,1}(n)$.

In order to study the turning point, investigations of the difference $f_{r,d}(n+1) - f_{r,d}(n)$ are needed. In Section 2 we introduce probabilistic preliminaries with Fourier analysis blended. In Section 3 we provide several representations of the difference function based on certain trigonometric integrals.

Throughout this work we adopt the commonly used convention for the generalized binomial coefficients: for $\alpha \in \mathbb{R}$, $j \in \mathbb{Z}$,

$$\begin{pmatrix} \alpha \\ j \end{pmatrix} = \begin{cases} \frac{\alpha(\alpha-1)\cdots(\alpha-j+1)}{j!}, & \text{if } j \ge 1; \\ 1, & \text{if } j = 0; \\ 0, & \text{if } j < 0. \end{cases}$$

2 Probabilistic analysis: Lens of Fourier method

To attack on $f_{r,d}(n + 1) - f_{r,d}(n)$, we adopt the Fourier analysis approach used in [4], where the special case p = q has been studied.

The following known fact [3, p. 95] will be useful in our studies. Let Z be an integervalued random variable. It holds that

$$\mathbb{P}(Z=k) = \frac{1}{2\pi} \int_0^{2\pi} \varphi_Z(t) e^{-ikt} dt, \qquad (2.1)$$

where $\varphi_Z(t)$ is the characteristic function of Z.

Lemma 2.1. For any $r, d, n \in \mathbb{N}$,

$$f_{r,d}(n+1) - f_{r,d}(n) = \sum_{j=0}^{r} (q(1-p)\mathbb{P}(T_n - S_n - k = j+1-d) - p(1-q))\mathbb{P}(T_n - S_n - k = j-d)\mathbb{P}(S_r = j).$$

Proof. For convenience, let $g(n,k) := \mathbb{P}(T_n - S_n - k = 0)$. Note that

$$f_{r,d}(n) = \mathbb{P}(S_{n+r} \ge T_n + d) = \mathbb{P}(S'_r \ge T_n - S_n + d) = \sum_{k=-n}^n g(n,k)\mathbb{P}(S'_r \ge k + d).$$

Here in this proof technically S'_r is independent of S_n and has the same distribution as S_r . Similarly,

$$f_{r,d}(n+1) = \mathbb{P}(S'_r \ge T_n - S_n + Y_1 - X_1 + d)$$
$$= \sum_{k=-n}^n g(n,k) \mathbb{P}(S'_r \ge Y_1 - X_1 + k + d)$$

Comparing the two formulae above, we arrive at

$$\begin{split} f_{r,d}(n+1) &- f_{r,d}(n) \\ &= \sum_{k=-n}^{n} g(n,k)(p(1-q)\mathbb{P}(S'_{r} \geq k+d+1) + q(1-p)\mathbb{P}(S'_{r} \geq k+d-1) \\ &+ (2pq-p-q)\mathbb{P}(S'_{r} \geq k+d)) \\ &= \sum_{k=-n}^{n} g(n,k)(q(1-p)\mathbb{P}(S'_{r} = k+d-1) - p(1-q)\mathbb{P}(S'_{r} = k+d)) \\ &= \sum_{j=0}^{r} (q(1-p)g(n,j+1-d) - p(1-q)g(n,j-d))\mathbb{P}(S'_{r} = j). \end{split}$$

Corollary 2.2. For any $r, d, n \in \mathbb{N}$, $f_{r,d}(n+1) - f_{r,d}(n) =$

$$\frac{1}{2\pi} \int_0^{2\pi} \varphi^n(t) \sum_{j=0}^r (\mathbb{P}(S_r=j)(q(1-p)e^{-i(j+1-d)t} - p(1-q)e^{-i(j-d)t}))dt,$$

where

$$\begin{split} \varphi(t) &= \varphi(t, p, q) := Ee^{it(Y_1 - X_1)} \\ &= (1 - p + pe^{it})(1 - q + qe^{-it}) \\ &= 1 - p - q + 2pq + (p + q - 2pq)\cos t + i(p - q)\sin t \end{split}$$

is the characteristic function of $Y_1 - X_1$ with that $Y_1 \sim Bin(1, p)$ and $X_1 \sim Bin(1, q)$.

Proof. This is an immediate consequence of (2.1) and Lemma 2.1.

Corollary 2.3. *More specifically, for* r = 0, d = 1, *and* $n \in \mathbb{N}$ *,*

$$f_{0,1}(n+1) - f_{0,1}(n) = \frac{1}{2\pi} \int_0^{2\pi} \varphi^n(t) (q(1-p) - p(1-q)e^{it}) dt.$$
 (2.2)

In the case r = 0 and d = 1, the formula of Corollary 2.2 reduces to the formula by Addona et al [1] as will be shown in Example 3.3.

3 Integral representations

The difference $f_{r,d}(n+1) - f_{r,d}(n)$ may be evaluated directly. In fact it depends on certain trigonometric integrals. Before we proceed the following fact is needed.

Lemma 3.1. For all nonnegative integers a, b, c, let $J(a, b, c) = \int_0^{2\pi} \cos^a t \sin^b t \cos(ct) dt$ and $K(a, b, c) = \int_0^{2\pi} \cos^a t \sin^b t \sin(ct) dt$. Then

$$J(a,b,c) = 2\pi \sum_{s} \frac{(-1)^{b/2+s}}{2^{a+b+1}} {b \choose s} \left[{a \choose (a+b-c)/2-s} + {a \choose (a+b+c)/2-s} \right]$$

$$K(a,b,c) = 2\pi \sum_{s} \frac{(-1)^{(b-1)/2+s}}{2^{a+b+1}} {b \choose s} \left[{a \choose (a+b-c)/2-s} - {a \choose (a+b+c)/2-s} \right],$$

where for convenience we assume that $(-1)^u = 0$ if $u \notin \mathbb{Z}$.

Proof. Note that J(a, b, c) = 0 whenever b is odd, and that

$$\int_0^{2\pi} e^{itm} dt = \begin{cases} 2\pi, & \text{if } m = 0; \\ 0, & \text{otherwise.} \end{cases}$$

Hence we have

$$\begin{split} J(a,b,c) &= \int_{0}^{2\pi} \cos^{a} t \sin^{b} t \cos(ct) dt \\ &= \int_{0}^{2\pi} (\frac{e^{it} + e^{-it}}{2})^{a} (\frac{e^{it} - e^{-it}}{2i})^{b} (\frac{e^{ict} + e^{-ict}}{2}) dt \\ &= \sum_{l,s} \frac{(-1)^{b-s}}{2^{a+b+1} i^{b}} \int_{0}^{2\pi} {a \choose l} e^{itl - it(a-l)} {b \choose s} e^{its - it(b-s)} (e^{ict} + e^{-ict}) dt \\ &= \sum_{l,s} \frac{(-1)^{b/2-s} {a \choose l} {b \choose s}}{2^{a+b+1}} (\int_{0}^{2\pi} e^{it(2l-a+2s-b+c)} dt + \int_{0}^{2\pi} e^{it(2l-a+2s-b-c)} dt) \\ &= 2\pi \sum_{s} \frac{(-1)^{b/2+s}}{2^{a+b+1}} {b \choose s} \left[{a \choose (a+b-c)/2-s} + {a \choose (a+b+c)/2-s} \right]. \end{split}$$

A similar calculation yields the result for K(a, b, c).

Now we rewrite Corollary 2.2 in a more explicit form:

Theorem 3.2. For any $r, d, n \in \mathbb{N}$,

$$f_{r,d}(n+1) - f_{r,d}(n) = \frac{1}{2\pi} \int_0^{2\pi} \varphi^n(t) \sum_{j=0}^r [\binom{r}{j} q^j (1-q)^{r-j} (q(1-p)\cos(j+1-d)t - p(1-q)\cos(j-d)t) - q(1-p)i\sin(j+1-d)t + p(1-q)i\sin(j-d)t] dt,$$

where

$$\varphi(t) = 1 - p - q + 2pq + (p + q - 2pq)\cos t + i(p - q)\sin t.$$

Note that by Theorem 3.2, $f_{r,d}(n+1) - f_{r,d}(n)$ reduces to

$$\frac{1}{2\pi} \sum_{j=0}^{r} \binom{r}{j} q^{j} (1-q)^{r-j} (I_1 + I_2 + I_3 + I_4)$$

where the integrals I_k 's $(1 \le k \le 4)$ are defined as,

$$I_{1} = \int_{0}^{2\pi} \varphi^{n}(t)q(1-p)\cos(j+1-d)tdt$$

$$I_{2} = -\int_{0}^{2\pi} \varphi^{n}(t)p(1-q)\cos(j-d)tdt$$

$$I_{3} = -\int_{0}^{2\pi} \varphi^{n}(t)q(1-p)i\sin(j+1-d)tdt$$

$$I_{4} = \int_{0}^{2\pi} \varphi^{n}(t)p(1-q)i\sin(j-d)t)dt.$$

All results reduce to such integrals. We shall represent $f_{r,d}(n+1) - f_{r,d}(n)$ by the "basis" $\int_0^{2\pi} \cos^{2k} t dt$, $k \ge 0$. To do this, we partition the real parts of $\varphi^n(t)(q(1-p)\cos(j+1-d)t)$, etc, according to the "order" 2k, i.e., those of the form constant times $\cos^a t \sin^b t \cos(ct)$ or $\cos^a t \sin^b t \sin(ct)$ where $2k-1 \le a+b \le 2k$. The notation $[\cos^{2k} t]_I f$ means that in the expansion of f, we group all "homogeneous" terms (of form $\cos^a t \sin^b t \cos(ct)$ or $\cos^a t \sin^b t \sin(ct)$ where $2k-1 \le a+b \le 2k$) and take the ratio of the integrals $\frac{\sum_{a,b} \int_0^{2\pi} \cos^a t \sin^b t \cos(ct) dt}{\int_0^{2\pi} \cos^{2k} t dt}$ or $\frac{\sum_{a,b} \int_0^{2\pi} \cos^2 t t \sin^b t \sin(ct) dt}{\int_0^{2\pi} \cos^{2k} t dt}$ as the corresponding coefficient. For example, based on Lemma 3.1, we have

$$\begin{split} &[\cos^{2k}t]_{I}(\cos^{2k-1-2m}t\sin^{2m}t\cos(ct))\\ &= \frac{(2k)!!}{(2k-1)!!}\sum_{s}\frac{(-1)^{m+s}}{2^{2k}}\binom{2m}{s}(\binom{2k-1-2m}{(2k-1-c)/2-s} + \binom{2k-1-2m}{(2k-1+c)/2-s})),\\ &[\cos^{2k}t]_{I}(\cos^{2k-2m}t\sin^{2m}t\cos(ct))\\ &= \frac{(2k)!!}{(2k-1)!!}\sum_{s}\frac{(-1)^{m+s}}{2^{2k+1}}\binom{2m}{s}(\binom{2k-2m}{(2k-c)/2-s} + \binom{2k-2m}{(2k+c)/2-s})). \end{split}$$

Similarly we obtain the formulas for $[\cos^{2k} t]_I(\cos^{2k-2m} t \sin^{2m-1} t \sin(ct))$ and $[\cos^{2k} t]_I(\cos^{2k+1-2m} t \sin^{2m-1} t \sin(ct))$. Consequently, $[\cos^{2k} t]_I\{I_1\}$, etc, may be found and the following theorem follows. To keep the cleanness we omit the proof details.

Theorem 3.3. For $r, d \in \mathbb{N}$,

$$f_{r,d}(n+1) - f_{r,d}(n) = \frac{1}{2\pi} \sum_{j} {\binom{r}{j}} q^{j} (1-q)^{r-j} \sum_{k} a_{n,k}(j,d) \int_{0}^{2\pi} \cos^{2k}(t) dt,$$

where (i) $a_{n,k}(j,d) =$

$$\frac{n!}{(2k)!(n+1-2k)!} \frac{(2k)!!\binom{2k}{k+(j-d+1)/2}}{(2k-1)!!} (1-p-q+2pq)^{n-2k} (q(1-p)p(1-q))^k (q^{-1}(1-p)^{-1}p(1-q))^{\frac{j-d+1}{2}} \{(k+(j-d+1)/2)p+(n+1-k+(j-d+1)/2)q - (n+2+j-d)pq - (k+(j-d+1)/2)\}, if j-d is odd;$$

and (ii) $a_{n,k}(j,d) =$

$$\frac{n!}{(2k)!(n+1-2k)!} \frac{(2k)!!\binom{2k}{k+(j-d)/2}}{(2k-1)!!} (1-p-q+2pq)^{n-2k} (q(1-p)p(1-q))^k (q^{-1}(1-p)^{-1}p(1-q))^{\frac{j-d}{2}} \{(-n-1+k+(j-d)/2)p - (k-(j-d)/2)q + (n+1-j+d)pq + k\}, \text{ if } j-d \text{ is even.}$$

We conclude with three examples.

Example 3.1.

$$f_{1,1}(n+1) - f_{1,1}(n) = \sum_{k} a_{n,k}(1,1) \frac{1}{2\pi} \int_{0}^{2\pi} \cos^{2k}(t) dt,$$

where

$$a_{n,k}(1,1) = \frac{n!}{(2k)!(n+1-2k)!}(1-p-q+2pq)^{n-2k}2^{2k}(1-q)$$
$$(pq(1-p)(1-q))^k((-n-1+k)p-kq+(n+1)pq+k).$$

Example 3.2. For $m \in \mathbb{N}$,

(i)
$$f_{0,2m}(n+1) - f_{0,2m}(n) = \sum_{k} a_{n,k}(0,2m) \frac{1}{2\pi} \int_{0}^{2\pi} \cos^{2k}(t) dt$$
,

where $a_{n,k}(0, 2m) :=$

$$\frac{n!}{(2k)!(n+1-2k)!}(1-p-q+2pq)^{n-2k}\frac{(2k)!!\binom{2k}{k+m}}{(2k-1)!!}(pq(1-p)(1-q))^k$$
$$(q(1-p)p^{-1}(1-q)^{-1})^{-m}((-n-1+k-m)p-(k-m)q+(n+1+2m)pq+k).$$

(*ii*)
$$f_{0,2m+1}(n+1) - f_{0,2m+1}(n) = \sum_{k} a_{n,k}(0,2m+1) \frac{1}{2\pi} \int_{0}^{2\pi} \cos^{2k}(t) dt$$
,

where $a_{n,k}(0, 2m + 1) :=$

$$\frac{n!}{(2k)!(n+1-2k)!}(1-p-q+2pq)^{n-2k}\frac{(2k)!!\binom{2k}{k+m}}{(2k-1)!!}(pq(1-p)(1-q))^k$$
$$(q(1-p)p^{-1}(1-q)^{-1})^{-m}((k-m)p+(n+1-k-m)q+(n+1-2m)pq+m-k).$$

Theorem 3.3 actually provides a perspective to generalize the Legendre type representations discussed in [1].

Finally we exhibit the equivalence of Corollary 2.3 and (1.4).

Example 3.3.

$$f_{0,1}(n+1) - f_{0,1}(n) = \frac{1}{\pi} \int_0^\pi \psi^n(t)(q - pq - \sqrt{pq(1-p)(1-q)}\cos t)dt,$$

where $\psi(t) = 1 - p - q + 2pq + 2\sqrt{pq(1-p)(1-q)}\cos t$.

Proof. In fact, specializing Theorem 3.3,

$$f_{0,1}(n+1) - f_{0,1}(n) = \frac{1}{2\pi} \sum_{k=0}^{\lfloor (n+1)/2 \rfloor} a_{n,k}(0,1) \int_0^{2\pi} \cos^{2k} t dt$$
$$= \frac{1}{\pi} \int_0^{\pi} \sum_{k=0}^{\lfloor (n+1)/2 \rfloor} a_{n,k}(0,1) \cos^{2k} t dt$$
$$= \frac{1}{\pi} \int_0^{\pi} \psi^n(t) (q - pq - \sqrt{pq(1-p)(1-q)} \cos t) dt.$$

Thus we have rediscovered (1.4).

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Saturation number of nanotubes

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Abstract

In the present paper we are interested in the saturation number of closed benzenoid chains and certain families of nanotubes. The saturation number of a graph is the cardinality of a smallest maximal matching in the graph. The problem of determining the saturation number is related to the edge dominating sets and efficient edge dominating sets in a graph. We establish the saturation number of some closed benzenoid chains and C_4C_6 -tubes. Further, upper and lower bounds for the saturation number of armchair, zig-zag, $TUC_4C_8(S)$ and $TUC_4C_8(R)$ nanotubes are calculated.

Keywords: Saturation number, maximal matching, edge domination number, efficient edge dominating set, closed benzenoid chain, armchair nanotube, zig-zag nanotube, tubulene, $TUC_4C_8(S)$ nanotube, $TUC_4C_8(R)$ nanotube.

Math. Subj. Class.: 92E10, 05C70, 05C69

1 Introduction

The saturation number s(G) of a graph G is the cardinality of a smallest maximal matching in G. Maximal matchings serve as models of adsorption of dimers (those that occupy two adjacent atoms) to a molecule. It can occur that the double bonds in a molecule are not efficiently saturated by dimers, and therefore, their number is below the theoretical maximum. Hence, the saturation number provides an information on the worst possible

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case of adsorption. Besides in chemistry the saturation number has a list of interesting applications in engineering and networks.

A lot of work has been done on enumeration problems of different matchings in some chemical graphs, for example see [4, 5], but not much has been done on the smallest maximal matchings. Previous work on the saturation number includes research on benzenoid systems [8] and fullerenes [6, 1, 2]. Recent results on related concepts can be found in [3, 7].

The saturation number is closely related to the edge dominating sets. Actually, for any graph, the saturation number equals the edge domination number. The problem of determining the saturation number of a graph is NP-complete [13].

In this paper we show how to use an efficient edge dominating set in a graph to determine its saturation number. Also, the saturation number is established for certain closed benzenoid chains. Further, some bounds for the saturation number of different families of nanotubes are calculated.

2 Preliminaries

A matching M in a graph G is a set of edges of G such that no two edges from M share a vertex. A matching M is a maximum matching if there is no matching in G with greater cardinality. The cardinality of any maximum matching in G is denoted by $\nu(G)$ and called the matching number of G. If every vertex of G is incident with an edge of M, the matching M is called a perfect matching (in chemistry perfect matchings are known as Kekulé structures).

A matching M in a graph G is *maximal* if it cannot be extended to a larger matching in G. Obviously, every maximum matching is also maximal, but the opposite is generally not true. A matching M is a *smallest maximal matching* if there is no maximal matching in G with smaller cardinality. The cardinality of any smallest maximal matching in G is the *saturation number* of G.

The following lemma is very useful for proving lower bounds for the saturation number. The proof can be found online, but for the sake of completeness we provide it.

Lemma 2.1. Let G be a graph and let A and B be maximal matchings in G. Then $|A| \ge \frac{|B|}{2}$ and $|B| \ge \frac{|A|}{2}$.

Proof. First note that each edge in $B \setminus A$ can be adjacent to at most two edges in $A \setminus B$ since A is a matching. Moreover, each edge in $A \setminus B$ is adjacent to an edge in $B \setminus A$ by maximality of B. Therefore,

$$|A \setminus B| \le 2|B \setminus A|.$$

Hence, we obtain

$$|A| = |A \cap B| + |A \setminus B| \le 2|B \cap A| + 2|B \setminus A| = 2|B|.$$

 \square

The other inequality can be proven analogously.

An *independent set* is a set of vertices in a graph G, no two of which are adjacent. A *maximum independent set* is an independent set of largest possible cardinality for a given graph G. This cardinality is called the *independence number* of G, and denoted $\alpha(G)$. It is obvious that if M is a maximal matching and A is the set of endpoints of edges in

M, then the set of vertices in V(G) - A is an independent set of vertices in *G*. Therefore, $\alpha(G) \ge |V(G)| - 2s(G)$. Hence, we obtain another lower bound for the saturation number:

$$s(G) \ge \frac{|V(G)| - \alpha(G)}{2}.$$

Another graph invariant closely related to the saturation number is the edge domination number. An *edge dominating set* for a graph G is a subset $D \subseteq E(G)$ such that every edge not in D is incident to at least one edge in D. An *independent edge dominating set* is an edge dominating set in which no two elements are adjacent. An independent edge dominating set is in fact a maximal matching and a smallest independent edge dominating set is a smallest maximal matching, i.e. the cardinality of a smallest independent edge dominating set is the saturation number. The *edge domination number* of a graph G, $\gamma'(G)$, is the smallest cardinality taken over all edge dominating sets of G. If M is a smallest maximal matching of G, then M is also an edge dominating set, therefore $\gamma'(G) \leq s(G)$. For the contrary, if D is a smallest edge dominating set with k elements, we can construct a maximal matching of cardinality k (for the details see [13]). Therefore, $s(G) \leq \gamma'(G)$. Hence, for every graph G it holds

$$s(G) = \gamma'(G). \tag{2.1}$$



Figure 1: Illustration of a (4, -3)-type tubulene.

Since the paper focuses on nanotubes, we will formally define open-ended carbon nanotubes, also called *tubulenes* (see [11]). Choose any lattice point in the hexagonal lattice as the origin O. Let $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$ be the two basic lattice vectors. Choose a vector $\overrightarrow{OA} = n\overrightarrow{a_1} + m\overrightarrow{a_2}$ such that n and m are two integers and |n| + |m| > 1, $nm \neq -1$. Draw two straight lines L_1 and L_2 passing through O and A perpendicular to OA, respectively. By rolling up the hexagonal strip between L_1 and L_2 and gluing L_1 and L_2 such that Aand O superimpose, we can obtain a hexagonal tessellation \mathcal{HT} of the cylinder. L_1 and L_2 indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a *tubulene* T is defined to be the finite graph induced by all the hexagons of \mathcal{HT} that lie between c_1 and c_2 , where c_1 and c_2 are two vertex-disjoint cycles of \mathcal{HT} encircling the axis of the cylinder. The vector \overrightarrow{OA} is called the *chiral vector* of T and the cycles c_1 and c_2 are the two open-ends of T.

For any tubulene T, if its chiral vector is $n\overrightarrow{a_1} + m\overrightarrow{a_2}$, T will be called an (n,m)-type tubulene (see Figure 1). A tubulene T is called *zig-zag* if n = 0 or m = 0 and *armchair* if n = m.

3 Graphs with an efficient edge dominating set

One other concept is also very useful in studying the saturation number. A matching D of a graph G is called an *efficient edge dominating set* if for each edge $e \in E(G) \setminus D$ there is exactly one edge f in D such that e and f are incident (this concept is equivalent to the efficient dominating set in the line graph of G, for the details see [10]). Using the following theorem we can exactly determine the saturation number for some graphs.

Theorem 3.1. If a graph G has an efficient edge dominating set D, then

$$s(G) = |D|.$$

Proof. It follows from Equation 2.1 that $s(G) = \gamma'(G)$. Hence it is enough to show that $\gamma'(G) = |D|$ (see [9]).

Obviously, if D is an efficient edge dominating set then D is also an edge dominating set. Therefore, $\gamma'(G) \leq |D|$. Conversely, let P be a smallest edge dominating set and let $e \in D$. It follows that either $e \in P$ or there is an edge $f \in P$ such that e and f are incident. Therefore, for an edge $e \in D$ there always exists $f_e \in P$ such that $e = f_e$ or e and f_e are incident. It is also clear that since D is an efficient edge dominating set, for given edges e and e' in D, $e \neq e'$, it follows that $f_e \neq f_{e'}$. Hence, $|D| \leq |P| = \gamma'(G)$. The proof is complete.

Example 3.2. One infinite family of graphs with an efficient edge dominating set are C_4C_6 -tubes, which are constructed of cycles C_4 and C_6 - see Figure 2. Let T(p,q) be a C_4C_6 -tube with p layers of hexagons and with q hexagons in every layer. The set of double edges in Figure 2 is obviously an efficient edge dominating set of cardinality pq = 15. Therefore, by Theorem 3.1, the saturation number of T(p,q) is s(T(p,q)) = pq.



Figure 2: A C_4C_6 -tube T(3,5). Edges e_1 , e_2 and e_3 are joined with edges e'_1 , e'_2 and e'_3 , respectively.

For example, polyacenes and closed polyacenes are also such graphs (see Section 4). However, not many graphs posses an efficient edge dominating set.

4 Closed benzenoid chains

Recall that *benzenoid graphs* are 2-connected subgraphs of the hexagonal lattice such that every bounded face is a hexagon. The vertices lying on the border of the non-hexagonal face of a benzenoid graph are called *external*; other vertices, if any, are called *internal*. A benzenoid graph without internal vertices is called *catacondensed*. If no hexagon in a catacondensed benzenoid is adjacent to three other hexagons, we say that the benzenoid is a *chain*. In each benzenoid chain there are exactly two hexagons adjacent to one other hexagon; those two hexagons are called *terminal*, while any other hexagons are called *interior*. An interior hexagon is called *straight* if the two edges it shares with other hexagons are parallel, i.e., opposite to each other. If the shared edges are not parallel, the hexagon is called *kinky*. If all interior hexagons of a benzenoid chain are straight, we call the chain a *polyacene*.

Let B be a benzenoid chain with terminal hexagons h and h'. Let e = uv and e' = u'v' be edges of h and h', respectively, such that vertices u, v, u', v' have degree 2 in B. Furthermore, suppose that there exist a path from u to u' in the perimeter of B, which does not contain neither v nor v'. A graph obtained by identifying edges e and e' is called a *closed benzenoid chain*. For example see Figure 3.



Figure 3: A closed benzenoid chain. Edges e and e' are joined together.

Similar as before, a hexagon of a closed benzenoid chain is called *straight* if the two edges it shares with other hexagons are opposite to each other. If the shared edges are not parallel, the hexagon is called *kinky*.

Remark 4.1. Note that not every closed benzenoid chain is a tubulene in the sense of the definition in the preliminaries. In fact, if we consider benzenoid chain embedded in the hexagonal lattice, it is not difficult to see that a closed benzenoid chain is a tubulene if and only if the distance from u to u' in the hexagonal lattice is an even number and the edge e is parallel to e'.

In this section we compute the saturation number of some closed benzenoid chains. The following lemma claims that every closed benzenoid chain has a perfect matching.

Lemma 4.2. Let B be a closed benzenoid chain. Then B has a perfect matching.

Proof. Let G be a benzenoid chain from which B is obtained by identifying edges e and e'. Since every internal hexagon in G has exactly 4 edges on the perimeter and both terminal hexagons have 5 edges on the perimeter, there is always an even number of edges on the perimeter of G. Therefore, let M be a perfect matching of the perimeter of G such that $e \in M$. Obviously, M is a perfect matching of G. Now we consider two cases:

- 1. If $e' \in M$, then after identifying e and e' into the new edge f, the set $(M \setminus \{e, e'\}) \cup \{f\}$ is a perfect matching of B.
- 2. If $e' \notin M$, then after identifying e and e', the set $M \setminus \{e\}$ is a perfect matching of B.

 \square

Hence, we have seen that B has a perfect matching.

In the next proposition we prove a lower bound for the saturation number of closed benzenoid chains.

Proposition 4.3. Let B be a closed benzenoid chain with h hexagons. Then $s(B) \ge h$.

Proof. Let M be a perfect matching of B. Since there is 4h vertices in B and every edge in M covers exactly 2 vertices, perfect matching M contains 2h edges. Therefore, by Lemma 2.1, any maximal matching contains at least half of the number of edges in M. Hence, $s(B) \ge \frac{2h}{2} = h$.

A closed benzenoid chain *B* is called a *closed polyacene* (or a *hexagonal belt*) if it does not contain kinky hexagons (see Figure 4).



Figure 4: A maximal matching of a closed polyacene with 5 hexagons.

Proposition 4.4. Let B be a closed polyacene with h hexagons. Then s(B) = h.

Proof. Obviously, the set of vertical edges of B (see the edges in matching M from Figure 4) is an efficient edge dominating set and |M| = h. Therefore, by Theorem 3.1 it follows s(B) = h.

The following theorem completely characterizes closed polyacenes among closed benzenoid chains according to saturation number.

Theorem 4.5. Let B be a closed benzenoid chain with h hexagons. Then s(B) = h if and only if B is a closed polyacene.

Proof. Let B be a closed polyacene with h hexagons. It follows from Proposition 4.4 that s(B) = h.

For the converse suppose that B is a closed benzenoid chain with h hexagons and s(B) = h. Let M be a maximal matching with h edges. Those edges cover exactly 2h vertices. Let A be the set of vertices that are not covered by edges in M. Since B has 4h vertices, there are 2h vertices in A. Since M is a maximal matching, no two vertices in A are adjacent. Let A' be the set of edges that are incident to vertices in A. Since the degree of every vertex in B is at least 2, it follows $|A'| \ge 4h$. But $A' \subseteq E(B) \setminus M$ and therefore, $|A'| \le 5h - h = 4h$. Hence, every vertex in A has degree 2 and every hexagon contains exactly two elements of A. Therefore, every hexagon of B has 2 non-adjacent vertices of degree 2. It follows that B is a closed polyacene.
In the next theorem we compute the saturation number of closed benzenoid chains with exactly one kinky hexagon. However, such closed benzenoid chain is never a tubulene since the distance between u and u' is odd.

Theorem 4.6. Let B be a closed benzenoid chain with h hexagons such that exactly one of them is a kinky hexagon. Then s(B) = h + 1.

Proof. Let M be the set of edges in B that lie on exactly two hexagons. Moreover, let one other edge of the kinky hexagon be in M. Then it is easy to see that M is a maximal matching and therefore, $s(B) \le h + 1$.

Since B is not a closed polyacene, $s(B) \ge h + 1$ and the proof is complete. \Box

Proposition 4.7. Let B be a closed benzenoid chain with exactly two kinky hexagons which are consecutive. Then s(B) = h + 1.

Proof. Let M be a maximal matching with h+1 edges from Figure 5. Hence, $s(B) \le h+1$.



Figure 5: A closed benzenoid chain with two consecutive kinky hexagons and its maximal matching.

Since B is not a closed polyacene, $s(B) \ge h + 1$ and the proof is complete.

5 Zig-zag tubulenes



Figure 6: Zig-zag tubulene ZT(3, 4).

Let T be a zig-zag tubulene such that c_1, c_2 are the shortest possible cycles encircling the axis of the cylinder (see Figure 6). If T has n layers of hexagons, each containing exactly h hexagons, then we denote it by ZT(n,h). Note that ZT(n,h) is a (0,h) or (h,0)-type tubulene. First we show an upper bound for the saturation number of ZT(n,h), which is essentially of order $\frac{2nh}{3}$.

Theorem 5.1. Let ZT(n, h) be a zig-zag tubulene. Then

$$s(ZT(n,h)) \le \begin{cases} \frac{h(2n+3)}{3}, & 3 \mid n\\ \frac{h(2n+1)}{3}, & 3 \mid n-1\\ \frac{h(2n+2)}{3}, & 3 \mid n-2. \end{cases}$$

Proof. Let ZT(n,h) be drawn in a plane such that some edges are vertical and such that cycles c_1 and c_2 lie on the bottom and on the top. To show an upper bound, we construct a maximal matching of ZT(n,h). This maximal matching is obtained by alternating two different layers of edges - vertical and non-vertical. We start with vertical edges in the first layer (at the bottom of a tubulene) and we need 2 layers of edges for every 3 layers of hexagons. Obviously we have exactly h edges in every layer. Now consider three different cases.



Figure 7: A maximal matching of zig-zag tubulenes. Lines L_1 and L_2 are joined together.

- 1. If $3 \mid n$: then we need $\frac{2n}{3}$ layers of edges and one additional layer at the top of a tubulene. Hence, we obtain $\frac{h(2n+3)}{3}$ edges in M. See Figure 7(a).
- 2. If $3 \mid n 1$: in this case we need $\frac{2(n-1)}{3}$ layers of edges and we have to add one vertical layer. Hence, $|M| = \frac{h(2n+1)}{3}$. See Figure 7(b).

3. If $3 \mid n-2$: in this case we have $\frac{2(n-2)}{3}$ layers of edges and we have to add 2 additional layers (one vertical and one non-vertical) to obtain a maximal matching. Hence, $|M| = \frac{h(2n+2)}{3}$. See Figure 7(c).

It is obvious that in such a way we always obtain a maximal matching. Therefore, the proof is complete. $\hfill \Box$

In the next lemma we prove a lower bound.

Lemma 5.2. Let ZT(n,h) be a zig-zag tubulene. Then

$$s(ZT(n,h)) \ge \frac{(n+1)h}{2}.$$

Proof. Obviously ZT(n,h) has a perfect matching with (n + 1)h edges. Therefore, by Lemma 2.1, any maximal matching contains at least $\frac{(n+1)h}{2}$ edges.

Theorem 5.1 and Lemma 5.2 together imply the following corollary.

Corollary 5.3. Let ZT(n, h) be a zig-zag tubulene. Then

$$\frac{(n+1)h}{2} \le s(ZT(n,h)) \le \begin{cases} \frac{h(2n+3)}{3}, & 3 \mid n\\ \frac{h(2n+1)}{3}, & 3 \mid n-1\\ \frac{h(2n+2)}{3}, & 3 \mid n-2. \end{cases}$$

6 Armchair tubulenes

Let T be an armchair tubulene such that c_1 and c_2 are the shortest possible cycles encircling the axis of the cylinder and such that there is the same number of hexagons in every column of hexagons (see Figure 8). If T has n vertical layers of hexagons, each containing exactly p hexagons, then we denote it by AT(n,p). Obviously, n must be an even number. Note that AT(n,p) is a $(\frac{n}{2}, \frac{n}{2})$ -type tubulene. In the following theorem we prove an upper bound for the saturation number of AT(n,p).

Theorem 6.1. Let AT(n, p) be an armchair tubulene. Then

$$s(AT(n,p)) \le \begin{cases} \frac{2n(p+1)}{3}, & 3 \mid n\\ \frac{(2n+1)(p+1)}{3}, & 3 \mid n-1\\ \frac{2(n+2)(p+1)}{3}, & 3 \mid n-2. \end{cases}$$

Proof. Let AT(n, p) be drawn in a plane such that some edges are horizontal and such that cycles c_1 and c_2 lie on the bottom and on the top. To show an upper bound, we construct a maximal matching of AT(n, p). This maximal matching is obtained by alternating two different columns of edges - horizontal and non-horizontal. We start with horizontal edges in the first column (at the left side of a tubulene) and we need 2 columns of edges for every 3 columns of hexagons. Obviously we have exactly p + 1 edges in every column. Now consider three different cases.

1. If $3 \mid n$: then we need $\frac{2n}{3}$ columns of edges to obtain a maximal matching. Hence, we obtain $\frac{2n(p+1)}{3}$ edges in M. See Figure 8.



Figure 8: A maximal matching of armchair tubulene AT(6,4). Curves L_1 and L_2 are joined together.

- 2. If $3 \mid n-1$: in this case we need $\frac{2(n-1)}{3}$ columns of edges and we have to add one horizontal column. Hence, $|M| = \frac{(2n+1)(p+1)}{3}$.
- 3. If 3 | n 2: in this case we have $\frac{2(n-2)}{3}$ columns of edges and we have to add 2 additional horizontal layers of edges to obtain a maximal matching. Hence, $|M| = \frac{2(n+2)(p+1)}{3}$. See Figure 9.



Figure 9: A maximal matching of armchair tubulene AT(8,4). Curves L_1 and L_2 are joined together.

It is obvious that in such a way we always obtain a maximal matching. Therefore, the proof is complete. $\hfill \Box$

In the next lemma we prove a lower bound.

Lemma 6.2. Let AT(n, p) be an armchair tubulene. Then

$$s(AT(n,p)) \ge \frac{n(p+1)}{2}.$$

Proof. Obviously AT(n, p) has a perfect matching with n(p + 1) edges (we can put all horizontal edges in a perfect matching). Therefore, by Lemma 2.1, any maximal matching contains at least $\frac{n(p+1)}{2}$ edges.

Theorem 6.1 and Lemma 6.2 together imply the following corollary.

Corollary 6.3. Let AT(n, h) be an armchair tubulene. Then

$$\frac{n(p+1)}{2} \le s(AT(n,p)) \le \begin{cases} \frac{2n(p+1)}{3}, & 3 \mid n\\ \frac{(2n+1)(p+1)}{3}, & 3 \mid n-1\\ \frac{2(n+2)(p+1)}{3}, & 3 \mid n-2. \end{cases}$$

7 $TUC_4C_8(S)$ nanotubes

A C_4C_8 net is a trivalent pattern made by alternating squares C_4 and octagons C_8 . Identifying some edges in such a lattice we obtain a $TUC_4C_8(S)$ nanotube (see Figure 10). Such nanotubes could appear by successive low energy Stone-Wales edge flipping [12] in polyhex nanotubes. In this section we prove an upper and a lower bound for the saturation number of $TUC_4C_8(S)$ nanotubes. We denote nanotube with q layers and p squares (or octagons) in every layer with TS(p,q).



Figure 10: TS(4, 4) with a maximal matching.

Theorem 7.1. Let TS(p,q) be a $TUC_4C_8(S)$ nanotube. Then

$$s(TS(p,q)) \le \begin{cases} \frac{4pq}{3}, & 3 \mid p \\ \frac{(4p+2)q}{3}, & 3 \mid p-1 \\ \frac{(4p+1)q}{3}, & 3 \mid p-2. \end{cases}$$

Proof. To prove the theorem we construct a maximal matching for nanotube TS(p,q). In every layer we put every third edge in the matching M. In layer with k = 1 we put the first edge in M and in layer with k = 2 we start with the second edge (see Figure 10). Next, in the third layer, we repeat the first layer.

Now consider the following cases:

- 1. If $3 \mid p$, then we have $\frac{4pq}{3}$ edges in M.
- 2. If 3 | p-1: in this case we have $\frac{4(p-1)q}{3}$ edges and we have to add 2 additional edges in every layer to obtain a maximal matching. Hence, $|M| = \frac{4(p-1)q}{3} + 2q = \frac{(4p+2)q}{3}$.
- 3. If $3 \mid p-2$: in this case we have $\frac{4(p-2)q}{3}$ edges and we have to add 3 additional edges in every layer to obtain a maximal matching. Hence, $|M| = \frac{4(p-2)q}{3} + 3q = \frac{(4p+1)q}{3}$.

In the next proposition we prove a lower bound.

Lemma 7.2. Let TS(p,q) be a $TUC_4C_8(S)$ nanotube. Then $s(TS(p,q)) \ge pq$.

Proof. First notice that TS(p,q) always has a perfect matching. For example, we can take every second edge in every layer. Since the number of vertices in TS(p,q) is 4pq, a perfect matching of TS(p,q) contains 2pq edges, since every edge covers two vertices. Now it follows from Lemma 2.1 that every maximal matching contains at least pq edges. Hence, $s(TS(p,q)) \ge pq$.

Theorem 7.1 and Lemma 7.2 together imply the next corollary.

Corollary 7.3. Let TS(p,q) be a TUC_4C_8 nanotube. Then

$$pq \le s(TS(p,q)) \le \begin{cases} \frac{4pq}{3}, & 3 \mid p \\ \frac{(4p+2)q}{3}, & 3 \mid p-1 \\ \frac{(4p+1)q}{3}, & 3 \mid p-2. \end{cases}$$

8 $TUC_4C_8(R)$ nanotubes

Again we begin with a C_4C_8 net, but this time squares are not in the horizontal position. Identifying some edges in such a lattice we obtain a $TUC_4C_8(R)$ nanotube (see Figure 11). In this section we prove an upper and a lower bound for the saturation number of $TUC_4C_8(R)$ nanotubes. We denote a nanotube with p octagons in every layer and q octagons in every column with TR(p, q).



Figure 11: TR(4,3) with a maximal matching. Left and right side are joined.

Theorem 8.1. Let TR(p,q) be a $TUC_4C_8(R)$ nanotube. Then

$$s(TR(p,q)) \le \begin{cases} \frac{4qp}{3} + p, & 3 \mid q\\ \frac{4(q-1)p}{3} + 3p, & 3 \mid q-1\\ \frac{4(q-2)p}{3} + 4p, & 3 \mid q-2. \end{cases}$$

Proof. We construct a maximal matching M for nanotube TR(p,q). For every 3 rows of octagons we put 4 layers of edges in the matching M. Of course, every layer contains exactly p edges. See Figure 11.

Now consider the following cases:

- 1. If $3 \mid q$: in this case we have $\frac{4qp}{3}$ edges in M and we need one additional layer of horizontal edges at the top see Figure 11.
- 2. If 3 | q-1: in this case we have $\frac{4(q-1)p}{3}$ edges and we have to add 3 additional layers of edges to obtain a maximal matching. Hence, $|M| = \frac{4(q-1)p}{3} + 3p$.
- 3. If $3 \mid q-2$: in this case we have $\frac{4(q-2)p}{3}$ edges and we have to add 4 additional layers of edges to obtain a maximal matching. Hence, $|M| = \frac{4(q-2)p}{3} + 4p$.

In the next lemma we prove a lower bound.

Lemma 8.2. Let TR(p,q) be a $TUC_4C_8(R)$ nanotube. Then $s(TR(p,q)) \ge p(q+1)$.

Proof. First notice that TR(p,q) always has a perfect matching. Since the number of vertices in TR(p,q) is 4p(q+1), a perfect matching of TR(p,q) contains 2p(q+1) edges, since every edge covers two vertices. Now it follows from Lemma 2.1 that every maximal matching contains at least p(q+1) edges. Hence, $s(TR(p,q)) \ge p(q+1)$.

Theorem 8.1 and Lemma 8.2 together imply the next corollary.

Corollary 8.3. Let TR(p,q) be a $TUC_4C_8(R)$ nanotube. Then

$$p(q+1) \le s(TR(p,q)) \le \begin{cases} \frac{4qp}{3} + p, & 3 \mid q\\ \frac{4(q-1)p}{3} + 3p, & 3 \mid q-1\\ \frac{4(q-2)p}{3} + 4p, & 3 \mid q-2. \end{cases}$$

Concluding remarks

In the paper we have established some bounds for the saturation number of certain families of nanotubes. However, the exact values are unknown. There are still many open problems regarding the saturation number of molecular graphs, for example coronenes, coronoids, polyomino chains, etc.

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From NMNR-coloring of hypergraphs to homogenous coloring of graphs

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Abstract

An NMNR-coloring of a hypergraph is a coloring of vertices such that in every hyperedge at least two vertices are colored with distinct colors, and at least two vertices are colored with the same color. We prove that every 3-uniform 3-regular hypergraph admits an NMNR-coloring with at most 3 colors. As a corollary, we confirm the conjecture that every bipartite cubic graph admits a 2-homogenous coloring, where a k-homogenous coloring of a graph G is a proper coloring of vertices such that the number of colors in the neigborhood of any vertex equals k. We also introduce several other results and propose some additional problems.

Keywords: Homogenous coloring, mixed hypergraph, bi-hypergraph, NMNR-coloring. Math. Subj. Class.: 05C15, 05C65

1 Introduction

In this paper we continue the study of homogenous colorings of graphs initiated in [8], specifically focusing on regular bipartite graphs. We consider only finite graphs and hype-graphs. Every graph G = (V, E) is determined by the set of vertices V = V(G) and the set of edges E = E(G). For any undefined notions used in the paper we refer to the standard monograph [1]. Given a vertex-coloring φ of a graph G, the *palette of a vertex* v, P(v), is the set of colors appearing in the neighborhood N(v) of v, i.e. $P(v) = \{\varphi(u) \mid u \in N(v)\}$. The cardinality of P(v) is denoted by p(v).

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A *k*-homogenous coloring of a graph G is a proper coloring of its vertices such that the palette of every vertex is of size k. The smallest number of colors (if it exists), for which G admits a k-homogenous coloring is called k-homogenous chromatic number and denoted $\chi_{h}^{k}(G)$.

As observed in [8], only bipartite graphs admit a 1-homogenous coloring: every proper coloring of a bipartite graph with two colors is admissible. Additionally, every *d*-regular graph admits a *d*-homogenous coloring: assigning distinct color to every vertex does the job. In fact, the *d*-homogenous chromatic number of a *d*-regular graph *G* is equal to the chromatic number of the square graph G^2 , i.e. the graph with $V(G^2) = V(G)$ where two vertices are adjacent if they are at distance at most 2 in *G*.

In the other cases, the question whether a graph admits a homogenous k-coloring becomes harder. In particular, two types of problems arise: (a) for a given integer k and a graph G, does G admit a k-homogenous coloring; and (b) if (a) is answered in affirmative, what is the value of $\chi_{b}^{k}(G)$?

A *d*-regular graph *G* is *completely homogenous* if it admits a *k*-homogenous coloring for every $k, 1 \le k \le d$. The motivation for this paper was given by the following conjecture.

Conjecture 1.1 (Janicová, 2015). Every cubic bipartite graph is completely homogenous.

As the cases with $k \in \{1,3\}$ are trivial as remarked above, it only remains to prove that there exists a 2-homogenous coloring of every cubic bipartite graph. To prove this, we make use of the results from the rich field of hypergraph colorings.

A hypergraph $H = (V, \varepsilon)$ is determined by a set of vertices V = V(H) and a set of (hyper)edges $\varepsilon = \varepsilon(H)$, where every edge is an arbitrary subset of vertices. For an edge e, let V(e) denote the set of vertices incident to e. We say that H is *k*-uniform if every edge is incident to exactly k vertices, *k*-regular if every vertex is contained in exactly k edges, and *linear* if every two edges share at most one vertex.

Similarly as in the case of graphs, by a *coloring* φ of a hypergraph H we mean an assignment of colors to the vertices of H. For an edge $e \in \varepsilon$, the palette of e, P(e), is the set of colors given to the vertices incident to e. Again, we define p(e) = |P(e)|. We say that an edge e of H is monochromatic if p(e) = 1, i.e. all the vertices incident to e are colored with the same color, and an edge is rainbow if p(e) = |V(e)|, i.e. no two vertices of e are colored with the same color. A coloring of H is non-monochromatic non-rainbow coloring (or a NMNR-coloring in short) if there is neither monochromatic edge nor rainbow edge in H.

The notion of NMNR-colorings arose from more general concepts of color-bounded hypergraphs introduced by Bujtás and Tuza in [2], where for every edge the lower and the upper bound on the palette size is given, and pattern hypergraphs introduced by Dvořák et al. in [6], where every hyperedge is assigned a set of admissible colors. Color-bounded hypergraphs generalize many coloring concepts in hypergraphs; they were inspired by the work of Drgas-Burchardt and Łazuka [5], who only set the lower bounds on the sizes of palettes, and the notion of mixed hypergraphs introduced by Voloshin [12, 13]. A *mixed hypergraph M* consists of the set of vertices and two families of edges, the C-edges and the D-edges. A coloring of the vertices of M is *proper* if no C-edge is rainbow and no D-edge is monochromatic. Study of mixed hypergraphs received considerable attention in the last two decades¹ (cf. [10]). Interestingly, colorings of mixed hypergraphs are strongly related

¹See also the web-page http://spectrum.troy.edu/voloshin/mh.html for more details.

to various types of graph colorings as shown e.g. by Král' in [9].

If every edge of M is a C-edge and a D-edge, then M is called a *bi-hypergraph*. When a mixed hypergraph M is a bi-hypergraph, then a proper coloring of M is precisely an NMNR-coloring. We refer an interested reader to [3] and [4] for the most recent results in this field.

Now, we present the main results of the paper, thus solving Conjecture 1.1 in affirmative.

Theorem 1.2. Every cubic bipartite graph G admits a 2-homogenous coloring. Moreover,

$$\chi^2_h(G) \le 6$$
 .

Theorem 1.2 is in fact a corollary of the following theorem:

Theorem 1.3. Every 3-regular 3-uniform hypergraph admits an NMNR-coloring with at most 3 colors.

The rest of the paper is structured as follows: in Section 2, we introduce some auxiliary results we use in the proofs of the main results. In Section 3, we prove Theorem 1.3, and in the last section, we present several additional results and conclude the paper with some open problems.

2 Auxiliaries

In this section we present some auxiliary results. First, we show how the problem of 2homogenous coloring of a cubic bipartite graphs can be modeled with an NMNR-coloring of 3-uniform hypergraphs. Let G be a cubic bipartite graph and H_G be a hypergraph with the vertex set $V(H_G) = V(G)$ and the edge set $\varepsilon(H_G) = \{N(v) | v \in V(G)\}$. Clearly, H_G is 3-uniform, hence an NMNR-coloring of H_G is a coloring assigning exactly two different colors to the vertices incident to every edge of H_G , meaning that the palette of every vertex in G is of size 2. Hence, we immediately obtain the next proposition.

Proposition 2.1. Every cubic bipartite graph G admits a 2-homogenous coloring if and only if the hypergraph H_G admits an NMNR-coloring.

Note that the bipartiteness of G is necessary to ensure that the coloring of G is proper, as we now see. The hypergraph H_G is not connected, since no pair of vertices from distinct parts of G is incident to a common edge of H_G . Let φ be an NMNR-coloring of H_G . Then, a 2-homogenous coloring φ' of G is obtained by assigning the color $(i, \varphi(v))$ to the vertex v in G, where $i \in \{1, 2\}$ denotes the part of G the vertex v belongs to. This in particular means that at most twice the number of colors used for an NMNR-coloring of H_G are used for a 2-homogenous coloring of G. On the other hand, each 2-homogenous coloring of H_G .

As G is cubic, H_G is also 3-regular, which enables us to use the following results on bipartite hypergraphs. A hypergraph is *bipartite* or 2-*colorable* if it admits a coloring of vertices with 2 colors such that no edge is monochromatic.

Theorem 2.2 (Henning and Yeo, 2013). For an integer $k \ge 4$, every k-regular k-uniform hypergraph is bipartite.

The proof of Theorem 2.2 was given in [7], but the result was mentioned already earlier in [11].

For k = 3, there exist infinite families of non-bipartite 3-regular 3-uniform hypergraphs (cf. [7]), the Fano plane being the most famous example (see Fig. 1). The result however holds if the hypergraph is not regular.

Theorem 2.3 (Henning and Yeo, 2013). *Every connected* 3-*uniform hypergraph with maximum degree at most* 3 *that is not* 3-*regular is bipartite.*



Figure 1: The hypergraph of Fano plane is not bipartite.

Theorem 2.3 immediately implies the following corollary.

Corollary 2.4. Every connected 3-regular 3-uniform hypergraph is either bipartite or becomes bipartite after deleting any edge from it.

3 Proof of Theorem 1.3

First we prove a lemma about NMNR-colorings of linear 3-regular 3-uniform hypergraphs.

Lemma 3.1. Every linear 3-regular 3-uniform hypergraph admits an NMNR-coloring with at most three colors.

Proof. Let H be a connected 3-regular 3-uniform linear hypergraph. By Corollary 2.4, H is either bipartite, or H - e is bipartite, for any $e \in E(H)$. In the former case, the lemma trivially holds, so we may asume that H is not bipartite.

We prove the lemma by contradiction. Suppose that H does not admit an NMNRcoloring with at most three colors. Let $e_s = (u, v, w)$ be an edge of H and φ be a 2coloring (with colors 0 and 1) of $H - e_s$. Consequently, e_s is monochromatic, and, without loss of generality, we may assume that $\varphi(u) = \varphi(v) = \varphi(w) = 0$.

We distinguish two types of edges of H regarding φ : an edge e is of type 0 if two vertices of e are colored with 0, and the third vertex is colored with 1, and analogously, e is of type 1, if one of its vertices is colored with 0, and the other two are colored with 1. Define $\overline{\varphi}(v) = 1 - \varphi(v)$ and call it the *complementary color* of a vertex v.

First, we discuss the types of the edges incident to the vertices of a monochromatic edge.

Claim 3.2. Every vertex incident to a monochromatic edge is incident to an edge of type 0 and an edge of type 1.

Proof: Let e be a monochromatic edge of H. Without loss of generality, we may assume all the vertices of e are of color 0. Suppose to the contrary that there is a vertex of e, say x, incident to two edges of the same type. If x is incident to two edges of type 0, then we can recolor x to 1 (see the left case in Fig. 2), obtaining a 2-coloring of H, a contradiction. In the case when x is incident to two edges of type 1, we color x with the color 2 (see the



Figure 2: Recoloring of a vertex x incident to two edges of type 0 (on the left), and type 1 (on the right). Vertices of color 0 are depicted with empty circles, vertices of color 1 with full, and the vertex of color 2 as a cross.

right case in Fig. 2). Notice that all three edges incident to x are now bichromatic, and so we obtain an NMNR-coloring of H with at most 3 colors, a contradiction.

An alternating chain $C = e_0 v_1 e_1 v_2 e_2 \dots e_{k-1} v_k$ with respect to the coloring φ , is a sequence of vertices and edges, where e_0 is a monochromatic edge incident to v_1 , the vertices v_i, v_{i+1} are incident to the edge e_i , for $1 \le i \le k-1$, and e_i is of type $\overline{\varphi}(v_i)$. The third vertex incident to e_i is denoted v'_{i+1} . We say that an edge e, distinct from the edges of C, is a bow edge for C if at least two of its vertices are incident to some edges of C. An alternating chain C is wrapped if one of the vertices v_k and v'_k , say v_k , is incident to some bow edge $e_k = (v_k, x, y)$ and there is no bow edge for the alternating chain $C' = e_0 v_1 e_1 v_2 e_2 \dots e_{k-2} v_{k-1}$. Consequently, if, say, x is incident to e_i , then y is not incident to any edge of C, as H is linear and C' does not have bow edges.

In the following claim, we discuss the edges incident to the vertices of alternating chains without bow edges.

Claim 3.3. Let $C = e_0v_1e_1v_2e_2 \dots e_{\ell-1}v_\ell$ be an alternating chain without bow edges. Then, for every e_i , $1 \le i \le \ell - 1$, each of the vertices v_{i+1} and v'_{i+1} is incident to another edge of the same type as e_i , and an edge of the opposite type.

Proof: Suppose to the contrary, that there exists $i, 1 \le i \le l - 1$, for which the claim does not hold and choose the smallest such i. Then, we recolor each $v_j, 1 \le j \le i$, with its complementary color, and obtain a 2-coloring of H with precisely one monochromatic edge e_i , due to minimality of i. By applying Claim 3.2 to e_i and v_{i+1} or v'_{i+1} , we obtain a contradiction on non-bipartiteness of H.

From Claims 3.2 and 3.3, and the fact that H is finite, it directly follows that there exists a wrapped alternating chain $C = e_s v_1 e_1 v_2 e_2 \dots e_{k-1} v_k$, for some $k \ge 2$ in H starting in some vertex of e_s , say $u = v_1$. In what follows, we show that we can recolor some vertices of H using colors 0, 1, and 2 to obtain an NMNR-coloring with at most three colors. At every step of recoloring, at most one edge of H is monochromatic and the other ones are bichromatic. Note that, for simplicity, we always adjust the coloring φ , so φ changes after every recoloring. Let $i, 0 \le i \le k - 2$, be the smallest integer such that the edge e_i is incident to a vertex of the edge $e_k = (v_k, x, y)$. Let x be the vertex incident to the edges e_i and e_k . Additionally, denote the edge incident to v_k distinct from e_{k-1} and e_k by e_{k+1} . It is possible that e_{k+1} is also incident to some vertex of C, but, by the minimality of i, it may be incident only to some vertex incident to the edges e_j , for $j \ge i$. As H is linear, e_{k+1} is not incident to x.

First, recolor all the vertices v_j , for $1 \le j \le i$, with the color $\overline{\varphi}(v_j)$. Note that only e_i becomes a monochromatic edge (see Fig. 3). Next, consider two cases regarding the vertex



Figure 3: In a wrapped alternating chain we recolor the vertices from v_1 to v_i to their complementary colors, where e_i is the edge to which e_k is wrapped.

- x. In both cases, we may, without loss of generality, assume that $\varphi(v_k) = 0$.
 - (i) $x = v_{i+1}$. Suppose first that $\varphi(x) = 0$. Then, $\varphi(y) = 1$, for otherwise e_k would be monochromatic. If the edge e_{k+1} is of type 0, then recolor the vertex x to 2 and the vertex v_k to 1. If the edge e_{k+1} is of type 1, then we consider two subcases. If i+2 < k-1, then recolor the vertices x and v_k to 2, and the vertex v_{k-1} to 0. Otherwise, if i+2 = k-1, recolor x to 1, v_{k-1} to 0, and v_k to 2. As v_{k-1} is not incident to e_{k+1} , φ is an NMNR-coloring in both subcases.

We may thus assume that $\varphi(x) = 1$. By Claim 3.3, we have that $\varphi(y) = 1$. Note that i + 1 < k - 1 in this case as H is linear. If the edge e_{k+1} is of type 1, then recolor x and v_k to 2, and v_{k-1} to 0. In the case when e_{k+1} is of type 0, recolor x to 2, and v_k to 1. This establishes the case (i).

(*ii*) $x = v'_{i+1}$. Suppose that $\varphi(x) = 0$. As above, $\varphi(y)$ must be 1. Note that by Claim 3.2, the third edge x is incident to is of type 1. If the type of e_{k+1} is 0, then recolor x to 2 and v_k to 1. If the type of e_{k+1} is 1, then recolor the vertices x and v_k to 2, and the vertex v_{k-1} to 0.

Therefore, we may assume that $\varphi(x) = 1$. Suppose first that $\varphi(y) = 1$. Then, the third edge incident to x is of type 0. If e_{k+1} is of type 0, then recolor v_k to 1, and x

to 2. If e_{k+1} is of type 1, then recolor v_{k-1} to 0 and v_k to 2, and, in the case when i+1 < k-1, recolor also x to 2.

Suppose now that $\varphi(y) = 0$. Then, the third edge incident to x is of type 1. If e_{k+1} is of type 0, then recolor v_k to 1, and x to 0. Therefore, we may assume that the type of e_{k+1} is 1. Then, we recolor v_k to 2, and x and v_{k-1} to 0.

This establishes the lemma.

Now, we are ready to prove Theorem 1.3 by considering non-linear 3-regular 3-uniform graphs.

Proof of Theorem 1.3. We prove the theorem by contradiction. Let H be a 3-regular 3uniform hypergraph with the minimum number of vertices such that it does not admit an NMNR-coloring with at most 3 colors. By Lemma 3.1, H is not linear. Thus, we may assume that there exists a pair of edges $e, f \in E(H)$ having at least two vertices in common. If e and f are incident to the same three vertices, then H - e is bipartite by Corollary 2.3. Consequently, H is bipartite also and the theorem holds.

Hence, it remains to consider the case where e and f are incident to precisely two common vertices. Let e = (u, v, w) and f = (v, w, z). Suppose first that there is another edge g = (v, w, x) of H incident to the vertices v and w. Then, let H^* be the hypergraph obtained from H by replacing the edges e, f and g with an edge $e^* = (u, z, x)$ and removing the vertices v and w. By the minimality of H, there exists an NMNR-coloring φ^* of H^* with at most 3 colors. Without loss of generality, we may assume that $\varphi^*(u) = \varphi^*(z) = 0$ and $\varphi^*(x) = 1$. However, we can obtain an NMNR-coloring of H from φ^* by coloring the vertex v with 0 and w with 1.

Thus, we may assume that there is no edge of H, apart from e and f, incident to both v and w. Now, let H^* be the hypergraph obtained from H by identifying the edges e and f into an edge $e^* = (u, v^*, z)$ (where v^* corresponds to the vertices v and w in H). Again, since H^* is smaller than H, there exists an NMNR-coloring φ^* of H^* with at most 3 colors. In what follows, we show that φ^* can be extended to the vertices v and w. Denote the third edge of H containing v (resp. w) by g = (a, b, v) (resp. h = (w, c, d)). There are three possible configurations of g and h (up to symmetry) in terms of the vertices a, b and c, d, namely:

- (*i*) g = (a, u, v), h = (w, z, c);
- (ii) g = (a, u, v), h = (w, c, d), with $d \neq z$; and
- (*iii*) g = (a, b, v), h = (w, c, d), with $b \neq u, d \neq z$.

Note also that it is possible that some vertices of g and h coincide.

Without loss of generality, we may again assume that the vertices of e^* are colored by the colors 0 and 1 only in φ^* . Clearly, if $\varphi^*(u) = \varphi^*(z) = 1$ and $\varphi^*(v^*) = 0$, then we color both, v and w, with 0 and obtain an NMNR-coloring of H with at most 3 colors. So, we may assume that $\varphi^*(v^*) = 0$ and either $\varphi^*(u) = 0$ and $\varphi^*(z) = 1$, or $\varphi^*(u) = 1$ and $\varphi^*(z) = 0$. In both cases, if $\{\varphi^*(a), \varphi^*(b)\} \neq \{1\}$ and $\{\varphi^*(a), \varphi^*(b)\} \neq \{0, 2\}$, then color v with 1 and w with 0. Otherwise, if $\{\varphi^*(c), \varphi^*(d)\} \neq \{1\}$ and $\{\varphi^*(c), \varphi^*(d)\} \neq \{0, 2\}$, then color v with 0 and w with 1. In the remaining cases, i.e. when $\{\{\varphi^*(a), \varphi^*(b)\}, \{\varphi^*(c), \varphi^*(d)\}\} \in \{\{1\}, \{0, 2\}\}$, color v and w with the color 2. It is easy to verify that such a coloring results in an NMNR-coloring of H with at most 3 colors, which establishes the theorem. \Box

 \square

Finally, from Theorem 1.3, we derive the proof of Theorem 1.2.

Proof of Theorem 1.2. Let G be a cubic bipartite graph and H_G the 3-regular 3-uniform hypergraph H_G , whose existence is guaranteed by Proposition 2.1. By Theorem 1.3, there exists an NMNR-coloring of H_G with at most 3 colors, and thus also a 2-homogenous coloring of G with at most 6 colors.

4 Conclusion

We have shown that every cubic bipartite graph G is completely homogenous and that $\chi_h^2(G) \leq 6$. For the latter, we used a simple construction of coloring obtained by NMNR-coloring with at most 3 colors of the hypergraph H_G modeling the neighborhoods in two parts of G. At least 3 colors must be used to color H_G , but one does not always need to double the number of colors to guarantee that the coloring of G is proper. In fact, we believe that the following holds.

Conjecture 4.1. Let G be a cubic bipartite graph. Then

$$\chi_h^2(G) \le 4$$
.

A computer verification shows that the conjecture is true for cubic bipartite graphs of order at most 26, and is tight as $\chi_h^2(K_{3,3}) = 4$.

When considering k-regular bipartite graphs for $k \ge 4$, the proof that they all admit a 2-homogenous coloring is much easier. Similarly as cubic bipartite graphs, by Proposition 2.1, one can model the ones with higher degree. Let G be a k-regular bipartite graph and H_G the k-regular k-uniform hypergraph modeling G. By Theorem 2.2, H_G is bipartite, implying that no edge of H_G is monochromatic, and clearly not rainbow, as only two colors are used. It immediately proves the following theorem.

Theorem 4.2. Every k-regular bipartite graph G, with $k \ge 4$, admits a 2-homogenous coloring. Moreover,

$$\chi_h^2(G) \le 4.$$

It is natural to ask, what if, for $k \ge 4$, the sizes of palettes are bigger than 2. Already in the class of 4-regular bipartite graphs, there are graphs which do not admit 3-homogenous colorings. However, among all 4-regular bipartite graphs of order at most 22, there are precisely two graphs not admitting a 3-homogenous coloring: the complete bipartite graph $K_{5,5}$ without a perfect matching, and the bipartite complement of the Heawood graph, i.e. the complete bipartite graph $K_{7,7}$ with a copy of the Heawood graph removed. Both graphs are depicted in Fig. 4.

An ℓ -proper coloring of a hypergraph H is such that the palette size of every edge equals ℓ . One can trivially generalize Proposition 2.1 into the following form.

Proposition 4.3. Every k-regular bipartite graph G admits an ℓ -homogenous coloring if and only if the hypergraph H_G admits an ℓ -proper coloring.

A complete k-uniform hypergraph \mathcal{H}_n^k is a hypergraph on n vertices with the edge set consisting of all k-element subsets of the vertex set. Let G be isomorphic to the complete bipartite graph $K_{n,n}$ without a perfect matching. Then, each of the two components of the hypergraph H_G is isomorphic to the complete (n - 1)-uniform hypergraph \mathcal{H}_n^{n-1} .



Figure 4: The only two 4-regular bipartite graphs on at most 22 vertices which do not admit a 3-homogenous coloring. A $K_{5,5}$ without a perfect matching on the left, and the bipartite complement of the Heawood graph on the right.

In [2], the authors, considered a more general notion of complete uniform color-bounded hypergraphs, with given lower and upper bounds for the sizes of edge palettes. Here, we only present the result, where the lower and the upper bounds are equal.

Proposition 4.4 (Bujtás, Tuza, 2009). *The complete* (n - 1)*-uniform hypergraph* \mathcal{H}_n^{n-1} admits an ℓ -proper coloring if and only if $\ell \in \{1, n - 1\}$ or

$$2 \le \frac{n-2}{\ell-1} \,.$$

Hence, the above inequality holds whenever $\ell \leq n/2$. Proposition 4.4 implies that the complete bipartite graph $K_{n,n}$ without a perfect matching is not completely homogenous for any $n \geq 4$. However, as discussed already above, it is not known if there exists some other infinite family of regular bipartite graphs which are not completely homogenous. Thus, the directions of further work are straightforward.

Question 1. Which k-regular bipartite graphs admit ℓ -homogenous colorings, for $k \ge 4$ and $3 \le \ell \le k - 1$?

Problem 4.5. Classify completely homogenous k-regular bipartite graphs, for $k \ge 4$.

Question 2. For a k-regular bipartite graph G admitting an ℓ -homogenous coloring, what is the order of $\chi_h^{\ell}(G)$ as a function of k and ℓ ?

We conclude with a conjecture about 4-regular bipartite graphs.

Conjecture 4.6. Every 4-regular bipartite graph, distinct from $K_{5,5}$ without a perfect matching and the bipartite complement of the Heawood graph, is completely homogenous.

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A normal quotient analysis for some families of oriented four-valent graphs

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Abstract

We analyse the normal quotient structure of several infinite families of finite connected edge-transitive, four-valent oriented graphs. These families were singled out by Marušič and others to illustrate various different internal structures for these graphs in terms of their alternating cycles (cycles in which consecutive edges have opposite orientations). Studying the normal quotients gives fresh insights into these oriented graphs: in particular we discovered some unexpected 'cross-overs' between these graph families when we formed normal quotients. We determine which of these oriented graphs are 'basic', in the sense that their only proper normal quotients are degenerate. Moreover, we show that the three types of edge-orientations studied are the only orientations, of the underlying undirected graphs in these families, which are invariant under a group action which is both vertex-transitive and edge-transitive.

Keywords: Edge-transitive graph, oriented graph, cyclic quotient graph, transitive group.

Math. Subj. Class.: 05C25, 20B25, 05C20

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1 Introduction

The graphs we study are simple, connected, undirected graphs of valency four, admitting an orientation of their edges preserved by a vertex-transitive and edge-transitive subgroup of the automorphism group, that is, graphs of valency four admitting a *half-arc-transitive* group action. Many of these graphs arise as medial graphs for regular maps on Riemann surfaces [8, 9]. The work of Marušič, summarised in [8], demonstrated the importance of a certain family of cyclic subgraphs for understanding the internal structure of these graphs, namely their *alternating cycles*. These are cycles in which each two consecutive edges have opposite orientations. They were introduced in [7] and their basic properties were studied in [7, 10].

The families of oriented graphs studied in this paper were singled out in [9, 10] because they demonstrate three different extremes for the structure of their alternating cycles: namely the alternating cycles are 'loosely attached', 'antipodally attached' or 'tightly attached' (see Subsection 1.2). These families are based on one of two infinite families of underlying unoriented valency four graphs (called X(r) and Y(r) for positive integers r), and for each family three different edge-orientations are induced by three different subgroups of their automorphism groups (Section 1.3); the three different edge-orientations correspond to the three different attachment properties of their alternating cycles. In this paper it is shown in Theorem 1.1 that these are essentially the only edge-orientations of the underlying graphs which are invariant under a half-arc-transitive group action.

Our approach is to study the normal quotients of these 'X-graphs' and 'Y-graphs' (as explained below), and in doing so we discover that graphs from a third family arise, the 'Z-graphs'. We find (Theorem 1.3) that normal quotients of the X-graphs are sometimes X-graphs, sometimes Y-graphs, and sometimes Z-graphs, and the same is true for normal quotients of the Y-graphs. In addition we determine in Theorem 1.2 those oriented graphs in these families which are 'basic' in the sense that all their proper normal quotients are degenerate (see Subsection 1.1).

1.1 Graph-group pairs and their normal quotients

The normal quotient approach was introduced in [2] to study oriented graphs, focusing on the structure of certain quotient graphs rather than subgraphs. For a connected oriented four-valent graph Γ with corresponding vertex- and edge-transitive group G preserving the edge-orientation, a *normal quotient* of (Γ, G) is determined by a normal subgroup N of G. It is the graph Γ_N with vertices the N-orbits on the vertices of Γ , and with distinct Norbits B, C adjacent provided there is some edge of Γ between a vertex of B and a vertex of C. The normal quotient theory in [2] asserts (with specified degenerate exceptions) that the normal quotient Γ_N has valency four, and inherits an edge-orientation from Γ which is preserved by the quotient group G/N acting transitively on vertices and edges, and, moreover, Γ is a cover of Γ_N (that is, for adjacent N-orbits B, C, each vertex of B is adjacent to exactly one vertex of C).

We call a pair (Γ, G) basic if the only proper normal quotients (that is, taking $N \neq 1$) are degenerate. Each pair (Γ, G) has at least one basic normal quotient, (more details are given in Section 2, and see [1, 2]). For the pairs (Γ, G) we study in this paper, there is always a basic normal quotient which lies in one of the families (possibly a different family from the family containing (Γ, G)). Thus, although all the graph-group pairs in a given family share the same properties of their alternating cycles (Remark 1.4), the structure of the family can be further elucidated by studying the much smaller subfamily of basic pairs.

1.2 The alternating cycles of Marušič

Let $\mathcal{OG}(4)$ denote the set of all graph-group pairs (Γ, G) , where Γ is a connected graph of valency four, G is a vertex-transitive and edge-transitive subgroup of automorphisms, and G preserves an orientation of the edges. In particular G is not transitive on the arcs of Γ (ordered pairs of vertices which form an edge), and such a group action is called *half-arc-transitive*.

Alternatively we could interpret each pair $(\Gamma, G) \in O\mathcal{G}(4)$ as consisting of a connected, undirected graph Γ of valency four, and a group G of automorphisms acting halfarc-transitively. Such a group action determines an edge-orientation of Γ (up to reversing the orientation on every edge). It is possible for a single graph to have different edgeorientations determined by different subgroups of automorphisms. This is the case with the examples in Subsection 1.3 (a) and (b). By viewing the fundamental objects of study as undirected graphs endowed with (perhaps several) edge-orientations, we are able to give a unified discussion of all possible edge-orientations preserved by half-arc-transitive group actions. Our notation is therefore slightly different from the papers [9, 10] where different names for the same graph are used for different edge-orientations.

The alternating cycles of (Γ, G) (defined above), are determined by the edge-orientation. They partition the edge set, they all have the same even length, denoted by $2 \cdot r(\Gamma, G)$, where $r(\Gamma, G)$ is called the *radius* of (Γ, G) , and if two alternating cycles share at least one vertex, then they intersect in a constant number $a(\Gamma, G)$ of vertices, called the *attachment number*, such that $a(\Gamma, G)$ divides $2 \cdot r(\Gamma, G)$ [7, Proposition 2.4]. The radius can be any integer greater than 1 ([7, Section 3] and [10, Section 4]), and the attachment number can be any positive integer [12, Theorem 1.5]. It is possible that $a(\Gamma, G) = 2 \cdot r(\Gamma, G)$ and all such pairs (Γ, G) were characterised by Marušič in [7, Proposition 2.4(ii)].

Otherwise, if $a(\Gamma, G) < 2 \cdot r(\Gamma, G)$, then Γ is a cover of a (possibly smaller) quotient graph Γ' admitting a (possibly unfaithful) action G' of G such that $(\Gamma', G') \in O\mathcal{G}(4)$ and the attachment number $a(\Gamma', G')$ is either 1, 2 or $r(\Gamma', G')$, [10, Theorem 1.1 and Theorem 3.6]. For this reason attention has focused on families of examples $(\Gamma, G) \in O\mathcal{G}(4)$ for which $a(\Gamma, G)$ is 1, 2 or $r(\Gamma, G)$, and such pairs are said to be *loosely attached*, *antipodally attached* or *tightly attached*, respectively. As we already mentioned, graphs in the families we examine have one of these properties, and the structure of their alternating cycles was studied by Marušič and others [4, 6, 7, 9, 10, 11, 12, 13].

1.3 The families of oriented graphs and our results

We describe the underlying graphs and their edge-orientations.

(a) The first three families of oriented graphs are all based on the same family of graphs, namely the Cartesian product $X(r) = C_{2r} \Box C_{2r}$ of two cycles of length 2r, for a positive integer r. The graph X(r) has vertex set $\mathbb{Z}_{2r} \times \mathbb{Z}_{2r}$, such that (i, j) is adjacent to $(i \pm 1, j)$ and $(i, j \pm 1)$ for all $i, j \in \mathbb{Z}_{2r}$. If r = 1 then $X(1) = C_4$, a 4-cycle. If $r \ge 2$, then X(r)has valency 4 and its automorphism group is $G(r) = \operatorname{Aut} X(r) = D_{4r} \wr Z_2 = D_{4r}^2 \rtimes Z_2$, with generators

$$\mu_1: (i,j) \longrightarrow (i+1,j), \qquad \mu_2: (i,j) \longrightarrow (i,j+1), \sigma_1: (i,j) \longrightarrow (-i,j), \qquad \sigma_2: (i,j) \longrightarrow (i,-j), \tau: (i,j) \longrightarrow (j,i).$$

The group G(r) is arc-transitive of order $32r^2$, and the stabiliser of the vertex x = (0,0) is $G(r)_x = \langle \sigma_1, \sigma_2, \tau \rangle$, a dihedral group of order 8. In 1999, Marušič and the fourth author [10] defined three edge-orientations on the graphs X(r), each of which corresponds to a half-arc-transitive action of a certain subgroup of G(r), as follows. The second edge-orientation was also studied by Marušič and Nedela [9]. As mentioned above, by Theorem 1.1, these are the only edge-orientations preserved by a half-arc-transitive subgroup of Aut X(r), up to conjugation in the automorphism group, and reversing the orientations on all edges. We note that elements of \mathbb{Z}_{2r} have a well-defined parity (even or odd).

(a.1) Define the first edge-orientation by

$$(i,j) \rightarrow (i,j+1)$$
 if *i* is even, $(i,j) \leftarrow (i,j+1)$ if *i* is odd

$$(i,j) \rightarrow (i+1,j)$$
 if j is even, $(i,j) \leftarrow (i+1,j)$ if j is odd

and the corresponding group

$$G_1(r) := \langle \mu_1 \sigma_2, \mu_2 \sigma_1, \tau \rangle.$$

Note that $G_1(r)_x = \langle \tau \rangle \cong Z_2$, and $|G_1(r)| = 8r^2$. (a.2) Define the second edge-orientation by

> $(i,j) \rightarrow (i,j+1), \quad (i,j) \leftarrow (i+1,j) \text{ if } i+j \text{ is even}$ $(i,j) \leftarrow (i,j+1), \quad (i,j) \rightarrow (i+1,j) \text{ if } i+j \text{ is odd}$

and the corresponding group

$$G_2(r) := \langle \mu_1 \mu_2, {\mu_1}^2, \sigma_1, \sigma_2, \tau \mu_1 \rangle.$$

Note that $G_2(r)_x = \langle \sigma_1, \sigma_2 \rangle \cong Z_2^2$, and $|G_2(r)| = 16r^2$.

(a.3) Define the third edge-orientation by

$$(i,j) \rightarrow (i,j+1), \quad (i,j) \rightarrow (i+1,j) \text{ for all } i \text{ and } j$$

and the corresponding group

$$G_3(r) := \langle \mu_1, \mu_2, \tau \rangle.$$

Note that $G_3(r)_x = \langle \tau \rangle \cong Z_2$, and $|G_3(r)| = 8r^2$.

In Remark 3.1 we discuss briefly how these three edge-orientations may be visualised. In neither of the papers [9, 10] where these graphs were previously studied are the generators of the groups $G_k(r)$ defined explicitly, and we need this information for our analysis. Indeed in order to analyse these families of oriented graphs we need an additional graph family related to the third edge orientation.

Basic Type	Possible Γ_N for $1 \neq N \lhd G$	Conditions on G-action
		on vertices
quasiprimitive	K_1 only	quasiprimitive
biquasiprimitive	K_1 and K_2 only (Γ bipartite)	biquasiprimitive
cycle	at least one C_m $(m \ge 3)$	at least one quotient action
		D_{2m} or Z_m

Table 1: Types of basic pairs (Γ, G) in $\mathcal{OG}(4)$

(a.4) Let s be an odd integer, $s \ge 3$, and let $Z(s) = C_s \Box C_s$ (that is, the graph X(r) with 2r replaced by s); let μ_1, μ_2, τ have the same meanings as above (as permutations of the set $\mathbb{Z}_s \times \mathbb{Z}_s$); define the edge-orientation as in (a.3); and call the corresponding group $G_{3Z}(s) = \langle \mu_1, \mu_2, \tau \rangle$.

(b) The last three families of oriented graphs are all based on certain quotients of the graphs in part (a). Define the (undirected) graph Y(r) as the quotient of X(r) modulo the orbits of the normal subgroup $M(r) := \langle (\mu_1 \mu_2)^r \rangle$ of G(r). Thus the vertices of Y(r) are the 2-element subsets $\{(i, j), (i+r, j+r)\}$, for $i, j \in \mathbb{Z}_{2r}$, and the vertex $\{(i, j), (i+r, j+r)\}$ of Y(r) is adjacent to $\{(i \pm 1, j), (i+r \pm 1, j+r)\}$ and $\{(i, j \pm 1), (i+r, j+r \pm 1)\}$. The graph $Y(1) = K_2$ and, for $r \ge 2$, Y(r) has valency 4, and admits an arc-transitive action of the quotient H(r) := G(r)/M(r). Moreover, X(r) is a cover of Y(r). In particular, $Y(2) = K_{4,4}$, a complete bipartite graph.

For k = 2, 3 with $r \ge 2$, and also for k = 1 with r even, we have $M(r) \le G_k(r)$ and we define $H_k(r) := G_k(r)/M(r)$. Then the graph-group pair $(Y(r), H_k(r)) \in \mathcal{OG}(4)$ (Lemma 3.3). It is the normal quotient of the pair $(X(r), G_k(r))$ relative to M(r), and by [2, Theorem 1.1], Y(r) inherits the k^{th} -edge-orientation from X(r).

For any of the graphs X(r), Y(r), Z(s), each of the edge-orientations defined above is invariant under some edge-transitive subgroup of automorphisms (by Theorem 1.2), and these are essentially the only such edge-orientations for these graphs.

Theorem 1.1. Let $\Gamma = X(r)$ with $r \ge 2$, or $\Gamma = Y(r)$ with $r \notin \{1, 2, 4\}$, or $\Gamma = Z(s)$ with s odd, s > 1. Then, up to conjugation in Aut Γ , and up to reversing the orientation on each edge, the only edge-orientations of Γ invariant under a half-arc-transitive subgroup of Aut Γ are those defined in Subsection 1.3.

We prove Theorem 1.1 in Section 4. By [2, Lemma 3.3], each graph-group pair $(\Gamma, G) \in O\mathcal{G}(4)$ is a normal cover of at least one basic pair in $O\mathcal{G}(4)$. It turns out that the graphgroup pairs $(X(r), G_k(r)), (Y(r), H_k(r))$, and $(Z(s), G_{3Z}(s))$ all lie in $O\mathcal{G}(4)$, and are all normal covers of at least one basic pair from one of these families, but not necessarily from the same family (Remark 3.1 (c)). Our main results identify which of these pairs is basic (Theorem 1.2), and present some of their interesting normal quotients (Theorem 1.3). The types of basic graph-group pairs are defined according to the kinds of degenerate normal quotients they have. These are summarised in Table 1, taken from [2, Table 2].

Theorem 1.2. Let (Γ, G) be one of the graph-group pairs in Table 2. Then $(\Gamma, G) \in OG(4)$. Moreover (Γ, G) is basic if and only if the conditions in the 'Conditions to be Basic' column hold, and in this case, the basic type is given in the 'Basic Type' column.

(Γ, G)	Conditions	Conditions to be Basic	Basic Type
$(X(r), G_k(r))$	all k and r	k = 1, r odd prime	cycle
$(Y(r), H_k(r))$	all k and r even	all k and $r = 2$	cycle
$(Y(r), H_k(r))$	k > 1 and r odd	k = 2, r odd prime	biquasiprimitive
$(Z(s), G_{3Z}(s))$	$s \geq 3 \text{ odd}$	s odd prime	cycle

Table 2: Conditions for (Γ, G) to be basic in Theorem 1.2. (Refer to Lemma 6.2.)

We verify membership of $\mathcal{OG}(4)$ in Lemma 3.3, and prove the assertions in Table 2 in Lemma 6.2. The normal quotients we explore are those modulo the following subgroups of G(r) and/or $G_{3Z}(s)$. We note that $|\mu_i|$ is 2r or s, when interpreting μ_i as an element of G(r) or $G_{3Z}(s)$, respectively. For each divisor a of 2r or of s, as appropriate, define

$$N(a) = \langle \mu_1^a, \mu_2^a \rangle \qquad \text{if} \qquad a \mid |\mu_1| \qquad (1.1)$$
$$M(a) = \langle (\mu_1 \mu_2)^a, \mu_1^{2a} \rangle \qquad \text{if} \qquad 2a \mid |\mu_1|$$
$$N(2, +) = \langle \mu_1^2, \mu_2^2, \sigma_1, \sigma_2 \rangle \le G_2(r).$$

If $|\mu_1| = 2r$, then each of N(a), M(a) is normal in the full automorphism group G(r) of X(r), and if $a \mid r$, then N(2a) is a subgroup of M(a) of index 2; if $|\mu_1| = s$ is odd, then $N(a) \leq G_{3Z}(s)$ (and M(a) is not defined). We also consider:

$$J = \langle \mu_1 \mu_2 \rangle \cong Z_t, \qquad \text{and} \quad K = \langle \mu_1 \mu_2^{-1}, \tau \rangle \cong D_{2t} \qquad (1.2)$$

where $t = |\mu_1| \in \{2r, s\}$, and if $|\mu_1| = 2r$, also

$$J(+) = \langle \mu_1 \mu_2, \mu_1^r \rangle \qquad \text{and} \quad K(+) = \langle \mu_1 \mu_2^{-1}, \tau, \mu_1^r \rangle.$$
(1.3)

If t = 2r then the four subgroups in (1.2) and (1.3) all contain M(r) and are normal in $G_3(r)$, while if t = s then J, K are normal in $G_{3Z}(s)$. For an arbitrary subgroup L of G(r), we write $\overline{L} := LM(r)/M(r)$, so, for example, $H(r) = \overline{G(r)}$ and $H_k(r) = \overline{G_k(r)}$, and we also consider the subgroups $\overline{M(a)}$ and $\overline{N(a)}$. Note that

$$M(r) \leq N(a)$$
 if and only if $\frac{2r}{a}$ is odd if and only if $\overline{N(a)} = \overline{M(\frac{a}{2})}$. (1.4)

Theorem 1.3. Let (Γ, G) be a graph-group pair $(X(r), G_k(r))$, $(Y(r), H_k(r))$, or $(Z(s), G_{3Z}(s))$, where $k \in \{1, 2, 3\}$, $s \ge 3$ is odd, $r \ge 2$, and in the case of $(Y(r), H_1(r))$, r is even.

- (a) Then (Γ, G) has proper non-degenerate normal quotients $(\Gamma_N, G/N)$, for (Γ, G) , N and the 'Conditions' as in one of the lines of Table 3.
- (b) also (Γ, G) has degenerate normal quotients (Γ_N, G/N), for N, G as in one of the lines of Table 4.

We prove parts (a) and (b) of Theorem 1.3 in Lemmas 5.1 and 5.2, respectively. We do not claim that Theorem 1.3 classifies all the normal quotients for these graph-group pairs.

(Γ, G)	N	$(\Gamma_N, G/N)$	Conditions on k, a, r
$(X(r), G_k(r))$	N(2a)	$(X(a), G_k(a))$	a < r
$(X(r), G_k(r))$	M(a)	$(Y(a), H_k(a))$	$\frac{2r}{a}$ even, and a even if $k = 1$
$(X(r), G_3(r))$	N(a)	$(Z(a), G_{3Z}(a))$	a odd
$(Y(r), H_k(r))$	$\overline{N(2a)}$	$(X(a), G_k(a))$	$\frac{r}{a}$ even
$(Y(r), H_k(r))$	$\overline{M(a)}$	$(Y(a), H_k(a))$	$\frac{2r}{a} > 2$ even, and a even if $k = 1$
$(Y(r), H_3(r))$	$\overline{N(a)}$	$(Z(a), G_{3Z}(a))$	a odd
$(Z(s), G_{3Z}(s))$	N(a)	$(Z(a), G_{3Z}(a))$	a < s

Table 3: Non-degenerate normal quotients of (Γ, G) for Theorem 1.3, with N as in (1.1) and a > 1. (Refer to Lemma 5.1.)

Table 4: Degenerate normal quotients of (Γ, G) for Theorem 1.3, with N as in (1.1), (1.2) or (1.3). (Refer to Lemma 5.2.)

N in $G_k(r)$	$N \text{ in } H_k(r)$	$N \text{ in } G_{3Z}(s)$	$(\Gamma_N, G/N)$	Conditions
N(2)	$\overline{N(2)}$	_	(C_4, D_8)	k = 1, 3,
				with r even for $H_k(r)$
N(2, +)	$\overline{N(2,+)}$	_	(C_4, Z_4)	k = 2
				with r even for $H_k(r)$
-	$\overline{N(2,+)}$	_	(K_2, Z_2)	k = 2, r odd
_	$\overline{N(2)}$	_	(K_2, Z_2)	k = 3, r odd
J	\overline{J}	J	(C_t, D_{2t})	$k=3, t\in\{2r,s\}$
K	\overline{K}	K	(C_t, Z_t)	$k=3,t\in\{2r,s\}$
J(+)	$\overline{J(+)}$	_	(C_r, D_{2r})	k = 3
K(+)	$\overline{K(+)}$	-	(C_r, Z_r)	k = 3

Remark 1.4. (a) When defining $(Z(s), G_{3Z}(s))$ with s odd, we only consider the third edge-orientation since, for s odd, elements of \mathbb{Z}_s do not have a well-defined parity, and so the definitions of the first and second edge-orientations do not make sense for the graph Z(s).

Also, when defining $(Y(r), H_k(r))$, we require that r should be even when k = 1, since when k = 1 and r is odd, there are oriented edges in both directions between adjacent Y(r)-vertices, so the first edge-orientation of X(r) is not inherited by Y(r).

(b) The nomenclature in (a.4) may seem clumsy. However we decided to keep the same names for the graphs X(r), Y(r) in order to facilitate reference to [9, 10] for their other properties, as follows.

- (i) It is pointed out in [10, Section 2] and [9, Page 161], that for r ≥ 3, the oriented graph-group pairs (X(r), G_k(r)) are loosely attached with radius 2, antipodally attached with radius r, and tightly attached with radius 2r, for k = 1, 2, 3, respectively. Note that the graph X(r) with the kth edge-orientation is called X_k(r) in [10].
- (ii) It is remarked in [10, Section 2], that if $r \ge 3$, then the oriented graph-group pairs $(Y(r), H_k(r))$ (with r even if k = 1) are loosely attached with radius 2, antipodally attached with radius r, and tightly attached with radius r, for k = 1, 2, 3, respectively.
- (iii) The pairs $(X(r), G_2(r))$ and $(Y(r), H_2(r))$ were also studied by Marušič and Nedela, where they were characterised in [9, Props. 3.3, 3.4] as the only pairs with stabilisers of order at least 4, and such that every edge lies in precisely two oriented 4-cycles.

(c) By Theorems 1.2 and 1.3, the graph-group pairs all have basic normal quotients, sometimes more than one. We summarise our findings.

- (i) (X(r), G₁(r)), and also (Y(r), H₁(r))(r even), have basic normal quotients (Y(2), H₁(2)) if r is even and (X(a), G₁(a)) for odd primes a | r;
- (ii) $(X(r), G_2(r))$, and also $(Y(r), H_2(r))$, have as basic normal quotients $(Y(a), H_2(a))$ for primes $a \mid 2r$;
- (iii) $(X(r), G_3(r))$, and also $(Y(r), H_3(r))$, have as basic normal quotients $(Y(2), H_3(2))$ if r is even and $(Z(a), G_{3Z}(a))$ for odd primes $a \mid r$;
- (iv) $(Z(s), G_{3Z}(s))$ (s odd) has basic normal quotients $(Z(a), G_{3Z}(a))$ for odd primes $a \mid s$.

2 Preliminaries: normal quotients of pairs in $\mathcal{OG}(4)$

For fundamental graph theoretic concepts please refer to the book [5], and for fundamental notions about group actions please refer to the book [3]. For permutations g of a set X, we denote the image of $x \in X$ under g by x^g .

A permutation group on a set X is *semiregular* if only the identity element fixes a point of X; the group is *regular* if it is transitive and semiregular. If a permutation group G on X has a normal subgroup $K \leq G$ such that K is regular, then (see [3, Section 1.7]) G is a semidirect product $G = K.G_x$, where G_x is the stabiliser of a point $x \in X$. Moreover, we may identify X with K in such a way that $x = 1_K$, K acts by right multiplication and G_x acts by conjugation. Many of the groups we study in this paper have this form. As mentioned in Section 1, normal quotients of graph-group pairs $(\Gamma, G) \in O\mathcal{G}(4)$ are usually of the form $(\Gamma_N, G/N)$, they lie in $O\mathcal{G}(4)$, and Γ is a cover of Γ_N , where $N \leq G$. The only exceptions are the degenerate cases when Γ_N consists of a single vertex (if N is transitive), or a single edge (if the N-orbits form the bipartition of a bipartite graph Γ), or when Γ_N is a cycle possibly, but not necessarily, inheriting a G-orientation of its edges, [2, Theorem 1.1]. Thus $(\Gamma, G) \in O\mathcal{G}(4)$ is *basic* if all of its proper normal quotients (that is, the ones with $N \neq 1$) are degenerate.

For a graph-group pair $(\Gamma, G) \in \mathcal{OG}(4)$ and vertex x, the *out-neighbours* of x are the two vertices y such that $x \to y$ is a G-oriented edge of Γ .

An *isomorphism* between graph-group pairs $(\Gamma, G), (\Gamma', G')$ is a pair (f, φ) such that $f: \Gamma \to \Gamma'$ is a graph isomorphism, $\varphi: G \to G'$ is a group isomorphism, and $(x^g)f = (xf)^{(g)\varphi}$ for all vertices x of Γ and all $g \in G$.

Lemma 2.1. Suppose that $(\Gamma, G) \in O\mathcal{G}(4)$, $N \leq G$, and (f, φ) is an isomorphism from $(\Gamma_N, G/N)$ to (Γ', G') . Let \mathcal{M} be the set of all normal subgroups M of G such that $N \leq M$ and M is the kernel of the G-action on the M-vertex-orbits in Γ . Then, for each $M \in \mathcal{M}$, (f, φ) induces an isomorphism from $(\Gamma_M, G/M)$ to $(\Gamma'_{\overline{M}}, G'/\overline{M})$, where $\overline{M} = (M/N)\varphi$, and each normal quotient of (Γ', G') corresponds to exactly one such normal quotient $(\Gamma_M, G/M)$.

Proof. The isomorphism $\varphi : G/N \to G'$ determines a one-to-one correspondence $M \mapsto (M/N)\varphi$ between the set of all normal subgroups of G which contain N, and the set of all normal subgroups of G', and moreover, setting $\overline{M} = (M/N)\varphi$, φ induces an isomorphism $\varphi_M : G/M \to G'/\overline{M}$ given by $Mg \to \overline{M}(Ng)\varphi$. For normal quotient graphs Γ_M , the induced group action is G/\hat{M} , where \hat{M} is the kernel of the G-action on the M-orbits. Thus $\Gamma_M = \Gamma_{\hat{M}}$, and the normal quotients of (Γ, G) relative to normal subgroups M containing N are precisely the normal quotients $(\Gamma_M, G/M)$, for $M \in \mathcal{M}$.

For each $M \in \mathcal{M}$, the graph isomorphism $f: \Gamma_N \to \Gamma'$ induces a graph isomorphism $f_M: \Gamma_M \to \Gamma'_{\overline{M}}$, where f_M maps the M-vertex-orbit x^M in Γ to the \overline{M} -vertex-orbit in Γ' containing $(x^N)f$. By the definition of (f, φ) we have $((x^N)^{Ng})f = ((x^N)f)^{(Ng)\varphi}$ for each vertex x of Γ and each $g \in G$. It follows that $((x^M)^{Mg})f_M = ((x^M)f_M)^{(Mg)\varphi_M}$ for each vertex x of Γ and each $g \in G$, and hence (f_M, φ_M) is an isomorphism from $(\Gamma_M, G/M)$ to $(\Gamma'_{\overline{M}}, G'/\overline{M})$.

This property of (f, φ) implies that normal subgroups containing N with the same vertex-orbits in Γ correspond to normal subgroups of G' with the same vertex-orbits in Γ' , and vice versa. Thus, on the one hand, distinct subgroups in \mathcal{M} correspond to distinct normal quotients of (Γ', G') . Also, on the other hand, each $K \leq G'$ such that K is the kernel of the G'-action on the K-vertex-orbits in Γ' is of the form $K = (M/N)\varphi$, where $N \leq M$ and M is the kernel of the G-action on the M-vertex orbits in Γ .

3 Each graph-group pair (Γ, G) in Theorem 1.2 lies in $\mathcal{OG}(4)$

First we consider X(r) and $G_k(r)$ for $k \leq 3$ and $r \geq 3$. Recall the definitions of the edge orientations and the generators $\mu_1, \mu_2, \sigma_1, \sigma_2, \tau$, from Subsection 1.3 (a). We make a few comments about the various edge orientations.

Remark 3.1. We view the vertex set of X(r) as a $2r \times 2r$ grid with rows and columns labeled $0, 1, \ldots, 2r - 1$ (in this order, increasing to the right and increasing from top to

bottom), and with the vertex (i, j) in the row *i*, column *j* position. The edges of X(r) then are either *horizontal* if they join vertices with equal first entries, or vertical if they join vertices with equal second entries. It may be helpful to use this point of view when reading the proofs below. In particular it aids a description of the various edge orientations.

- (1) In the first edge-orientation, for *i* even, the horizontal edges in row *i* are oriented from left to right (except of course that the edge from (i, 2r 1) is joined to (i, 0)), and for *i* odd, the horizontal edges in row *i* are oriented from right to left. Similarly, for *j* even, the vertical edges in column *j* are oriented downwards and those in column *j*, for odd *j*, are oriented upwards.
- (2) In the second edge-orientation, both the rows and the columns are alternating cycles, arranged in such a way that, for each *i*, *j*, the sequence

$$(i, j), (i, j + 1), (i + 1, j + 1), (i + 1, j)$$

forms a directed 4-cycle, oriented from left to right if i + j is even, and from right to left if i + j is odd.

(3) Finally, in the third edge-orientation, all the horizontal edges are oriented from left to right, and all the vertical edges are oriented downwards.

Lemma 3.2. Let $k \leq 3$ and $r \geq 2$. Then the group $G_k(r)$ preserves the k^{th} edgeorientation of X(r).

Proof. We consider the cases k = 1, 2, 3 separately. In each case, for each generator of $G_k(r)$, we consider its actions on a horizontal edge E in row i joining (i, j) to (i, j + 1), and on a vertical edge D in column j joining (i, j) to (i + 1, j).

(1) Firstly $\mu_1 \sigma_2$ maps E to the horizontal edge E' joining (i+1, -j) to (i+1, -j-1), since $\mu_1 \sigma_2$ moves row i to row i + 1 (by μ_1) and then reflects it across a vertical axis through the 0^{th} -column (by σ_2). Thus if E is oriented from left to right, then E' is oriented from right to left (and vice versa), and since horizontal edges in row i and row i + 1 have opposite orientations (see Remark 3.1(1)), it follows that $\mu_1 \sigma_2$ preserves the orientation of horizontal edges. Also $\mu_1 \sigma_2$ maps D to the vertical edge joining (i+1, -j) to (i+2, -j), and since j, -j have the same parity, edges in columns j and -j have the same orientation (see Remark 3.1(1)). Thus $\mu_1 \sigma_2$ preserves the first edge-orientation on all edges. An exactly similar argument (interchanging the roles of rows and columns) shows that $\mu_2 \sigma_1$ also preserves the first edge-orientation.

Finally τ swaps the horizontal edge E in row i with the vertical edge E' in column i joining (j, i) to (j + 1, i). If i is even then E is oriented from left to right and E' is oriented downwards, so the orientation is preserved. Also, if i is odd then E is oriented from right to left and E' is oriented upwards, and again the orientation is preserved. (For example, the oriented edge $(1, 2) \leftarrow (1, 3)$ is swapped with the oriented edge $(2, 1) \leftarrow (3, 1)$.) Similarly the action of τ preserves the orientation of D. Thus τ preserves the first edge-orientation.

(2) Firstly μ_1^2 maps E to the horizontal edge E' joining (i + 2, j) to (i + 2, j + 1) and E, E' have the same orientation; and μ_1^2 maps D to the vertical edge D' joining (i + 2, j) to (i + 3, j) and D, D' have the same orientation. Thus μ_1^2 preserves the second edge-orientation. Similar arguments show that μ_2^2 and $\mu_1\mu_2$ also preserve the second edge-orientation. Next, σ_1 maps E to the horizontal edge E' in row -i joining (-i, j) to (-i, j + 1) and since i+j and -i+j have the same parity, the edges E, E' have the same orientation;

similarly σ_1 maps D to the vertical edge D', still in column j, joining (-i, j) to (-i-1, j)and we see again that D, D' have the same orientation. Thus σ_1 preserves the second edge-orientation. An exactly similar argument shows that also σ_2 preserves the second edge-orientation. Finally $\tau \mu_1$ maps E to the vertical edge E' joining (j+1,i) to (j+2,i)and since i + j and j + 1 + i have opposite parities, the orientation of E is preserved under the action of $\tau \mu_1$; and $\tau \mu_1$ maps D to the horizontal edge D' joining (j + 1, i) to (j + 1, i + 1) and for the same reason the orientation of D is preserved under the action of $\tau \mu_1$. Thus $\tau \mu_1$ preserves the second edge-orientation.

(3) Firstly, since μ_1 and μ_2 map E to a horizontal edge and D to a vertical edge, and since all horizontal edges have the same orientation, and all vertical edges have the same orientation (see Remark 3.1(3)), it follows that μ_1 and μ_2 preserve the third edge-orientation. Finally τ swaps horizontal and vertical edges, and since all horizontal edges are oriented from left to right, and all vertical edges are oriented downwards, it follows that τ also preserves the third edge-orientation.

Next we prove membership of $\mathcal{OG}(4)$. Recall that, for a subgroup $L \leq G(r)$ we write $\overline{L} = LM(r)/M(r)$ for the corresponding subgroup of H(r) = G(r)/M(r).

Lemma 3.3. Let $k \leq 3$, $r \geq 2$, and let s > 1 be odd. Let (Γ, G) be one of $(X(r), G_k(r))$, $(Y(r), H_k(r))$ (with r even if k = 1), or $(Z(s), G_{3Z}(s))$. Then $(\Gamma, G) \in OG(4)$.

Proof. It is easy to check that the graphs X(r) and Z(s) are connected. Thus, once we have proved that $G_k(r)$ acts half-arc-transitively on X(r), and $G_{3Z}(s)$ acts half-arc-transitively on Z(s), it follows from Lemma 3.2 that $(X(r), G_k(r)) \in \mathcal{OG}(4)$ and $(Z(s), G_{3Z}(s)) \in \mathcal{OG}(4)$. Further, as $(Y(r), H_k(r))$ is a normal quotient of $(X(r), G_k(r))$ relative to $M(r) \cong Z_2$, its membership in $\mathcal{OG}(4)$ follows from [2, Theorem 1.1]. It therefore remains to prove that the actions on X(r) and Z(s) are half-arc-transitive. First we consider X(r).

The subgroup $L := N(2) = \langle \mu_1^2 \rangle \times \langle \mu_2^2 \rangle \leq G(r)$ is contained in $G_k(r)$, for each k, and the L-orbits on vertices are the following four subsets.

$$\Delta_{ee} = \{(i,j) \mid i,j \text{ are both even}\}, \qquad \Delta_{eo} = \{(i,j) \mid i \text{ is even}, j \text{ is odd}\}, \quad (3.1)$$

$$\Delta_{oe} = \{(i,j) \mid i \text{ is odd}, j \text{ is even}\}, \qquad \Delta_{oo} = \{(i,j) \mid i,j \text{ are both odd}\}.$$

Writing $\bar{g} = Lg$ for each $g \in G(r)$, we note that $G(r)/L = \langle \bar{\mu}_1, \bar{\mu}_2, \bar{\sigma}_1, \bar{\sigma}_2, \bar{\tau} \rangle \cong (Z_2 \times Z_2) \wr Z_2$ of order 2^5 . Let $x := (0,0) \in \Delta_{ee}$. For each k we find a normal subgroup K of $G_k(r)$ such that K contains L and K is regular on vertices. Hence $G_k(r)$ is the semidirect product $G_k(r) = K \cdot (G_k(r))_x$. Then to prove half-arc-transitivity, it is sufficient to prove that $(G_k(r))_x$ fixes setwise and interchanges the two out-neighbours of x. (This is sufficient since, for two arbitrary oriented edges, say $y \to z$ and $y' \to z'$, there are elements $g, g' \in K$ such that $y^g = x, (y')^{g'} = x$, so that $z^g, (z')^{g'}$ are possibly equal out-neighbours of x.)

(1) For the first edge-orientation we see that $K := \langle \mu_1 \sigma_2, \mu_2 \sigma_1 \rangle$ is normalised by τ and hence K is normal in $G_1(r)$ with index 2, and $G_1(r) = K \cdot \langle \tau \rangle$. Since $|G_1(r)| = 8r^2$ (see Subsection 1.3), we have $|K| = 4r^2$. Moreover, since $x^{\mu_1 \sigma_2} = (1, 0) \in \Delta_{oe}, x^{\mu_2 \sigma_1} = (0, 1) \in \Delta_{eo}$, and $(0, 1)^{\mu_1 \sigma_2} = (1, -1) \in \Delta_{oo}$, it follows that K permutes the L-orbits transitively, and hence K is transitive on vertices. Now $|K| = 4r^2$, and hence K is regular on vertices. Thus the stabiliser $(G_1(r))_x$ has order 2 and so is equal to $\langle \tau \rangle \cong Z_2$. Finally τ interchanges the two out-neighbours (0, 1) and (1, 0) of x. (2) For the second edge-orientation, the subgroup $K := \langle \mu_1 \mu_2, \mu_1^2, \tau \mu_1 \rangle$ is normalised by σ_1 and σ_2 and hence is normal in $G_2(r)$. Also the subgroup $H := \langle \sigma_1, \sigma_2 \rangle \cong Z_2^2$ fixes the vertex x and $H \cap K = 1$. Since $|G_2(r)| = 16r^2 = |K| \cdot |H|$, this implies that $G_2(r)$ is the semidirect product $K \cdot H$, and $|K| = 16r^2/|H| = 4r^2$. Since $x^{\mu_1\mu_2} = (1,1) \in \Delta_{oo}$, $x^{\tau\mu_1} = (1,0) \in \Delta_{oe}$, and $(1,0)^{\mu_1\mu_2} = (2,1) \in \Delta_{eo}$, it follows that K permutes the Lorbits transitively, and hence K is transitive on vertices. Then since $|K| = 4r^2$, it follows that K is regular on vertices. Thus the stabiliser $(G_2(r))_x$ has order $|G_2(r) : K| = 4$ and so is equal to H. Finally $\sigma_2 \in H$ interchanges the two out-neighbours (0, 1) and (0, -1)of x.

(3) For the third edge-orientation, the subgroup $K := \langle \mu_1, \mu_2 \rangle$ is normalised by τ and hence is normal in $G_3(r)$ of index 2, and $G_3(r) = K \cdot \langle \tau \rangle$ so $|K| = 4r^2$. Moreover, since $x^{\mu_1} = (1,0) \in \Delta_{oe}, x^{\mu_2} = (0,1) \in \Delta_{eo}$, and $(0,1)^{\mu_1} = (1,1) \in \Delta_{oo}$, it follows that Kpermutes the *L*-orbits transitively, and hence K is transitive on vertices. Now $|K| = 4r^2$, and hence K is regular on vertices. Thus the stabiliser $(G_3(r))_x$ has order 2 and so is equal to $\langle \tau \rangle \cong Z_2$. Finally τ interchanges the two out-neighbours (0,1) and (1,0) of x.

(4) Now we consider Z(s) and $G = G_{3Z}(s)$ with s odd. It is straighforward to show that the subgroup $K = \langle \mu_1, \mu_2 \rangle$ is regular on vertices, and $G = K \cdot \langle \tau \rangle$ with $G_x = \langle \tau \rangle$. Also τ interchanges the two out-neighbours (0, 1) and (1, 0) of x.

4 Classifying the edge-orientations

In this section we prove Theorem 1.1. Suppose that Γ is one of the graphs X(r), Y(r), Z(s) defined in Subsection 1.3, and that $H \leq \operatorname{Aut} \Gamma$ acts half-arc-transitively. Then as discussed in Subsection 1.2, H preserves an edge-orientation of Γ , and this edge-orientation is determined by H up to reversing the orientation on each edge. Moreover, this edge-orientation and its 'reverse' will be the same as those preserved by a subgroup of $\operatorname{Aut} \Gamma$ which is maximal subject to containing H and acting half-arc-transitively on Γ . Thus proving Theorem 1.1 is equivalent to classifying all of the subgroups H of $\operatorname{Aut} \Gamma$ which are maximal subject to acting half-arc-transitively on Γ . First we show that a proof of Theorem 1.1 in the case of X(r) implies the result for the graph Y(r).

Lemma 4.1. If $r \notin \{1, 2, 4\}$, then $\operatorname{Aut} Y(r)$ is the group G(r)/M(r) discussed in Subsection 1.3(b). Moreover, if the assertions of Theorem 1.1 hold for X(r), then they hold also for Y(r).

Proof. Write $\overline{G(r)} = G(r)/M(r)$, so $\overline{G(r)}$ is an arc-transitive subgroup of $A := \operatorname{Aut} Y(r)$, where $M(r) = \langle (\mu_1 \mu_2)^r \rangle$ as in Subsection 1.3. We consider the vertex $\overline{x} = \{(0,0), (r,r)\}$ of Y(r), and its four neighbours $\overline{y} = \{(1,0), (r+1,r)\}, \overline{y'} = \{(-1, \underline{0}), (r-1,r)\},$ $\overline{z} = \{(0,1), (0,r+1)\}$ and $\overline{z'} = \{(0,-1), (r,r-1)\}$. The stabiliser in $\overline{G(r)}$ of the arc $(\overline{x}, \overline{y})$ is the subgroup $\langle \sigma_2 \rangle$. Since $r \notin \{1, 2, 4\}$, there are two paths of length 2 joining \overline{y} to the vertex v, for $v = \overline{z}$ and $v = \overline{z'}$ but only one such path for $v = \overline{y'}$. It follows that $A_{\overline{x},\overline{y}}$ must also fix $\overline{y'}$.

Thus $A_{\overline{x},\overline{y},\overline{z}}$ has index 2 in $A_{\overline{x},\overline{y}}$, and fixes each of the four neighbours of \overline{x} . Moreover, $A_{\overline{x},\overline{y},\overline{z}}$ fixes the second common neighbour $\{(1,1), (r+1,r+1)\}$ of \overline{y} and \overline{z} , and also the second common neighbour $\{(1,-1), (r+1,r-1)\}$ of \overline{y} and $\overline{z'}$. It follows that $A_{\overline{x},\overline{y},\overline{z}}$ fixes pointwise each of the neighbours of \overline{y} . Repeating this argument we conclude that $A_{\overline{x},\overline{y},\overline{z}} = 1$. Thus |A| is equal to twice the number of arcs, and hence $A = \overline{G(r)}$.

To prove the last assertion, suppose that $\overline{H} \leq A$ and \overline{H} is maximal subject to being half-arc-transitive on Y(r), and thus preserving a certain edge-orientation of Y(r) (and its reverse edge-orientation). Define an edge-orientation of X(r) by orienting each edge of X(r) according to the orientation of the corresponding edge of Y(r). Since X(r) is a double cover of Y(r), this means that both X(r)-edges corresponding to a Y(r)-edge will have the same orientation. Now $\overline{H} = H/M(r)$ where $M(r) \leq H \leq G(r)$, H is half-arctransitive on X(r), and H preserves this edge-orientation of X(r). Thus, by assumption, replacing H by a conjugate in Aut X(r) if necessary, this edge-orientation of X(r) is one of the three defined in Subsection 1.3 (a) or the reverse of one of these, and so $H \leq G_k(r)$ for some $k \in \{1, 2, 3\}$. Moreover if k = 1, then r is even, since in this case, if r were odd then the two X(r)-edges corresponding to a Y(r)-edge would have opposite orientations (see Remark 1.4 (a)).

By Lemma 4.1, we may assume that $\Gamma = X(r)$ or Z(s), or in other words, that $\Gamma = C_t \Box C_t$, where either t = 2r, or t = s (with s odd). Then $A := \operatorname{Aut} \Gamma = \langle \mu_1, \mu_2, \sigma_1, \sigma_2, \tau \rangle$, where the generators are defined as in Subsection 1.3 (a). We use this notation for the rest of this subsection and we assume that H is a half-arc-transitive subgroup of $\operatorname{Aut} \Gamma$. We let x = (0, 0), and denote its neighbours in Γ by y = (1, 0), y' = (-1, 0), z = (0, 1) and z' = (0, -1). First we obtain some restrictions on H.

- **Lemma 4.2.** (a) The group H contains none of the elements $\sigma_1\mu_1$, $\sigma_2\mu_2$, $\sigma_1\sigma_2\mu_1$, or $\sigma_1\sigma_2\mu_2$.
 - (b) Up to conjugation in A, the stabiliser H_x is one of $\langle \sigma_1 \sigma_2 \rangle$, $\langle \sigma_1, \sigma_2 \rangle$ or $\langle \tau \rangle$.

Proof. As noted in Subsection 1.3, $A_x = \langle \sigma_1, \sigma_2, \tau \rangle \cong D_8$, and $A_{x,y} = \langle \sigma_2 \rangle \cong Z_2$. There are thus exactly two elements of A which reverse the arc (x, y), and an easy computation shows these are the elements $\sigma_1\mu_1$ and $\sigma_1\sigma_2\mu_1$. Since H is vertex-transitive, and edge-transitive, but not arc-transitive, these two elements do not lie in H. The same argument for the arc (x, z) shows that H does not contain $\sigma_2\mu_2$ or $\sigma_1\sigma_2\mu_2$. This proves part (a).

Since *H* is not arc-transitive, it is a proper subgroup of *A*, so H_x is a proper subgroup of A_x , and H_x has two orbits on $\{y, y'z, z'\}$, the set of neighbours of *x*. If $|H_x| = 4$ these properties imply that $H_x = \langle \sigma_1, \sigma_2 \rangle$. The only other possibility is that $|H_x| = 2$, so suppose this is the case. Of the five involutions in A_x the only ones which act on $\{y, y'z, z'\}$ with two cycles of length 2 are $\sigma_1 \sigma_2, \tau$ and $\sigma_1 \sigma_2 \tau$. Since $\tau^{\sigma_1} = \sigma_1 \sigma_2 \tau$, part (b) follows.

This result allows us, in particular, to deal with the case where H contains the subgroup $M := \langle \mu_1, \mu_2 \rangle$.

Lemma 4.3. If H contains $M := \langle \mu_1, \mu_2 \rangle$, then up to conjugation in A,

$$H = \begin{cases} G_3(r) & \text{if } t = 2r \\ G_{3Z}(s) & \text{if } t = s \text{ is odd.} \end{cases}$$

In particular the edge-orientation is the one defined in Subsection 1.3 (a.3) or (a.4), or its reverse. Moreover, all assertions in Theorem 1.1 hold if $\Gamma = Z(s)$.

Proof. Suppose that $M \leq H$. Then $H = M \rtimes H_x$, as M is regular on vertices, and it follows from Lemma 4.2 that $H_x = \langle \tau \rangle$ (replacing H by a conjugate if necessary). Thus

H is as claimed and so is the edge-orientation. If $\Gamma = Z(s)$ then $|A| = 8s^2$ and the subgroup *M* is the unique Hall 2'-subgroup of *A*. Since *H* is vertex-transitive *H* must contain *M*.

We may therefore assume that $\Gamma = X(r)$, and that $M \not\subseteq H$. Next we consider the case $\tau \in H$.

Lemma 4.4. If $\Gamma = X(r)$, $M \not\subseteq H$, and $\tau \in H$, then up to conjugation in A, $H = G_1(r)$ and the edge-orientation is as defined in Subsection 1.3 (a.1) or its reverse.

Proof. Since $\tau \in H$, we have $H_x = \langle \tau \rangle$ by Lemma 4.2, and so |A : H| = 4. Also $|M : M \cap H| = |MH : H|$ divides |A : H| = 4.

We claim that $|M : M \cap H| = 4$. Suppose not. Then since $M \not\subseteq H$, the subgroup $M \cap H$ has index 2 in M, and as it is τ -invariant, it follows that $M \cap H = \langle \mu_1^2, \mu_2^2, \mu_1 \mu_2 \rangle$. Now $MH/M \cong H/(M \cap H)$ has order $|H|/|M \cap H| = 4$, and as A_x is a transversal for M in A, the M-cosets in MH/M have representatives from a subgroup of A_x of order 4 containing τ . The unique such subgroup is $\langle \tau, \sigma_1 \sigma_2 \rangle$. Since each of these M-cosets also has a representative from H, it follows that H contains an element $\sigma_1 \sigma_2 \mu_1^i \mu_2^j$, for some i, j. Since H contains μ_1^2, μ_2^2 and $\mu_1 \mu_2$, we may assume that j = 0 and $i \in \{0, 1\}$. Part (a) of Lemma 4.2 implies that $i \neq 1$, while the fact that $H_x = \langle \tau \rangle$ implies that $i \neq 0$. This is a contradiction, and hence $|M : M \cap H| = 4$. Thus $|MH/M| = |H|/|M \cap H| = 8$, so MH = A.

We next claim that $M \cap H = \langle \mu_1^2, \mu_2^2 \rangle$. Since $M \cap H$ is τ -invariant, this claim would follow if the projection of $M \cap H$ into $\langle \mu_1 \rangle$ were contained in $\langle \mu_1^2 \rangle$ (since this would imply that $M \cap H \subseteq \langle \mu_1^2, \mu_2^2 \rangle$). Suppose that this is not the case. Then $M \cap H$ is a τ -invariant, subdirect subgroup of $M = \langle \mu_1 \rangle \times \langle \mu_2 \rangle$ of index 4, and it follows that r is even and $M \cap H = \langle \mu_1^4, \mu_2^4, \mu_1 \mu_2^a \rangle$, where $a \in \{1, -1\}$. Since MH = A, H contains an element of the form $h = \sigma_2 \mu_1^i \mu_2^j$ for some i, j, and hence H contains $\mu_1 \mu_2^a (\mu_1 \mu_2^a)^h = \mu_1 \mu_2^a \mu_1 \mu_2^{-a} =$ μ_1^2 . This is a contradiction, proving our second claim.

Thus $M \cap H = \langle \mu_1^2, \mu_2^2 \rangle$. Since MH = A, the subgroup H contains an element $h' = \sigma_1 \mu_1^i \mu_2^j$ for some i, j, and since $M \cap H$ contains μ_1^2, μ_2^2 , we may assume that $i, j \in \{0, 1\}$. Since $\sigma_1 \notin H$, and also, by Lemma 4.2, $\sigma_1 \mu_1 \notin H$, it follows that j = 1. If $h' = \sigma_1 \mu_1 \mu_2$, then H also contains $(h')^{\tau} = \sigma_2 \mu_2 \mu_1$, and this implies that H contains $(h')^{\tau}(h')^{-1} = \sigma_2 \sigma_1 = \sigma_1 \sigma_2$, which is a contradiction. Thus $h' = \sigma_1 \mu_2$. Then H also contains $(h')^{\tau} = \sigma_2 \mu_1$, and so the group $G_1(r)$ is contained in H. These groups have the same order, so $H = G_1(r)$ and the lemma follows.

Thus from now on we may assume that $\tau \notin H$ and hence, by Lemma 4.2, that $H_x = \langle \sigma_1 \sigma_2 \rangle$ or $\langle \sigma_1, \sigma_2 \rangle$.

Lemma 4.5. If $\Gamma = X(r)$, $M \not\subseteq H$, and $H_x = \langle \sigma_1, \sigma_2 \rangle$ or $\langle \sigma_1 \sigma_2 \rangle$, then up to conjugation in A, $H \leq G_2(r)$ and the edge-orientation is as defined in Subsection 1.3 (a.2) or its reverse.

Proof. Here $H_x = \langle \sigma_1 \sigma_2 \rangle$ or $\langle \sigma_1, \sigma_2 \rangle$ and $|H| = 8r^2$ or $16r^2$ respectively. Let $\delta := |M : M \cap H|$, so $\delta > 1$ since $M \not\subseteq H$. Then $|H| = |H : M \cap H| \cdot |M \cap H| = |MH : M| \cdot (4r^2/\delta)$ divides $8 \cdot (4r^2/\delta)$, so $\delta \mid 4$ or $\delta = 2$ according as $|H| = 8r^2$ or $16r^2$. Note that it is sufficient to prove that $H \leq G_2(r)$ (up to conjugation in A), since the edge-orientations preserved by H and $G_2(r)$ are then the same as both act half-arc-transitively. Let $\pi_i : M \to \langle \mu_i \rangle$ denote the natural projection map, for i = 1, 2.

We claim that $\pi_i(M \cap H) = \langle \mu_i \rangle$ for at least one *i*. Suppose that this does not hold. Then, since $\delta \leq 4$, it follows that $M \cap H = \langle \mu_1^2, \mu_2^2 \rangle$, $\delta = 4$, so $H_x = \langle \sigma_1 \sigma_2 \rangle$ and A = MH. Since A = MH it follows that *H* contains elements of the form $h = \tau \mu_1^i \mu_2^j$ and $h' = \sigma_1 \mu_1^{i'} \mu_2^{j'}$, and we may assume that i, j, i', j' all lie on $\{0, 1\}$ since μ_1^2, μ_2^2 lie in *H*. Since neither τ nor σ_1 lies in *H*, $(i, j) \neq (0, 0) \neq (i', j')$. By Lemma 4.2 (a), *H* does not contain either $\sigma_1 \mu_1$ or $\sigma_2 \mu_2 = (\sigma_1 \sigma_2)(\sigma_1 \mu_2)$, and hence the only possibility for *h* is $\sigma_1 \mu_1 \mu_2$. If $h' = \tau \mu_1 \mu_2$, but then *H* contains $h'h^{-1} = \tau \sigma_1$, which is a contradiction, proving the claim.

Replacing H by its conjugate H^{τ} if necessary, we may assume that $M \cap H$ contains $\mu_1 \mu_2^a$ for some a. Then $|M \cap H| = 2r |H \cap \langle \mu_2 \rangle|$, and hence $H \cap \langle \mu_2 \rangle = \langle \mu_2^{\delta} \rangle$ and $M \cap H = \langle \mu_1 \mu_2^a, \mu_2^{\delta} \rangle$, where r is even if $\delta = 4$. We may also assume that $0 \le a < \delta$. Moreover $a \ne 0$, since otherwise H contains $(\sigma_1 \sigma_2) \mu_1$, contradicting Lemma 4.2.

We claim that $\delta = 2$. Suppose to the contrary that $\delta = 4$. Then r is even, $H_x = \langle \sigma_1 \sigma_2 \rangle$, and $M \cap H = \langle \mu_1 \mu_2^a, \mu_2^d \rangle$, with $a \in \{1, 2, 3\}$. The equations in the first paragraph imply that |MH : M| = 8 so A = MH, and hence H contains elements of the form $h = \sigma_1 \mu_2^b$ and $h' = \tau \mu_2^c$ for some $b, c \in \{1, 2, 3\}$ (adjusting by elements of $M \cap H$ and noting that $\tau, \sigma_1 \notin H$). Then $M \cap H$ contains $\mu_1 \mu_2^a (\mu_1 \mu_2^a)^h = \mu_2^{2a}$, which implies that a = 2, and hence that $M \cap H$ contains μ_1^2 . Therefore $M \cap H$ contains $(\mu_1 \mu_2^2)^{h'} \mu_1^{-2} = \mu_2$, which is a contradiction.

Thus $\delta = 2$, so $M \cap H = \langle \mu_1 \mu_2, \mu_2^2 \rangle$, and the equations in the first paragraph imply that |MH : M| = 4 or 8, when $|H| = 8r^2$ or $16r^2$ respectively. Then MH/M has order at least 4. Suppose that H contains an element of the form $h = \tau \mu_1^i \mu_2^j$; adjusting by an element of $M \cap H$ we may assume that $h = \tau \mu_1$ (since H does not contain τ). Then $H = \langle M \cap H, H_x, \tau \mu_1 \rangle \leq \langle \mu_1 \mu_2, \mu_2^2, \sigma_1, \sigma_2, \tau \mu_1 \rangle = G_2(r)$, and the lemma is proved in this case. If H contains no such element then |MH/M| = 4. Next, if H contains an element of the form $h = \tau \sigma_\ell \mu_1^i \mu_2^j$ (for $\ell = 1$ or 2), then adjusting by an element of $M \cap H$ we may assume that $h = \tau \sigma_\ell \mu_1$ (since H does not contain $\tau \sigma_\ell$), and again we find that $H = \langle M \cap H, H_x, \tau \sigma_\ell \mu_1 \rangle \leq G_2(r)$. The lemma follows in this case. Thus we may assume that MH/M projects to the subgroup $\langle \sigma_1, \sigma_2 \rangle$ of A_x , and now we obtain an element of the form $h = \sigma_1 \mu_1^i \mu_2^j$ in H, and $H = \langle M \cap H, H_x, h \rangle \leq G_2(r)$, completing the proof. \Box

All the assertions of Theorem 1.1 now follow from Lemmas 4.1, 4.3, 4.4, and 4.5, completing its proof.

5 Identifying normal quotients of (Γ, G) for Theorem 1.3

We identify some of the normal quotients of these graph-group pairs. Note that whenever a normal subgroup N of G(r) is contained in $G_k(r)$ we can use it to form a normal quotient of $(X(r), G_k(r))$, and moreover we can use Lemma 2.1 to deduce information about normal quotients of $(Y(r), H_k(r))$ (taking N = M(r)) and about $(Z(s), G_{3Z}(s))$ (taking r = s odd and N = N(s)). Recall the definitions of the subgroups in (1.1), (1.2) and (1.3). First we deal with normal quotients modulo N(a), M(a), and the corresponding subgroups of H(r) = G(r)/M(r).

Lemma 5.1. For Γ , G, N as in one of the lines of Table 3, the assertions about the normal quotient $(\Gamma_N, G/N)$ are valid.

Proof. Let $G = G_k(r)$ or $G_{3Z}(s)$, and let $\Gamma = X(r)$ or Z(s), so Γ has vertex set $\mathbb{Z}_t \times \mathbb{Z}_t$, where t = 2r or s respectively. Consider the action on vertices of the normal subgroup N = N(a) of G, where $a \mid t$ and 2 < a < t. The N-orbits are the a^2 subsets

$$\Delta_{i,j} = \{ (i'j') \mid i' \equiv i \pmod{a}, \ j' \equiv j \pmod{a} \}$$

for $i, j \in \mathbb{Z}_a$. Since (i', j') is adjacent in Γ to $(i' \pm 1, j')$ and $(i', j' \pm 1)$, for all $i', j' \in \mathbb{Z}_t$, it follows that $\Delta_{i,j}$ is adjacent in the quotient graph Γ_N to $\Delta_{i\pm 1,j}$ and $\Delta_{i,j\pm 1}$, for each $i, j \in \mathbb{Z}_a$. Thus, since a > 2, Γ_N has valency 4, and the mapping $f : \Delta_{i,j} \longrightarrow (i, j)$ defines a graph isomorphism from Γ_N to X(a/2) if a is even, or to Z(a) if a is odd. By [2, Theorem 1.1], the group induced by G on the quotient Γ_N is precisely G/N, and $(\Gamma_N, G/N) \in \mathcal{OG}(4)$. In particular N is the kernel of the G-action on the set of N-orbits in Γ . Write $\bar{g} := Ng$ for elements of the quotient group G/N.

If a is even, then it follows from the definitions of the generators $\mu_1, \mu_2, \sigma_1, \sigma_2, \tau$ of G(r), given in Subsection 1.3, that the induced maps $\bar{\mu}_1, \bar{\mu}_2, \bar{\sigma}_1, \bar{\sigma}_2, \bar{\tau}$ acting on Γ_N correspond to the respective generators for the smaller group G(a/2) acting on X(a/2). This natural correspondence defines a group isomorphism $G(r)/N \to G(a/2)$ which restricts to an isomorphism $\varphi : G/N \to G_k(a/2)$. We conclude that (f, φ) defines an isomorphism from $(\Gamma_N, G/N)$ to $(X(a/2), G_k(a/2))$. Thus the first line of Table 3 is valid.

Similarly if a is odd, then the maps $\bar{\mu}_1, \bar{\mu}_2, \bar{\tau}$ acting on Γ_N induced from the generators μ_1, μ_2, τ (for $G_3(r)$ or $G_{3Z}(s)$) correspond to the respective generators for the smaller group $G_{3Z}(a)$ acting on Z(a), and we obtain an isomorphism from $(\Gamma_N, G/N)$ to $(Z(a), G_{3Z}(a))$. Thus lines 3 and 7 of Table 3 are also valid.

Suppose now that t = 2r above, so $\Gamma = X(r)$. If a and $\frac{2r}{a}$ are both even then by (1.4), N(a) contains M(r), and it follows by Lemma 2.1 (taking N = M(r) in that result) that the quotient of $(Y(r), H_k(r))$ modulo $\overline{N(a)}$ is isomorphic to the quotient of $(X(r), G_k(r))$ modulo N(a), and we have just shown that this latter quotient is isomorphic to $(X(a/2), G_k(a/2))$. Thus line 4 of Table 3 is valid. Similarly if a is odd then $\frac{2r}{a}$ is even, and again by (1.4), N(a) contains M(r). The same argument now yields that the quotient of $(Y(r), H_k(r))$ modulo $\overline{N(a)}$ is isomorphic to $(Z(a), G_{3Z}(a))$, proving that line 6 of Table 3 is valid.

It remains to consider lines 2 and 5 of Table 3. We continue to let (Γ, G) be the pair $(X(r), G_k(r))$, and we note that, if a normal quotient of (Γ, G) modulo M is 4-valent, then by [2, Theorem 1.1], M is the kernel of the G-action on the set of M-vertex-orbits in Γ . Consider now M = M(a) where $a \mid r$ (so $\frac{2r}{a}$ is even) and $1 < a \leq r$. Since $M \subseteq G = G_k(r)$, we must have a even when k = 1. Applying Lemma 2.1 with $(\Gamma', G') = (X(a), G_k(a))$ and N = N(2a), we find that the quotient of (Γ, G) modulo M is isomorphic to the quotient of $(X(a), G_k(a))$ modulo the image of M under projection from G to $G/N \cong G_k(a)$, namely $\langle (\bar{\mu}_1 \bar{\mu}_2)^a \rangle$. Thus the latter normal quotient is $(Y(a), H_k(a))$, proving that line 2 of Table 3 is valid.

For the final line, line 5, we apply Lemma 2.1 with $(\Gamma', G') = (Y(r), H_k(r))$ and N = M(r), where r is even when k = 1. Consider M = M(a), where $a \mid r$ and 1 < a < r, and note that $N \leq M$. We wish to take the quotient of (Γ', G') modulo $\overline{M} = M(a)M(r)/M(r)$, and we note that $1 < \overline{M} \leq H_k(r)$ if and only if a < r, and also a is even when k = 1. Suppose this is the case. Then by Lemma 2.1, the quotient of (Γ, G) modulo M is isomorphic to the quotient of $(Y(r), H_k(r))$ modulo the image \overline{M} of M(a) under projection from G to $G/N \cong H_k(r)$. We already proved that the former normal

quotient $(\Gamma_M, G/M)$ is isomorphic to $(Y(a), H_k(a))$. This proves that line 5 of Table 3 is valid.

Next we consider normal quotients in Table 4. Recall the definitions of the subgroups in (1.1), (1.2) and (1.3).

Lemma 5.2. For Γ , G as in Theorem 1.3 (b), and for N as in one of the lines of Table 4, the assertions about the normal quotient (Γ_N , G/N) are valid.

Proof. The N(2)-vertex-orbits on X(r) are the four subsets given in (3.1). It is straightforward to check that the underlying quotient graph of X(r) modulo N(2) is a cycle C_4 . With the first and third edge-orientations (that is, k = 1 or 3), there are oriented edges in both directions between the adjacent N(2)-orbits, so the cyclic quotient is unoriented, N(2) is the kernel of the action on the N(2)-vertex-orbits, and the induced group is D_8 . Thus line 1 of Table 4 is valid for N in $G_k(r)$ with k = 1, 3. Moreover in these cases, if r is even, then N(2) contains M(r) by (1.4), and it follows from Lemma 2.1 that the quotient of $(Y(r), H_k(r))$ modulo $\overline{N(2)}$ is isomorphic to the quotient of $(X(r), G_k(r))$ modulo N(2), namely (C_4, D_8) , proving the rest of line 1 of Table 4.

On the other hand, if k = 2, then the edges of the quotient graph of X(r) modulo N(2)(which is a 4-cycle) are oriented $\Delta_{ee} \rightarrow \Delta_{eo} \rightarrow \Delta_{oo} \rightarrow \Delta_{oe} \rightarrow \Delta_{ee}$, the kernel of the $G_2(r)$ -action on the N(2)-vertex-orbits is N(2, +), and $G_2(r)/N(2, +) \cong Z_4$. Thus line 2 of Table 4 is valid for N in $G_2(r)$. If r is even, then $M(r) \leq N(2, +)$ and arguing as in the previous paragraph, the normal quotient of $(Y(r), H_2(r))$ modulo N(2, +) is also (C_4, Z_4) , proving the rest of line 2 of Table 4.

Next suppose that r is odd and k = 2, or 3. Then the preimage in $G_k(r)$ of N(2, +), or $\overline{N(2)}$, is equal to $\langle N(2, +), \mu_1 \mu_2 \rangle$, or M(1), respectively. Each of these preimage groups has vertex-orbits $\Delta_{ee} \cup \Delta_{oo}$ and $\Delta_{eo} \cup \Delta_{oe}$ in X(r), and hence the normal quotients of $(Y(r), H_2(r))$ modulo $\overline{N(2, +)}$, and of $(Y(r), H_3(r))$ modulo $\overline{N(2)}$, are both isomorphic to (K_2, Z_2) . This proves that lines 3 and 4 of Table 4 are valid.

Now let $(\Gamma, G) = (X(r), G_3(r))$ and $(\Gamma', G') = (Y(r), H_3(r))$. First consider $N = J = \langle \mu_1 \mu_2 \rangle$. Then the *N*-vertex-orbits in Γ are the sets $B_i = \{(i + j, j) \mid j \in \mathbb{Z}_{2r}\}$ for $i \in \mathbb{Z}_{2r}$. The quotient $(\Gamma_N, G/N)$ is the unoriented cycle C_{2r} with edges of both orientations between adjacent *N*-orbits B_i, B_{i+1} (for example, $(i, 0) \rightarrow (i + 1, 0)$ and $(i, 0) \leftarrow ((i + 1) - 1, -1))$. Hence *N* is the kernel of the *G*-action on the set of *N*-orbits, and $(\Gamma_N, G/N) = (C_{2r}, D_{4r})$, as in line 5 of Table 4 for 'N in $G_3(r)$ '. The same argument with 2r replaced by *s*, proves line 5 for 'N in $G_{3Z}(s)$ ' with N = J. Continuing with N = J in $G_3(r)$, since *N* contains M(r), it follows from Lemma 2.1 that the normal quotient of (Γ', G') modulo \overline{N} is also (C_{2r}, D_{4r}) , completing the proof of line 5 of Table 4. Moreover, if we replace N by $J(+) = \langle \mu_1 \mu_2, \mu_1^r \rangle$, then the *N*-vertex-orbits become $B_i \cup B_{i+r}$, for $0 \leq i < r$, and the quotients $(\Gamma_N, G/N)$ and $(\Gamma'_{\overline{N}}, G'/\overline{N})$ both become (C_r, D_{2r}) , proving line 7 of Table 4.

Now consider $M = \langle \mu_1 \mu_2^{-1} \rangle$ in $G = G_3(r)$. The *M*-vertex-orbits in Γ are the sets $D_i = \{(i + j, -j) \mid j \in \mathbb{Z}_{2r}\}$ for $i \in \mathbb{Z}_{2r}$. All the out-neighbours of vertices in B_i lie in B_{i+1} , and hence the quotient is (an oriented) cycle of length 2r and the induced group is Z_{2r} . Moreover the element $\tau \in G$ fixes each D_i setwise and the kernel of the *G*-action on the set of *M*-orbits is $N := K = \langle M, \tau \rangle$. Thus $(\Gamma_N, G/N) = (C_{2r}, Z_{2r})$, and since *N* contains M(r), it follows from Lemma 2.1 that the normal quotient of (Γ', G') modulo \overline{N} is also (C_{2r}, Z_{2r}) , as in line 6 of Table 4. If we replace 2r by *s* and (Γ, G) by

 $(Z(s), G_{3Z}(s))$, the argument above proves line 6 for N = K in $G_{3Z}(s)$, completing the proof of line 6 of Table 4. Finally, if we replace N by $K(+) = \langle \mu_1 \mu_2^{-1}, \tau, \mu_1^r \rangle$ in $G_3(r)$, then the N-vertex-orbits in X(r) become $D_i \cup D_{i+r}$ for $0 \le i < r$, and the quotients $(\Gamma_N, G/N)$ and $(\Gamma'_N, G'/\overline{N})$ both become (C_r, Z_r) , as asserted in line 8 of Table 4. \Box

Theorem 1.3 follows from Lemmas 5.1 and 5.2.

6 Identifying the basic pairs (Γ, G) for Theorem 1.2

Each of the pairs (Γ, G) in Theorem 2 lies in $\mathcal{OG}(4)$, by Lemma 3.3. Before competing the proof of Theorem 1.2 by determining the basic graph-group pairs, we prove a preliminary lemma. The *centraliser* of a subgroup N of a group G is the subgroup $C_G(N) = \{g \in G \mid gh = hg, \forall h \in N\}$. For a prime p, $O_p(G)$ is the (unique) largest normal p-subgroup of G. By Sylow's Theorem, $O_p(G)$ is contained in every Sylow p-subgroup of G. Possibly $O_p(G) = 1$.

Lemma 6.1. Suppose that $r \ge 3$.

- (a) Let N(2) be as in (1.1), a subgroup of G(r). Then $C_{G(r)}(N(2)) = \langle \mu_1, \mu_2 \rangle$.
- (b) For t odd, $O_2(G_2(t)) = M(t)$, $O_2(G_3(t)) = \langle \mu_1^t, \mu_2^t \rangle$, and $O_2(G_{3Z}(t)) = 1$.

Proof. (a) Let $C := C_{G(r)}(N(2))$. Recall that $N(2) = \langle \mu_1^2, \mu_2^2 \rangle$ and that $\langle \mu_1, \mu_2 \rangle$ is abelian, so $\langle \mu_1, \mu_2 \rangle \leq C$. Let $K = \langle \mu_1, \mu_2, \sigma_1, \sigma_2 \rangle$. Then each element of $G(r) \setminus K$ interchanges $\langle \mu_1 \rangle$ and $\langle \mu_2 \rangle$, and hence does not centralise N(2). Thus $C \leq K$. Similarly, for i = 1, 2, any element of K not lying in $\langle \mu_1, \mu_2, \sigma_i \rangle$ inverts $\langle \mu_{3-i} \rangle$, so does not lie in C since r > 2. It follows that $C = \langle \mu_1, \mu_2 \rangle$.

(b) Let $Q = O_2(G_k(t))$ with k = 2 or 3. Since $M(t) = \langle \mu_1^t \mu_2^t \rangle \cong Z_2$ is normal in $G_k(t)$, we have $M(t) \leq Q$. Moreover, since t is odd, the normal subgroups N(2) (of order t^2) and Q intersect in the identity subgroup. Hence $Q \leq C_{G(t)}(N(2)) \cap G_k(t) = L$, say, and by part (a), $L = \langle \mu_1, \mu_2 \rangle \cap G_k(t)$. In fact Q must be contained in the unique Sylow 2-subgroup P of L. If k = 2, then P = M(t) and hence Q = M(t). If k = 3, then $P = \langle \mu_1^t, \mu_2^t \rangle$, and since this subgroup P is a normal 2-subgroup of $G_3(t)$, it follows that Q = P. Finally consider $Q = O_2(G_{3Z}(t))$. Since $|G_{3Z}(t)| = 2t^2$ with t odd, we have $|Q| \leq 2$. Suppose for a contradiction that |Q| = 2. Then $Q \cap N = 1$, where $N = \langle \mu_1, \mu_2 \rangle$ (of odd order t^2). So Q centralises N, but this implies that $G_{3Z}(t) = NQ$ is abelian, which is not the case. Hence Q = 1.

Lemma 6.2. The 'Conditions to be Basic' in Table 2 are correct, namely,

- (a) $(X(r), G_k(r))$ is basic if and only if k = 1 and r is an odd prime;
- (b) $(Y(r), H_k(r))$ is basic if and only if either r = 2, or k = 2 and r is an odd prime;
- (c) $(Z(s), G_{3Z}(s))$ is basic if and only if s is an odd prime.

Moreover the 'Basic Type' entries in Table 2 are also correct.

Proof. (a) Suppose first that $(X(r), G_k(r))$ is basic, that is, $(X(r), G_k(r))$ has no proper nondegenerate normal quotients. It follows from lines 1 and 2 of Table 3 that k = 1 and r is an odd prime.
Conversely suppose that k = 1 and r is an odd prime, and assume, for a contradiction that $G_1(r)$ has a nontrivial normal subgroup N such that $(X(r)_N, G_k(r)/N)$ is nondegenerate. Then by [2, Theorem 1.1], N is semiregular on the vertices of X(r), and this quotient has valency 4, so N has at least five vertex-orbits. Without loss of generality we may assume that N is a minimal normal subgroup of $G_1(r)$. Now $N \cap N(2) = 1$ would imply that $N \leq C_{G_1(r)}(N(2))$, and hence by Lemma 6.1 that $N \leq \langle \mu_1, \mu_2 \rangle \cap G_1(r) = N(2)$, which in turn implies $N \leq N \cap N(2) = 1$, a contradiction. Hence $N \cap N(2) \neq 1$, so by the minimality of N, we have $N \leq N(2)$. Since N(2) has only four vertex orbits in X(r), N must be a proper subgroup of N(2), and since $|N(2)| = r^2$ and r is an odd prime, it follows that |N| = r. Since N is normalised by $\tau \in G_1(r)$, it follows that $N \neq \langle \mu_i^2 \rangle$ for i = 1 or i = 2, and hence that $N = \langle \mu_1^2 \mu_2^{2i} \rangle$ for some i such that $1 \leq i < r$. Now N must contain $(\mu_1^2 \mu_2^{2i})^{\tau} = \mu_2^2 \mu_1^{2i}$. Since the only element of N projecting to μ_1^{2i} is $(\mu_1^2 \mu_2^{2i})^i$, we have $\mu_2^2 \mu_1^{2i} = (\mu_1^2 \mu_2^{2i})^i$, and hence $\mu_2^{2(i^2-1)} = 1$, so $i^2 \equiv 1 \pmod{r}$. This implies that i = 1 or r - 1. However neither $\langle \mu_1^2 \mu_2^2 \rangle$ nor $\langle \mu_1^2 \mu_2^{2(r-1)} \rangle$ is normalised by $\mu_1 \sigma_2 \in G_1(r)$. This is a contradiction. Therefore $(X(r), G_k(r))$ is basic when k = 1 and r is an odd prime. Moreover $(X(r), G_1(r))$ is basic of cycle type, see line 1 of Table 4.

(b) Suppose next that $(\Gamma', G') = (Y(r), H_k(r))$ is basic, where r is even if k = 1. It follows from lines 4, 5 and 6 of Table 3 that either r = 2, or k = 2 and r is an odd prime. Now we prove the converse. Suppose that r = 2, or k = 2 and r is an odd prime. Let M be a minimal normal subgroup of $G' = H_k(r)$ and consider the quotient Γ'_M . If $(\Gamma'_M, G'/M)$ is nondegenerate (hence of valency 4), then by [2, Theorem 1.1], M is semiregular with at least five vertex-orbits on Γ' , and M is the kernel of the G'-action on the M-orbits. On the other hand if $(\Gamma'_M, G'/M)$ is degenerate, then we replace M by the kernel of the G'-action on the M-orbits. We consider the possibilities for $(\Gamma'_M, G'/M)$: in particular if none are nondegenerate then (Γ', G') is basic.

Suppose first that r = 2. Then the graph Γ' has only eight vertices, and hence M has at most four vertex-orbits, so all quotients $(\Gamma'_M, G'/M)$ are degenerate. Thus if r = 2, then (Γ', G') is basic. It is basic of cycle type, by lines 1 and 2 of Table 4.

Suppose now that k = 2 and r is an odd prime. Note that the normal subgroup N(2)of G' has just two vertex-orbits, each of size r^2 , on Γ' . If M contains $\overline{N(2)}$ then by the minimality of M, $M = \overline{N(2, +)}$ (the kernel of the G'-action on the $\overline{N(2)}$ -orbits) and $(\Gamma'_M, G'/M) = (K_2, Z_2)$ as in line 4 of Table 4. Suppose now that $M \not\supseteq \overline{N(2)}$. By Lemma 2.1, since (Γ', G') is isomorphic to the normal quotient of $(\Gamma, G) = (X(r), G_k(r))$ modulo the normal subgroup N = M(r) of G (Table 3, line 2), it follows that $(\Gamma'_M, G'/M)$ is isomorphic to a normal quotient $(\Gamma_L, G/L)$ for some normal subgroup L of G such that $N \leq L$ and L is the kernel of the G-action on the L-vertex-orbits on Γ , and $G/L \cong G'/M$. Moreover L/N corresponds to M under the isomorphism $G \to G'$. In particular, L/N is a minimal normal subgroup of G/N if M is a minimal normal subgroup of G', and since $M \not\supseteq \overline{N(2)}$ we have $L \not\supseteq N(2)$.

If |L| is not divisible by (the odd prime) r, then L is a normal 2-subgroup of $G = G_2(r)$ properly containing N = M(r). Hence $L \leq O_2(G)$ and $O_2(G) \neq M(r)$, contradicting Lemma 6.1(b). Thus |L| is divisible by r. Then $L' := L \cap N(2) \neq 1$, and $L' \neq N(2)$ since $L \not\supseteq N(2)$. Since $|N(2)| = r^2$, it follows that |L'| = r, and, being the intersection of two normal subgroups, L' is normal in $G = G_2(r)$. We argue as in the proof of part (a): $L' \neq \langle \mu_i^2 \rangle$ for i = 1 or i = 2 since L' is normalised by $\tau \mu_1$. So $L' = \langle \mu_1^2 \mu_2^{2i} \rangle$, for some i such that $1 \leq i < r$. However $\sigma_2 \in G_2(r)$ and σ_2 does not normalise L', contradiction. Thus there is no proper normal quotient $(\Gamma'_M, G'/M)$ with $M \not\supseteq \overline{N(2)}$. Hence (Γ', G') is basic and its only proper normal quotient is (K_2, Z_2) . This implies that (Γ', G') is basic of biquasiprimitive type, see Table 1, and completes the proof of part (b).

(c) Suppose now that $(\Gamma, G) = (Z(s), G_{3Z}(s))$, where s is odd. If (Γ, G) is basic then it follows from line 7 of Table 3 that s is an odd prime. Suppose conversely that s is an odd prime. Let M be a nontrivial normal subgroup of G which is equal to the kernel of the G-action on the M-orbits in Γ , and consider $(\Gamma_M, G/M)$. If M contains $N = N(1) = \langle \mu_1, \mu_2 \rangle$ (of order s^2), then since N is vertex-transitive on Z(s), we have M = G and $(\Gamma_M, G/M) = (K_1, 1)$. So assume that $N \not\subseteq M$. If $M \cap N = 1$, then M is a normal subgroup of G of order dividing |G|/|N| = 2, and so |M| = 2 and $M \leq O_2(G)$, contradicting Lemma 6.1. Thus $M \cap N$ must have order s, and must be normal in G. Since $M \cap N$ is normalised by $\tau \in G$, it follows that $M \cap N = \langle \mu_1 \mu_2^{\pm 1} \rangle$, that is, $M \cap N$ is either J or the derived subgroup K' of K, as defined in (1.2). If $M \cap N = K'$, then the orbits of $M \cap N$ and K are the same. Thus Γ_M is a quotient of $\Gamma_{M \cap N}$ which, in either case, is a cycle of length s, by lines 5 and 6 of Table 4. Thus (Γ, G) is basic of cycle type, completing the proof of part (c).

Finally we observe that Theorem 1.2 follows from Lemma 3.3 (for membership in $\mathcal{OG}(4)$), and Lemma 6.2.

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Vertex-transitive graphs and their arc-types

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Abstract

Let X be a finite vertex-transitive graph of valency d, and let A be the full automorphism group of X. Then the *arc-type* of X is defined in terms of the sizes of the orbits of the stabiliser A_v of a given vertex v on the set of arcs incident with v. Such an orbit is said to be *self-paired* if it is contained in an orbit Δ of A on the set of all arcs of X such that Δ is closed under arc-reversal. The arc-type of X is then the partition of d as the sum $n_1 + n_2 + \cdots + n_t + (m_1 + m_1) + (m_2 + m_2) + \cdots + (m_s + m_s)$, where n_1, n_2, \ldots, n_t are the sizes of the self-paired orbits, and $m_1, m_1, m_2, m_2, \ldots, m_s, m_s$ are the sizes of the non-self-paired orbits, in descending order. In this paper, we find the arc-types of several families of graphs. Also we show that the arc-type of a Cartesian product of two 'relatively prime' graphs is the natural sum of their arc-types. Then using these observations, we show that with the exception of 1 + 1 and (1 + 1), every partition as defined above is *realisable*, in the sense that there exists at least one vertex-transitive graph with the given partition as its arc-type.

Keywords: Symmetry type, vertex-transitive graph, arc-transitive graph, Cayley graph, Cartesian product, covering graph.

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1 Introduction

Vertex-transitive graphs hold a significant place in mathematics, dating back to the time of first recognition of the Platonic solids, and also now in other disciplines where symmetry (and even other properties such as rigidity) play an important role, such as fullerene chemistry, and interconnection networks.

A major class of vertex-transitive graphs is formed by Cayley graphs, which represent groups in a very natural way. (For example, the skeleton of the C_{60} molecule is a Cayley graph for the alternating group A_5 .) It is relatively easy to test whether a given vertextransitive graph is a Cayley graph for some group: by a theorem attributed to Sabidussi [23], this happens if and only if the automorphism group of the graph contains a subgroup that acts regularly on vertices. Vertex-transitive graphs that fail this test are relatively rare, the Petersen graph being a famous example. A recent study of small vertex-transitive graphs of valency 3 in [18] shows that among 111360 such graphs of order up to 1280, only 1434 of them are not Cayley graphs.

For almost every Cayley graph, the automorphism group itself acts regularly on vertices (see [1]). Any such graph is called a *graphical regular representation* of the group G, or briefly, a *GRR*. In a book by Coxeter, Frucht and Powers [8] devoted to the study of 3-valent GRRs, vertex-transitive 3-valent graphs were classified into four types, according to the action of the automorphism group on the *arcs* (ordered pairs of adjacent vertices) of the graph. One class consists of those graphs which are arc-transitive, another of those for which there are two orbits on arcs, and the other two are two classes of GRRs. Arc-transitive graphs are also called *symmetric*.

Symmetric graphs have been studied quite intensively, especially in the 3-valent case, by considering the action of the automorphism group on non-reversing walks of given length *s*, known as *s*-arcs. For example, it was shown by Tutte [26, 27] that every finite symmetric 3-valent graph is *s*-arc-regular for some $s \le 5$, and hence that the order of the stabiliser of a vertex in the automorphism group of every such graph is bounded above by 48. Tutte's theorem and related work have been used to determine all symmetric 3-valent graphs on up to 10,000 vertices; see [9, 6, 5]. Also Tutte's seminal theorem was generalised much later by Weiss, who used the classification of doubly-transitive permutation groups to prove that every finite symmetric graph of valency greater than 2 is *s*-arc-transitive but not (s+1)-arc-transitive for some $s \le 7$, and in particular, that there are no 8-arc-transitive finite graphs; see [29].

Another important class of vertex-transitive graphs was investigated by Tutte [28] and Bouwer [3], namely the graphs that are vertex- and edge-transitive but not arc-transitive. These are now called *half-arc-transitive graphs*. Every such graph has even valency, and its automorphism group has two orbits on arcs, with every arc (v, w) and its reverse (w, v)lying in different orbits; see [28, p. 59]. Bouwer [3] constructed a family of examples containing one half-arc-transitive graph of each even valency greater than 2, and the first and third authors of this paper have recently proved that other examples of the type considered by Bouwer produce infinitely many of every such valency; see [7].

According to Coxeter, Frucht and Powers [8], the idea of classifying cubic vertextransitive graphs with respect to the arc-orbits of the automorphism group originated in some work by Ronald Foster over half a century ago, which was presented to his friends in the form of unpublished notes. The classification is carried out rigorously in their book [8]. Although Foster's original idea of 'zero-symmetric' graphs was later expanded to other valencies under the term GRR, the classification by arc-orbits itself was never extended in a systematic way to graphs of other valencies. This paper provides a remedy for that omission. By introducing the concept of 'arc-type', we provide a language that can be used to unify the notions of arc-transitivity and half-arc-transitivity and the above-mentioned classification of symmetric 3-valent graphs, and also to extend this classification to vertex-transitive graphs of higher valency.

We can now define the notion of arc-type for a vertex-transitive graph. Let X be a d-valent vertex-transitive graph, with automorphism group A. We first make a critical observation about the pairing of arc-orbits. The orbit of an arc (v, w) under the action of A can be *paired* with the orbit of A containing the reverse arc (w, v), and if these orbits are the same, then the given orbit is said to be *self-paired*. This is similar to the definition of paired orbitals for transitive permutation groups. But here we will abuse notation and extend the definition to the orbits of the stabiliser A_v in A of a vertex v on the arcs emanating from v, and say that the orbit of A_v containing the arc (v, w) is *self-paired* if (v, w) lies in the same orbit of A as its reverse (w, v).

We define the *arc-type* of X as the partition Π of d as the sum

$$\Pi = n_1 + n_2 + \dots + n_t + (m_1 + m_1) + (m_2 + m_2) + \dots + (m_s + m_s) \qquad (\dagger)$$

where n_1, n_2, \ldots, n_t are the sizes of the self-paired arc-orbits of A_v on the arcs emanating from v, and $m_1, m_1, m_2, m_2, \ldots, m_s, m_s$ are the sizes of the non-self-paired arc-orbits, in descending order.

Similarly, the *edge-type* of X is the partition of d as the sum of the sizes of the orbits of A_v on edges incident with v, and can be found by simply replacing each bracketed term $(m_j + m_j)$ by $2m_j$ (for $1 \le j \le s$).

The number of possibilities for the arc-type Π depends on the valency d. For d = 1 there is just one possibility, namely with $n_1 = 1$, and this occurs for the complete graph K_2 . For d = 2, in principle there could be three possibilities, namely 2, 1 + 1 and (1 + 1), but every 2-valent connected graph is a cycle, and is therefore arc-transitive, with arc-type 2. In particular, 1 + 1 and (1 + 1) cannot occur as arc-types. For d = 3 there are four possibilities (namely 3, 2 + 1, 1 + 1 + 1 and 1 + (1 + 1)), and they all occur, as shown in [8]. A natural question arises as to what arc-types occur for higher valencies.

In this paper, we provide some basic theory for arc-types, which helps us to answer that question. In particular, we give for each positive integer d the number of different partitions of the above form (†) for d, by means of a generating function. This gives a closed form solution for the number of different possibilities in the case of a GRR of given valency d. (As a curiosity, we mention that there is also a connection with the different root types of polynomials with real coefficients.)

Then our main theorem states that with the exception of 1+1 and (1+1), every partition Π as defined in (†) is *realisable*, in the sense that there exists at least one vertex-transitive graph with Π as its arc-type. To prove this, we consider how to combine 'small' vertex-transitive graphs into a larger vertex-transitive graph, preserving (but increasing the number of) the summands in the arc-type. The key step is to show that the arc-type of a Cartesian product of such graphs is just the sum of their arc-types, when the graphs are 'relatively prime' with respect to the Cartesian product.

Our proof of the theorem then reduces to finding suitable 'building blocks', to use as base cases for the resulting construction. Several interesting families and examples of graphs are found to be helpful. In particular, we introduce the concept of a special kind of *thickened cover* of a graph, obtained by replacing some edges of the given graph by complete bipartite graphs, and other edges by ladder graphs (with 'parallel' edges). Under some special conditions, the thickened cover is vertex-transitive, and it is easy to compute its arc-type from the arc-type of the given base graph. Note that this does not work in general. It can happen that a group G acts transitively on the vertices of the graph, with given arc-type, but the full automorphism group is larger than G. The challenge is to ensure that no further automorphisms are admitted.

Finally, as a corollary of our main theorem, we show that every standard partition of a positive integer d is realisable as the *edge-type* of a vertex-transitive graph of valency d, except for 1 + 1 (when d = 2).

Vertex-transitive graphs are key players in algebraic graph theory, but also (as intimated earlier) they have important applications in other branches of mathematics. In group theory they play a crucial role as Cayley graphs. In geometry they are encountered in convex and abstract polytopes, incidence geometries, and configurations, and in manifold topology they feature in the study of regular and chiral maps and hypermaps, and Riemann and Klein surfaces with large automorphism groups.

Classification of vertex-transitive graphs by their edge- or arc-type gives a new viewpoint, and helps provide a better understanding of their structure. This approach can also be fruitful in terms of determining all small examples of various kinds of graphs, akin to the census of 3-valent symmetric graphs on up to 10000 vertices [9, 6, 5], the census of vertextransitive graphs up to 31 vertices [22], or the census of small 4-valent half-arc-transitive graphs and arc-transitive digraphs of valency 2 [20]. For example, the construction used by Potočnik, Spiga and Verret to obtain their census of vertex-transitive 3-valent graphs on up to 1280 vertices in [18] depends on the edge-type, and their census of all connected quartic arc-transitive graphs of order up to 640 (also in [18]) was obtained by associating some of them with vertex-transitive 3-valent graphs of edge-type 2+1 (and using cycle decompositions); see also [19, 21]. In these cases it was a stratified approach that enabled the limits of the census to be pushed so high, and it is likely that for graphs of higher valency or larger order, this kind of approach will be invaluable.

2 Preliminaries

All the graphs we consider in this paper are finite, simple, undirected and non-trivial. Given a graph X, we denote by V(X) and E(X) the set of vertices and the set of edges of X, respectively. We denote an edge of X with vertices u and v by $\{u, v\}$, or sometimes more briefly by uv. We will occasionally use *triangle* (respectively *quadrangle*) to denote an unoriented 3-cycle (resp. 4-cycle) in a graph, and will say that two triangles are disjoint if they have no vertex in common. For any vertex v of X, we denote by E(v) the set of edges of X incident with v. An *arc* is an ordered pair of adjacent vertices, and we denote by A(X) the set of all arcs of X. Associated with each edge $\{u, v\}$ there are two arcs, which we denote by (u, v) and its reverse (v, u). Also we define A(v) as the set of all arcs (v, w)of X emanating from a given vertex v.

The automorphism group of X is denoted by $\operatorname{Aut}(X)$. Note that the action of $\operatorname{Aut}(X)$ on the vertex-set V(X) also induces an action of $\operatorname{Aut}(X)$ on the edge-set E(X) and one on the arc-set A(X). If the action of $\operatorname{Aut}(X)$ is transitive on the vertex-set, edge-set, or arc-set, then we say that X is *vertex-transitive*, *edge-transitive* or *arc-transitive*, respectively. An arc-transitive graph is often also called *symmetric*. The graph X is *half-arc-transitive* if it is vertex-transitive, but not arc-transitive. Note that the valency of

a half-arc-transitive graph is necessarily even; see [28, p. 59].

In this paper we only consider vertex-transitive graphs. Obviously, vertex-transitive graphs are always regular. Moreover, because a disconnected vertex-transitive graph consists of pairwise isomorphic connected components, we may restrict our attention here to connected graphs. Also we will sometimes use 'VT' as an abbreviation for vertex-transitive.

Next, let G be a group, and let S be a subset of G that is inverse-closed and does not contain the identity element. Then the Cayley graph $\operatorname{Cay}(G, S)$ is the graph with vertexset G, and with vertices u and v being adjacent if and only if $vu^{-1} \in S$ (or equivalently, v = xu for some $x \in S$). Since we require S to be inverse-closed, this Cayley graph is undirected, and since S does not contain the identity, the graph has no loops. Also $\operatorname{Cay}(G,S)$ is regular, with valency |S|, and is connected if and only if S generates G. Furthermore, it is easy to see that G acts as a group of automorphisms of $\operatorname{Cay}(G,S)$ by right multiplication, and this action is transitive on vertices, with trivial stabiliser, and so this action of G on $\operatorname{Cay}(G,S)$ is sharply-transitive (or regular). Hence in particular, $\operatorname{Cay}(G,S)$ is vertex-transitive.

Indeed the following (which is attributed to Sabidussi [23]) shows how to recognise Cayley graphs:

Lemma 2.1. A graph X is a Cayley graph for the group G if and only if G acts regularly on V(X) as a group of automorphisms. More generally, a graph X is a Cayley graph if and only if some subgroup of Aut(X) acts regularly on V(X).

Observe that for a fixed $x \in S$, all the edges of form $\{u, xu\}$ and $\{u, x^{-1}u\}$ for $u \in G$ lie in the same edge-orbit (as each other) under the automorphism group of $\operatorname{Cay}(G, S)$, and similarly, that all the arcs of the form (u, xu) lie in the same arc-orbit. If all such arc-orbits are distinct, then G is the full automorphism group of $\operatorname{Cay}(G, S)$, and $\operatorname{Cay}(G, S)$ is called a graphical regular representation of the group G, or briefly a GRR for G. Another term for such a graph is zero-symmetric. Note that if X is a connected zero-symmetric graph (or GRR) with valency d, then X has d arc-orbits, and all the arcs emanating from a given vertex v lie in different arc-orbits. Moreover, if $G = \operatorname{Aut}(X)$, then the stabiliser G_v of any vertex v must fix each neighbour of v, and then by connectedness, it follows that G_v is trivial. Thus G acts regularly on V(X), and so by Lemma 2.1, the graph X is a Cayley graph for G.

Next, we describe another group-theoretic construction, for a special class of vertextransitive graphs. Let G be a group, let H be a subgroup of G, and let a be an element of G such that $a^2 \in H$. Now define a graph $\Gamma = \Gamma(G, H, a)$ by setting

$$V(\Gamma) = \{Hg : g \in G\}$$
 and $E(\Gamma) = \{\{Hx, Hy\} : x, y \in G \mid xy^{-1} \in HaH\}.$

This graph Γ is called a (*Sabidussi*) double coset graph. As with Cayley graphs, the given group G induces a group of automorphisms of $\Gamma(G, H, a)$ by right multiplication, since $(xg)(yg)^{-1} = xgg^{-1}y^{-1} = xy^{-1} \in HaH$ whenever $\{Hx, Hy\} \in E(\Gamma)$. Again this action is vertex-transitive, since $(Hx)x^{-1}y = Hy$. Moreover, the stabiliser of the vertex H is $G_H = \{g \in G | Hg = H\}$, which is H itself, and this acts transitively on the neighbourhood $\{Hah : h \in H\}$ of H, so in fact $\Gamma(G, H, a)$ is arc-transitive. Conversely, every non-trivial arc-transitive graph X can be constructed in this way, by taking $G = \operatorname{Aut}(X)$, and $H = G_v$ for some $v \in V(X)$, and a as any automorphism in G that interchanges v with one of its neighbours. Finally, we mention a convenient way to describe cubic Hamiltonian graphs, that will be helpful later. Let X be a cubic Hamiltonian graph on n vertices. Label the vertices of X with numbers $0, \ldots, n-1$, such that vertices i and i + 1 are consecutive in a given Hamilton cycle for $0 \le i < n$ (treated modulo n). Each vertex i is adjacent to i - 1 and $i + 1 \pmod{n}$, and to one other vertex, which has label v_i , say. Now define $d_i = v_i - i$ for $0 \le i < n$. Then the *LCF-code* of X is given by the sequence $[d_0, \ldots, d_{n-1}]$. Clearly the LCF-code defines the graph X, since the edges are $\{i, i + 1\}$ for all $i \pmod{n}$ and $\{i, i + d_i\}$ for all $i \pmod{n}$. On the other hand, the LCF is not necessarily unique for X, since it depends on the choice of Hamilton cycle. Note also that if the code sequence is periodic, then it is sufficient to list a sub-sequence and indicate how many times it repeats, using a superscript. For example, $[3, -3]^4$ is the LCF-code of a 3-dimensional cube.

3 Edge-types and integer partitions

Let X be a vertex-transitive graph of valency d, and let $\{\Delta_1, \ldots, \Delta_k\}$ be the set of orbits of $G = \operatorname{Aut}(X)$ on E(X). This partition of E(X) into orbits also induces a partition of the set E(v) of all edges incident with a given vertex v, namely into the sets $E(v) \cap \Delta_i$ for $1 \le i \le k$. These are simply the restrictions of the edge-orbits Δ_i to the set E(v).

If we let $\ell_i = |E(v) \cap \Delta_i|$ for each *i*, then we may define the *edge-type* of X to be the partition of the valency d as the sum

$$\ell_1 + \ell_2 + \dots + \ell_k,$$

where we assume the numbers ℓ_i are in descending order. Note that by vertex-transitivity, the numbers ℓ_i do not depend on the choice of v. (Indeed when X is finite, counting incident vertex-edge pairs (v, e) with $e \in \Delta_i$ gives $2|\Delta_i| = |V(X)|\ell_i$ and therefore $\ell_i = 2|\Delta_i|/|V(X)|$ for each i.) Hence in particular, the edge-type does not depend on the choice of v. We denote the edge-type of X by et(X).

It is not at all obvious as to which partitions can occur as the edge-type of a vertextransitive graph. The edge-type of a vertex-transitive cubic graph can be 3, or 2 + 1, or 1 + 1 + 1, while that of a vertex-transitive quartic graph can be 4, or 3 + 1, or 2 + 2, or 2 + 1 + 1, or 1 + 1 + 1 + 1. We will see instances of all of these in Section 5. Then later, in Section 9, we will show that with the exception of 1 + 1 (for d = 2), every standard partition of a given positive integer d can be realised as an edge-type.

To enumerate the possibilities for a given valency d, we may use generating functions for integer partitions. Let p(d, k) denote the number of partitions of d with k parts, and let p(d) denote the number of partitions of an integer d. Obviously, $p(d) = \sum_k p(d, k)$.

The generating functions for integer partitions are very well-known, and can be found in [30, p. 100] for example. In fact, the generating function P(x, y) for p(d, k) is given by

$$P(x,y) = \sum_{d} \sum_{k \ge 0} p(d,k) y^k x^d = \prod_{n \ge 1} \frac{1}{1 - yx^n},$$

and then by taking y = 1, we get

$$P(x) = \prod_{n \ge 1} \frac{1}{1 - x^n} = \sum_{d \ge 0} p(d) x^d$$

as the generating function for p(d) itself.

4 Arc-types and marked partitions

In this section we refine the notion of edge-type of a vertex-transitive graph X, by considering the action of Aut(X) on the arcs of X.

Let Δ be an orbit of $\operatorname{Aut}(X)$ on A(X), and let $\Delta^* = \{(v, u) : (u, v) \in \Delta\}$ be its *paired* orbit, in the same way that a permutation group on a set Ω has paired orbitals on the Cartesian product $\Omega \times \Omega$. Note that Δ^* is also an orbit of $\operatorname{Aut}(X)$ on A(X), and that the union $\Delta \cup \Delta^*$ consists of all the arcs obtainable from an orbit of $\operatorname{Aut}(X)$ on edges of X. We say that Δ is *self-paired* if $\Delta = \Delta^*$ and *non-self-paired* if $\Delta \neq \Delta^*$.

We can now write the orbits of Aut(X) on A(X) as

$$\Delta_1, \ldots, \Delta_t, \ \Delta_{t+1}, \Delta_{t+1}^*, \ldots, \Delta_{t+s}, \Delta_{t+s}^*,$$

where $\Delta_1, \ldots, \Delta_t$ are self-paired, while $\Delta_{t+1}, \ldots, \Delta_{t+s}$ are non-self-paired.

This partition of A(X) into the orbits of Aut(X) also induces a partition of the set of arcs emanating from a given vertex. For any vertex v of X, define $n_i = |A(v) \cap \Delta_i|$ for $1 \le i \le t$, and $m_j = |A(v) \cap \Delta_j|$ for $t+1 \le j \le t+s$. Again since X is vertex-transitive, these numbers do not depend on the choice of v, and then furthermore, arc-reversal gives $|A(v) \cap \Delta_j| = |A(v) \cap \Delta_j| = m_j$ for $t+1 \le j \le t+s$.

Hence the n_i are the sizes of the self-paired arc-orbits restricted to A(v), while the m_j are the sizes of the non-self-paired arc-orbits restricted to A(v), and thus we obtain

 $d = |A(v)| = n_1 + \dots + n_t + (m_1 + m_1) + \dots + (m_s + m_s),$

just as in (†) in the Introduction. This is the *arc-type* of X, and we denote it by at(X).

We may call the expression on the right-hand-side of the above a *marked partition* of the integer d. By this, we mean simply a partition in which some pairs of equal-valued summands are placed in parentheses. Note that the parentheses in a marked partition Π are important, because when Π represents the arc-type of a VT graph, they indicate that the two numbers summed between the parentheses are the sizes of two paired arc-orbits corresponding to the same edge-orbit.

Since the order of the arc-orbits of each of the two kinds (self-paired and non-selfpaired) can be chosen arbitrarily, we may consider two marked partitions to be equal if they have the same summands, possibly in a different order. Usually we will assume that the summands of each kind (unbracketed and bracketed) are in descending order, so that $n_1 \ge \cdots \ge n_t$ and $m_1 \ge \cdots \ge m_s$.

In a sense, the three most important classes of vertex-transitive graphs are the arctransitive, half-arc-transitive and zero-symmetric graphs, and their arc-types are as follows:

- Arc-transitive graphs of valency d have arc-type d;
- Half-arc-transitive graphs of even valency d have arc-type (d/2 + d/2);
- Zero-symmetric graphs have arc-type $1 + \ldots + 1 + (1+1) + \ldots + (1+1)$.

In particular, it follows that there are $\lfloor d/2 \rfloor + 1$ possibilities for the arc-type of a *d*-valent zero-symmetric graph (or GRR).

At this point, we recall that the arc-type of a VT graph X depends on the action of the G = Aut(X) on the arcs of X, and in particular, the action of the vertex-stabiliser G_v on the neighbourhood X(v) of a given vertex v. The summands in the arc-type of X are just

the sizes of the orbits of G_v on the neighbourhood of a vertex v of X, while the brackets depend on the pairings of arc-orbits of G.

By finding the generating function for the set of marked partitions, we can count the (maximum) number of possible arc-types for each valency d.

Let t'(d, k) denote the number of marked partitions of d with k parts, and let t(d) denote the number of marked partitions of an integer d. Obviously, $t(d) = \sum_k t'(d, k)$. We can obtain the generating function T'(x, y) for t'(d, k) by adapting the generating function for standard partitions, to take account of the bracketed pairs. This can be found from [30, p. 95], for example, and is as follows:

$$T'(x,y) = \sum_{d \ge 0} \sum_{k \ge 0} t'(d,k) x^d y^k = \prod_{n \ge 1} \frac{1}{(1-yx^n)(1-y^2x^{2n})}.$$

Then by taking y = 1, we get

$$T(x) = T'(x, 1) = \prod_{n \ge 1} \frac{1}{(1 - x^n)(1 - x^{2n})} = \sum_{d \ge 0} t(d)x^d$$

as the generating function for t(d) itself.

Here we remark that a different combinatorial approach can be taken for the generating function T(x), namely through refining integer partitions by labelling some even parts (with an asterisk). For example, the partition 6 = 2 + 2 + 1 + 1 gives rise to three labelled partitions: 6 = 2 + 2 + 1 + 1, $6 = 2 + 2^* + 1 + 1$, and $6 = 2^* + 2^* + 1 + 1$.

Now let $t^*(d, k)$ denote the number of labelled partitions of an integer d having k parts. Then the generating function for $t^*(d, k)$ is

$$T^*(x,y) = \sum_{d \ge 0} \sum_{k \ge 0} t^*(d,k) x^d y^k = \prod_{n \ge 1} \frac{1}{(1-yx^n)(1-yx^{2n})},$$

and we find that $T^*(x, 1) = T'(x, 1) = T(x)$.

Also we note that the generating function T(x) defines the sequence

 $1, 1, 3, 4, 9, 12, 23, 31, 54, 73, 118, \ldots,$

which is denoted by A002513 in The On-Line Encyclopedia of Integer Sequences [24].

Finally, it should come as no surprise that marked partitions of a positive integer d can be used also to count different types of solutions of a real polynomial equation of degree d, when attention is paid whether the roots are real and unequal, real and equal (in various combinations) or simple or multiple complex conjugate; see [4].

5 Edge-types and arc-types for small valency

In this section we give examples of vertex-transitive graphs with every possible edge-type and arc-type, for valencies up to 4, and summarise the information in Table 1 at the end. Note that it is enough to find examples of VT graphs for each arc-type, since the same graphs will give also all the possible edge-types. We do not give a proof that the arc-type is as claimed in each case, since that can be easily verified by computer (using for example Magma [2]), or in some cases by hand. Graphs with arc-type 1 + 1 + 1 of order up to 120 are given in [8, Part III], and graphs with arc-type (1 + 1) + 1 of order up to 120 are given in [8, Part II]. The other zero-symmetric graphs listed here were found with the help of Magma [2], by checking the Cayley graphs for certain kinds of generating sets for small groups. In some cases, we give the smallest possible example with the given arc-type. Some examples were found by also checking tables of vertex-transitive graphs on up to 31 vertices; see [22].

Valency d = 1 (one case):

(P1) There is only one marked partition of 1, namely 1, and only one VT graph with this arc-type, namely the complete graph K_2 .

Valency d = 2 (three cases):

- (P2) 2 = 2: For every $n \ge 3$, the simple cycle C_n has arc-type 2.
- (P3) 2 = 1 + 1: No VT graph has arc-type 1 + 1, because cycles are the only connected regular graphs with valency 2.
- (P4) 2 = (1+1): No VT graph has arc-type (1+1), because cycles are the only connected regular graphs with valency 2.

Valency d = 3 (four cases):

- (P5) 3 = 3: The VT graphs with arc-type 3 are precisely the arc-transitive cubic graphs, and there are infinitely many examples, the smallest of which is the complete graph K_4 . Numerous other small examples, including the ubiquitous Petersen graph, are given in the Foster census [9], which was later expanded by Conder and Dobcsányi [6], and again further by Conder [5] up to order 10000.
- (P6) 3 = 2 + 1: The smallest VT graph with arc-type 2 + 1 is the triangular prism, on 6 vertices; see Figure 1. It is easy to see that the edges on the two triangles form one edge-orbit, while all the other edges form another orbit.



Figure 1: The triangular prism, which has arc-type 2 + 1

(P7) 3 = 1 + 1 + 1: The smallest VT graph with arc-type 1 + 1 + 1 is the zero-symmetric graph on 18 vertices from [8, p. 4]; see also Figure 2. This is the Cayley graph of a group of order 18 generated by three involutions, and it can also be described as a cubic Hamiltonian graph with LCF-code $[5, -5]^9$.



Figure 2: The smallest VT graph with arc-type 1 + 1 + 1, on 18 vertices

(P8) 3 = 1+(1+1): The smallest VT graph with arc-type 1+(1+1) is the zero-symmetric graph on 20 vertices from [8, p. 35]; see Figure 3. This is the Cayley graph of a group of order 20, generated by one involution and one non-involution, and it can also be described as a cubic Hamiltonian graph with LCF-code $[6, 6, -6, -6]^5$. For more properties of this graph, see Lemma 8.4.



Figure 3: The smallest VT graph with arc-type 1 + (1 + 1), on 20 vertices

Valency d = 4 (nine cases):

- (P9) 4 = 4: The VT graphs with arc-type 4 are arc-transitive quartic graphs. The smallest example is the complete graph K_5 .
- (P10) 4 = (2 + 2): The VT graphs with arc-type (2 + 2) are half-arc-transitive quartic graphs. The smallest example is the Holt graph [12], of order 27; see Figure 4.



Figure 4: The Holt graph (the smallest 4-valent half-arc-transitive graph)

- (P11) 4 = 3 + 1: The smallest VT graph with arc-type 3 + 1 is $K_4 \square K_2$, which is the Cartesian product of K_4 and K_2 . The two summands K_4 and K_2 have arc-types 3 and 1, respectively, and are 'relatively prime'. The example will be generalised in Theorem 6.6.
- (P12) 4 = 2 + 2: The smallest VT graph with arc-type 2 + 2 is the circulant graph $Cay(\mathbb{Z}_7; \{1, 2\})$ on 7 vertices, where \mathbb{Z}_7 is viewed as an additive group. This graph is shown in Figure 5. Each of the edges on the outer 7-cycle lies in two triangles while each edge of the inner 7-cycle lies in only one triangle, and it follows that $Cay(\mathbb{Z}_7; \{1, 2\})$ has two edge orbits.



Figure 5: The circulant $Cay(\mathbb{Z}_7; \{1, 2\})$, which has arc-type 2 + 2

(P13) 4 = 2 + (1 + 1): The graph on 40 vertices in Figure 6 is the smallest known VT graph with arc-type 2 + (1 + 1). It is a thickened cover of the trivalent graph on 20 vertices with arc-type (1 + 1) + 1; see Section 7 for generalisations of this.



Figure 6: A VT graph with arc-type 2 + (1 + 1), on 40 vertices

(P14) 4 = (1+1) + (1+1): The graph on 42 vertices in Figure 7 is the smallest VT graph with arc-type (1+1) + (1+1). As a GRR, it is a Cayley graph of the group $C_7 \rtimes C_6$ with generating set that contains an element of order 6, an element of order 7, and their inverses. For more details on this graph see Lemma 8.6.



Figure 7: On the left is the smallest VT graph with arc-type (1+1)+(1+1), on 42 vertices — and on the right is an illustration of an embedding of this graph on the torus, using a hexagon with opposite sides identified

(P15) 4 = 2 + 1 + 1: The graph on 12 vertices in Figure 8 is the smallest VT graph with arc-type 2 + 1 + 1. It can be obtained from the hexagonal prism by adding diagonals to three non-adjacent quadrangles.



Figure 8: The smallest VT graph with arc-type 2 + 1 + 1, on 12 vertices

(P16) 4 = 1 + 1 + (1 + 1): The graph on 20 vertices in Figure 9 is the smallest VT graph with arc-type 1 + 1 + (1 + 1). If G is the Frobenius group $C_5 \rtimes C_4$ of order 20, generated by the permutations a = (1, 2, 3, 4, 5) and b = (2, 3, 5, 4), which satisfy the relations $a^5 = b^4 = 1$ and $b^{-1}ab = a^2$, then this graph is the Cayley graph (in fact a GRR) for G given by the generating set $S = \{ab^2, a^2b^2, b, b^{-1}\}$.



Figure 9: The smallest VT graph with arc-type 1 + 1 + (1 + 1), on 20 vertices

(P17) 4 = 1 + 1 + 1 + 1: The graph on 16 vertices in Figure 10 is the smallest VT graph with arc-type 1 + 1 + 1 + 1. It is the Cayley graph (in fact a GRR) for the dihedral group $D_8 = \langle x, y | x^2 = y^8 = (xy)^2 = 1 \rangle$ of order 16 with generating set $S = \{x, xy, xy^2, xy^4\}$.



Figure 10: The smallest VT graph with arc-type 1 + 1 + 1 + 1, on 16 vertices

Valency	Edge-type	Arc-type	Example	Case
1	1	1	K_2	P1
2	2	2	C_3	P2
		(1+1)	[Impossible]	P3
2	1 + 1	1 + 1	[Impossible]	P4
3	3	3	K_4	P5
3	2 + 1	2 + 1	prisms	P6
		(1+1)+1	$LCF[6, 6, -6, -6]^5$	P7
3	1 + 1 + 1	1 + 1 + 1	$LCF[5, -5]^9$	P8
4	4	4	K_5	P9
		(2+2)	Holt graph	P10
4	3 + 1	3 + 1	$K_4 \square K_2$	P11
4	2 + 2	2 + 2	$Cay(\mathbb{Z}_7; \{1, 2\})$	P12
		2 + (1 + 1)	Figure 6	P13
		(1+1) + (1+1)	Figure 7	P14
4	2 + 1 + 1	2 + 1 + 1	Figure 8	P15
		(1+1)+1+1	Figure 9	P16
4	1 + 1 + 1 + 1	1 + 1 + 1 + 1	Figure 10	P17

The above examples are summarised in Table 1.

Table 1: Edge-types and arc-types of VT graphs with valency up to 4

6 Arc-types of Cartesian products

Given a pair of graphs X and Y (which might or might not be distinct), the Cartesian product $X \Box Y$ is a graph with vertex set $V(X) \times V(Y)$, such that two vertices (u, x) and (v, y) are adjacent in $X \Box Y$ if and only if u = v and x is adjacent with y in Y, or x = y and u is adjacent with v in X.

This definition can be extended to the Cartesian product $X_1 \Box \ldots \Box X_k$ of a larger number of graphs X_1, \ldots, X_k . The terms X_i are called the *factors* of the Cartesian product $X_1 \Box \ldots \Box X_k$. The Cartesian product operation \Box is associative and commutative. A good reference for studying this and other products is the book by Imrich and Klavžar [13].

There are many properties of Cartesian product graphs that can be easily derived from the properties of their factors. For example, we have the following:

Proposition 6.1. A Cartesian product graph is connected if and only if all of its factors are connected.

Proposition 6.2. Let X_1, \ldots, X_k be regular graphs with valencies d_1, \ldots, d_k . Then their Cartesian product $X_1 \Box \ldots \Box X_k$ is also regular, with valency $d_1 + \cdots + d_k$.

A graph X is called *prime* (with respect to the Cartesian product) if it is not isomorphic to the Cartesian product of a pair of smaller, non-trivial graphs. It is well-known that every connected graph can be decomposed to a Cartesian product of prime graphs, which is unique up to reordering and isomorphism of the factors; for a proof, see [13, Theorem 4.9]. Similarly, two graphs are said to be *relatively prime* (with respect to the Cartesian product) if there is no non-trivial graph that is a factor of both. Note that two prime graphs are relatively prime unless they are isomorphic.

We are interested in the question of how the symmetries of individual graphs are involved in the symmetries of their product. Let $X = X_1 \square ... \square X_k$, and let α be an automorphism of one of the X_i . Then α induces an automorphism β of X, given by

$$\beta: (v_1, \ldots, v_k) \mapsto (v_1, \ldots, v_{i-1}, v_i^{\alpha}, v_{i+1}, \ldots, v_k).$$

The set of all automorphisms of X induced in this way forms a subgroup of Aut(X), and if some of the factors of X are isomorphic, then Aut(X) contains also other automorphisms that permute these factors among themselves, but if the factors of X are relatively prime, then there are no other automorphisms. Indeed we have the following:

Theorem 6.3. ([13, Corollary 4.17]) Let X be the Cartesian product $X = X_1 \Box \ldots \Box X_k$ of connected pairwise relatively prime graphs X_1, \ldots, X_k . Then every automorphism φ of X has the property that

 $\varphi: (v_1, \dots, v_k) \mapsto (v_1^{\varphi_1}, \dots, v_k^{\varphi_k}) \quad \text{for all } (v_1, \dots, v_k) \in V(X),$

where φ_i is an automorphism of X_i for $1 \leq i \leq k$.

Corollary 6.4. If X be the Cartesian product $X_1 \Box \ldots \Box X_k$ of connected pairwise relatively prime graphs X_1, \ldots, X_k , then $\operatorname{Aut}(X) \cong \operatorname{Aut}(X_1) \times \cdots \times \operatorname{Aut}(X_k)$.

Corollary 6.5. A Cartesian product of connected graphs is vertex-transitive if and only if every factor is vertex-transitive.

Corollary 6.5 follows directly from Theorem 6.3 when the factors are pairwise relatively prime. But it is also true in the general case — for a proof, see [13, Proposition 4.18].

We now come to the key observation we need to prove our main theorem.

Theorem 6.6. Let X_1, \ldots, X_k be non-trivial connected vertex-transitive graphs, with arctypes τ_1, \ldots, τ_k . Then also $X = X_1 \Box \ldots \Box X_k$ is a connected vertex-transitive graph, and if X_1, \ldots, X_k are pairwise relatively prime, then the arc-type of X is $\tau_1 + \cdots + \tau_k$. *Proof.* First, the graph X is connected by Proposition 6.1, and vertex-transitive by Corollary 6.5. For the second part, suppose that X_1, \ldots, X_k are pairwise relatively prime. Then by Corollary 6.4, we know that $\operatorname{Aut}(X) \cong \operatorname{Aut}(X_1) \times \cdots \times \operatorname{Aut}(X_k)$. Moreover, by Theorem 6.3, the stabiliser in $\operatorname{Aut}(X)$ of a vertex (v_1, \ldots, v_k) of X is isomorphic to $\operatorname{Aut}(X_1)_{v_1} \times \cdots \times \operatorname{Aut}(X_k)_{v_k}$.

We will now show that two arcs incident with a given vertex $u = (u_1, \ldots, u_k)$ in X are in the same orbit of Aut(X) if and only if the corresponding arcs are in the same orbit of $Aut(X_i)$ for some *i*, and that two such arcs are in paired orbits of Aut(X) if and only if the corresponding arcs of X_i belong to paired orbits of $Aut(X_i)$ for some *i*. This will imply that the sizes of arc-orbits of Aut(X) on X match the sizes of arc-orbits of the subgroups $Aut(X_i)$ on the corresponding X_i , for $1 \le i \le k$, and hence that the arc-type of X is just the sum of the arc-types of X_1, \ldots, X_k .

So suppose that $u' = (u'_1, \ldots, u'_k)$ and $u'' = (u''_1, \ldots, u''_k)$ are adjacent to $u = (u_1, \ldots, u_k)$ in X, and that the arcs (u, u') and (u, u'') lie in the same orbit of Aut(X). Then there exists an automorphism φ of X taking (u, u') to (u, u''), and since φ stabilises u, we know that $\varphi = (\varphi_1, \ldots, \varphi_k)$ where $\varphi_i \in \text{Aut}(X_i)_{u_i}$ for $1 \le i \le k$. Also u' differs from u in only one coordinate, say the *i*-th one, in which case $u'_j = u_j$ for $j \ne i$, and then since $\varphi = (\varphi_1, \ldots, \varphi_k)$ takes u' to u'' (and φ_j fixes u_j), we find that $u''_j = u_j$, so that u'' differs from u only in the *i*-th coordinate as well. In particular, φ_i fixes u_i and takes u'_i to u''_i , so the arcs (u_i, u'_i) and (u_i, u''_i) lie in the same orbit of Aut(X_i).

The converse is easy. For suppose the arcs (u_i, u'_i) and (u_i, u''_i) lie in the same orbit of $\operatorname{Aut}(X_i)$, and φ_i is an automorphism of X_i taking (u_i, u'_i) to (u_i, u''_i) . Then letting $u'_j = u''_j = u_j$ for $j \neq i$, and $u' = (u'_1, \ldots, u'_k)$ and $u'' = (u''_1, \ldots, u''_k)$, we find that the automorphism of X induced by φ_i takes (u, u') to (u, u''), and so these two arcs lie in the same orbit of $\operatorname{Aut}(X)$.

On the other hand, suppose the arcs (u, u') and (u, u'') lie in different but paired orbits of Aut(X). Then there exists an automorphism φ of X taking (u, u') to (u'', u), and $\varphi = (\varphi_1, \ldots, \varphi_k)$ where $\varphi_i \in Aut(X_i)$ for $1 \le i \le k$. Again, u' differs from u in only one coordinate, say the *i*-th one, in which case $u'_j = u_j$ for $j \ne i$. Then since φ takes u' to u, we find that φ_j fixes u_j , and since φ takes u to u'', also $u''_j = u_j$. Thus, as before, u''differs from u only in the *i*-th coordinate, and the arcs (u_i, u'_i) and (u_i, u''_i) lie in the same orbit of Aut (X_i) . The converse is analogous to the previous case, and this completes the proof.

Our final observations in this section are often helpful when proving that a given graph is prime with respect to the Cartesian product. The first two are easy, and the third one is proved in [14], for example.

Lemma 6.7. Let $X = X_1 \Box X_2$ be a Cartesian product of two connected graphs, each of which has at least two vertices. Then every edge of X is contained in a 4-cycle.

Corollary 6.8. Let X be a connected graph. If some edge of X is not contained in any 4-cycle, then X is prime. In particular, if X has no 4-cycles, then X is prime.

Lemma 6.9. Let X be a Cartesian product of connected graphs.

- (a) All the edges in a cycle of length 3 in X belong to the same factor of X.
- (b) Let (v, u, w, x) be any 4-cycle in X. Then the edges {v, u} and {w, x} belong to the same factor of X, as do the edges {u, w} and {x, v}.

(c) If e and f are incident edges that are not in the same factor of X, then there exists a unique 4-cycle that contains e and f, and this 4-cycle has no diagonals.

7 Thickened covers

In this section we explain the general notion of a thickened cover of a graph, and show how it can be used to build larger vertex-transitive graphs from a given one.

Let X be any simple graph, F any subset of the edge-set of X, and m any positive integer. Then we define X(F,m) to be the graph with vertex set $V(X) \times \mathbb{Z}_m$, and with edges of two types:

- (a) an edge from (u, i) to (v, i), for every $i \in \mathbb{Z}_m$ and every $\{u, v\} \in E(X) \setminus F$,
- (b) an edge from (u, i) to (v, j), for every $(i, j) \in \mathbb{Z}_m \times \mathbb{Z}_m$ and every $\{u, v\} \in F$.

We call X(F,m) a thickened m-cover of X over F.

In other words, a thickened *m*-cover of a graph X over a given set F of edges of X is obtained by replacing each vertex of X by m vertices, and each edge by the complete bipartite graph $K_{m,m}$ if the edge lies in F, or by mK_2 (a set of m 'parallel' edges) if the edge does not lie in F.

For example, the thickened 3-cover of the path graph P_6 on 6 vertices over the unique 1-factor of P_6 is shown in Figure 11.



Figure 11: A thickened 3-cover of P_6 (over its 1-factor)

Here we note that X(F, 1) is isomorphic to X, while $X(\emptyset, m)$ is isomorphic to mX (the union of m copies of X).

Also the base graph X is a quotient of X(F, m), obtainable by identifying all vertices (u, i) that have the same first coordinate, but X(F, m) is not a covering graph of X in the usual sense of that term when F is non-empty and m > 1, because in that case the valency of a vertex (u, i) of X(F, m) is greater than the valency of u.

On the other hand, if $X^{(m)}$ is the multigraph obtained from X by replacing each edge from F by m parallel edges, then X(F,m) is a regular covering graph of $X^{(m)}$, with voltages taken from \mathbb{Z}_m : we may choose the voltages of the edges not in F to be 0, and for each set of m parallel edges, choose a direction and then assign distinct voltages from \mathbb{Z}_m to these edges. The derived graph of $X^{(m)}$ with this voltage assignment is a covering graph of $X^{(m)}$ that is isomorphic to X(F,m).

(For the definitions of voltage graphs and covering graphs, see the book on topological graph theory by Gross and Tucker [10].)

For each $u \in V(X)$, we may call the set $\{(u, i) : i \in \mathbb{Z}_m\}$ of vertices of X(F, m) the *fibre* over the vertex u of X. Similarly the *fibre* over the edge $\{u, v\}$ of X is the set $\{\{(u, i), (v, i)\} : i \in \mathbb{Z}_m\}$ of edges of X(F, m) if $\{u, v\} \in E(X) \setminus F$, or the set

 $\{\{(u,i),(v,j)\}: i, j \in \mathbb{Z}_m\}$ if $\{u,v\} \in F$. Also for each $i \in \mathbb{Z}_m$ we call the subgraph of X(F,m) induced by the vertices $\{(u,i): u \in V(X)\}$ the *i*-th layer of X(F,m).

We now define three families of bijections on the vertex set of X(F, m). The first is $\tilde{\varphi}$, which is induced by addition of 1 mod m on \mathbb{Z}_m , and given by the rule

$$\tilde{\varphi}: (u,i) \mapsto (u,i+1) \quad \text{for all } u \in V(X) \text{ and all } i \in \mathbb{Z}_m.$$
 (7.1)

Next, if ψ is any automorphism of X, then we define $\tilde{\psi}$ by the rule

$$\widetilde{\psi}: (u,i) \mapsto (u^{\psi},i) \quad \text{for all } u \in V(X) \text{ and all } i \in \mathbb{Z}_m.$$
(7.2)

Finally, if $i, j \in \mathbb{Z}_m$ and $\{u, v\}$ is an edge in F such that u and v lie in different components of $X \setminus F$ (the graph obtained from X by deleting all the edges in F), then we define the bijection $\tilde{\theta} = \tilde{\theta}(u, v, i, j)$ by

$$\tilde{\theta}: (w,k) \mapsto \begin{cases} (w,j) & \text{if } k = i \text{ and } w \text{ lies in the same component of } X \setminus F \text{ as } v, \\ (w,i) & \text{if } k = j \text{ and } w \text{ lies in the same component of } X \setminus F \text{ as } v, \\ (w,k) & \text{otherwise.} \end{cases}$$
(7.3)

Lemma 7.1. If X is any graph, $F \subseteq E(X)$ and $m \ge 2$, then $\tilde{\varphi}$ is an automorphism of X(F,m).

Proof. The mapping $\tilde{\varphi}$ is a bijection and obviously sends edges of X(F,m) to edges, so is an automorphism of X(F,m).

Lemma 7.2. If $\psi \in Aut(X)$ and ψ preserves F setwise, then $\tilde{\psi}$ is an automorphism of X(F,m) for all m.

Proof. The given mapping $\tilde{\psi}$ is clearly a bijection. Next, if $\{u, v\} \in F$ then also $\{u^{\psi}, v^{\psi}\} \in F$ by hypothesis, and so $\{(u, i), (v, j)\}^{\tilde{\psi}} = \{(u^{\psi}, i), (v^{\psi}, j)\}$ is an edge of X(F, m), for all $i, j \in \mathbb{Z}_m$. Similarly, if $\{u, v\} \in E(X) \setminus F$, then $\{u^{\psi}, v^{\psi}\} \in E(X) \setminus F$, and so $\{(u, i), (v, i)\}^{\tilde{\psi}} = \{(u^{\psi}, i), (v^{\psi}, i)\}$ is an edge of X(F, m), for all $i \in \mathbb{Z}_m$. \Box

Corollary 7.3. If X is a vertex-transitive graph, and $F \subseteq E(X)$ is a union of some edgeorbits of X, then X(F,m) is vertex-transitive for every $m \ge 2$.

Proof. The subgroup of $\operatorname{Aut}(X(F,m))$ generated by $\tilde{\varphi}$ and $\{\tilde{\psi} : \psi \in \operatorname{Aut}(X)\}$ acts transitively on the vertex set of X(F,m).

Here we note that X(F, m) is vertex-transitive also when F is the union of edge-orbits of some vertex-transitive subgroup of Aut(X).

Lemma 7.4. If X is any graph, $F \subseteq E(X)$ and $m \ge 2$, and $\{u, v\}$ is any edge in F such that u and v lie in different components of $X \setminus F$, then $\tilde{\theta} = \tilde{\theta}(u, v, i, j)$ is an automorphism of X(F, m), for all $i, j \in \mathbb{Z}_m$.

Proof. The mapping $\hat{\theta}$ is clearly a bijection, and to prove it is an automorphism of X(F, m), all we have to do is show that it preserves the set E' of edges incident with one or more vertices not fixed by $\tilde{\theta}$. So suppose w is any vertex of X lying in the same component of $X \setminus F$ as v, and consider the effect of $\tilde{\theta}$ on an edge from (say) the vertex (w, i) to a vertex

(z, k) in X(F, m). If $\{w, z\} \in E(X) \setminus F$ and k = i, then z lies in the same component of $X \setminus F$ as w and hence in the same one as v, and therefore $\tilde{\theta}$ takes (w, i) to (w, j), and (z, k) = (z, i) to (z, j), which is a neighbour of (w, j). On the other hand, if $\{w, z\} \in F$ and k is arbitrary, then $\tilde{\theta}$ takes (w, i) to (w, j), and (z, k) to (z, k), which is a neighbour of (w, j). The analogous things happen for edges incident with (w, j) in place of (w, i), and so the set E' is preserved by $\tilde{\theta}$, as required. \Box

Next, we note that under the assumptions of Lemma 7.4, the automorphism $\tilde{\theta}(u, v, i, j)$ fixes the vertex (u, k), for every $k \in \mathbb{Z}_m$, and therefore the stabiliser of every such (u, k) contains the automorphisms $\tilde{\theta}(u, v, i, j)$ for all $i, j \in \mathbb{Z}_m$.

We now give a helpful example of an application of this thickened cover construction, to cycles of even order.

Theorem 7.5. Let X be the cycle on n vertices, where n is even and n > 2, and let F be a 1-factor of X. Then X(F,m) is vertex-transitive for all $m \ge 2$, with arc-type m + 1 (that is, with two self-paired arc orbits of lengths m and 1) whenever $(n,m) \ne (4,2)$. Also X(F,m) is prime with respect to the Cartesian product, for $m \ge 2$ and $n \ne 4$.

Proof. We may take $V(X) = \mathbb{Z}_n$ and $E(X) = \{\{r, r+1\} : r \in \mathbb{Z}_n\}$, and assume without loss of generality that $F = \{\{2r, 2r+1\} : r \in \mathbb{Z}_n\}$. By Lemma 7.1 and Lemma 7.4, we know that $\tilde{\varphi}$ and $\tilde{\theta}(2r, 2r+1, i, j)$ are automorphisms of X(F, m), for all $r \in \mathbb{Z}_n$ and all $i, j \in \mathbb{Z}_m$. Also let $\tilde{\rho}$ and $\tilde{\tau}$ be the permutations of V(X(F, m)) given by

 $\tilde{\rho}: (u,i) \mapsto (u+2,i) \text{ and } \tilde{\tau}: (u,i) \mapsto (1-u,i) \text{ for all } u \in V(X) \text{ and all } i \in \mathbb{Z}_m.$

By Lemma 7.2, these are automorphisms of X(F, m), induced by the automorphisms ρ and τ of X taking $u \mapsto u + 2$ and $u \mapsto 1 - u$, and from this is clear that $\tilde{\rho}$ and $\tilde{\tau}$ generate a dihedral subgroup of $\operatorname{Aut}(X(F, m))$ of order n (with n/2 'rotations' and n/2 'reflections'). Moreover, this subgroup acts transitively on the vertices of the *i*-th layer $\{(u, i) : u \in \mathbb{Z}_n\}$ of X(F, m), for every $i \in \mathbb{Z}_m$. It follows that the subgroup of $\operatorname{Aut}(X(F, m))$ generated by the automorphisms $\tilde{\varphi}$, $\tilde{\rho}$ and $\tilde{\tau}$ acts transitively on the set of all vertices of X(F, m), and therefore X(F, m) is vertex-transitive.

Now let Δ_1 and Δ_2 be the sets of arcs associated with edges of the types (a) and (b) from the construction of X(F, m). Specifically, let Δ_1 be the set of arcs associated with edges of the form $\{(2r + 1, i), (2r + 2, i)\}$ for $r \in \mathbb{Z}_n$ and $i \in \mathbb{Z}_m$, and let Δ_2 be the set of arcs associated with edges of the form $\{(2r, i), (2r + 1, j)\}$ for $r \in \mathbb{Z}_n$ and $i, j \in \mathbb{Z}_m$. Note that by the thickening construction, every vertex of X(F, m) is incident with one arc from Δ_1 , and with m arcs from Δ_2 .

All the arcs in Δ_1 lie in the same orbit of $\operatorname{Aut}(X(F, m))$. In fact Δ_1 is an arc-orbit of the subgroup generated by $\tilde{\varphi}$, $\tilde{\rho}$ and $\tilde{\tau}$, and here we may note that $\tilde{\tau}\tilde{\rho}$ reverses each arc ((1,i), (2,i)), and so $\tilde{\rho}^{-r}(\tilde{\tau}\tilde{\rho})\tilde{\rho}^r$ reverses each arc ((2r+1,i), (2r+2,i)) in Δ_1 . Similarly, all the arcs associated with edges of the form $\{(2r,i), (2r+1,i)\}$ for $r \in \mathbb{Z}_n$ and $i \in \mathbb{Z}_m$ lie in the same orbit of the subgroup generated by $\tilde{\varphi}$, $\tilde{\rho}$ and $\tilde{\tau}$, and then since $\tilde{\theta}(2r, 2r+1, i, j)$ interchanges the vertices (2r, i) and (2r, j) while fixing (2r+1, i) and (2r+1, j), we find that all the arcs in Δ_2 lie in the same orbit of $\operatorname{Aut}(X(F, m))$.

Next, we show there is no automorphism taking an arc in Δ_1 to an arc in Δ_2 , unless (n, m) = (4, 2). To see this, we consider the number of quadrangles containing a given edge. Every edge of the form $\{(2r, i), (2r + 1, j)\}$ is contained in at least $(m - 1)^2$ quadrangles, namely those with vertices (2r, i), (2r + 1, j), (2r, k) and $(2r + 1, \ell)$, for given

 $k \in \mathbb{Z}_m \setminus \{i\}$ and $\ell \in \mathbb{Z}_m \setminus \{j\}$. On the other hand, if n > 4 then no edge of the form $\{(2r + 1, i), (2r + 2, i)\}$ is contained in a quadrangle, because the other neighbours of (2r + 1, i) and 2r + 2, i) are all of the form (2r, j) and (2r + 3, j) respectively, and no two of these are adjacent, while if n = 4, then every edge of the form $\{(2r + 1, i), (2r + 2, i)\}$ is contained in exactly m quadrangles, namely those with vertices (2r + 1, i), (2r + 2, i), (2r + 3, j) and (2r, j), for given $j \in \mathbb{Z}_m$. Since $(m - 1)^2 > m$ for all m > 2, the numbers of quadrangles are different when $(n, m) \neq (4, 2)$.

Hence if $(n,m) \neq (4,2)$, we find that Δ_1 and Δ_2 are arc-orbits of X(F,m). Then since every vertex is incident with one arc from Δ_1 and m arcs from Δ_2 , the arc-type of X(F,m) is m + 1 in this case. Finally, if n > 4, then by Corollary 6.8, the fact that not every edge of X(F,m) is contained in a quadrangle implies that X(F,m) is prime with respect to the Cartesian product.

In the exceptional case (n, m) = (4, 2), the graph $C_4(F, 2)$ is isomorphic to the 3-cube Q_3 , which is arc-transitive (with arc-type 3). Also for every $m \ge 2$, the graph $C_4(F, m)$ is isomorphic to the Cartesian product of $K_{m,m}$ and K_2 , and hence is not prime.

Thickened covers of cycles belong to the family of cyclic Haar graphs [11], which are regular covering graphs over a dipole. Indeed the graph $C_{2k}(F,m)$ we considered in Theorem 7.5 is a covering graph over a dipole with n + 1 edges, and voltage assignments $1, 0, m, 2m, \ldots, (n-1)m$ from the additive group \mathbb{Z}_{mn} .

Next, we prove the following, which will be very helpful later.

Theorem 7.6. Let X be a vertex-transitive graph, let F be union of edge-orbits of X, and let m be any integer with $m \ge 2$. Also suppose that for every edge $\{u, v\} \in F$, the vertices u and v lie in different components of $X \setminus F$, and let (x, y) and (z, w) be two arcs lying in the same arc-orbit of X. Then

- (a) the arcs ((x,i), (y,i)) and ((z,j), (w,j)) lie in the same arc-orbit of X(F,m) for all $i, j, \in \mathbb{Z}_m$, and
- (b) the arcs ((x,i), (y, j)) and ((z,k), (w, l)) lie in the same arc-orbit of X(F,m) for all i, j, k, l ∈ Z_m, when {x, y} ∈ F.

Proof. First, there exists an automorphism ψ that maps (x, y) to (z, w). Now let $\tilde{\varphi}$ and ψ be the mappings defined earlier in this section in (7.1) and (7.2). These are automorphisms, by Lemma 7.1 and Lemma 7.2, and $\tilde{\varphi}^{j-i}\tilde{\psi}$ takes the arc ((x,i),(y,i)) to ((z,j),(w,j)), and so these two arcs lie in the same orbit of Aut(X(F,m)).

Next, suppose $\{x, y\} \in F$. Then also $\{z, w\} \in F$, since $\{x, y\}$ and $\{z, w\}$ are in the same edge-orbit, and the vertices z and w lie in different components of $X \setminus F$, by hypothesis. Note that the automorphism $\tilde{\varphi}^{k-i}\tilde{\psi}$ takes ((x, i), (y, i)) to ((z, k), (w, k)), Now let $\tilde{\theta} = \tilde{\theta}(z, w, k, \ell)$, as defined in (7.3). This is an automorphism of X(F, m), by Lemma 7.4, which takes ((z, k), (w, k)) to $((z, k), (w, \ell))$. Thus $\tilde{\varphi}^{k-i}\tilde{\psi}\tilde{\theta}$ takes ((x, i), (y, i)) to $((z, k), (w, \ell))$, and so these two arcs lie in the same of $\operatorname{Aut}(X(F, m))$.

Note that Theorem 7.6 cannot be pushed much further. For example, if F is a 1-factor in $X = C_6$, then the graph $Y = C_6(F, 2)$ has arc-type 2 + 1, by Theorem 7.5. Now one might expect that if Φ_1 is the smaller edge-orbit of Y, then the 4-valent graph $Y(\Phi_1, 2)$ has arc-type 2 + 2, but this does not happen: it turns out that $Y(\Phi_1, 2)$ is arc-transitive, and so has arc-type 4.

8 Building blocks

In this section we produce families of examples (and a few single examples) of vertextransitive graphs with certain arc-types, which we will use as building blocks for the Cartesian product construction, to prove our main theorem in the final section. The marked partitions that occur as arc-types in these cases have a small number of summands. We begin with the arc-transitive case, for which there is just one summand.

Lemma 8.1. For every integer $m \ge 2$, there exist infinitely many VT graphs that have arc-type m and are prime with respect to the Cartesian product.

Proof. First, when m = 2 we can take the cycle graphs C_n , for $n \ge 5$. These are vertex-transitive, with arc-type 2, and taking n > 4 ensures that C_n contains no 4-cycles and is therefore prime, by Lemma 6.7.

Now suppose $m \ge 3$. We construct infinitely many *m*-valent arc-transitive graphs, using a theorem of Macbeath [16] which gives the following: for almost all positive integer triples (m_1, m_2, m_3) with $1/m_1 + 1/m_2 + 1/m_3 < 1$, there exist infinitely many odd primes *p* for which the simple group PSL(2, *p*) is generated by two elements *x* and *y* such that *x*, *y* and *xy* have orders m_1, m_2 and m_3 , respectively.

Here we can take $(m_1, m_2, m_3) = (2, m, m+4)$, and then for each such prime p > m, take G = PSL(2, p) and let H be the cyclic subgroup of G generated by y. Then |H| = m, and the double coset graph $\Gamma = \Gamma(G, H, x)$ is an arc-transitive graph of order |G|/m = p(p-1)(p+1)/(2m). This graph has valency m, because the stabiliser in G of the arc (H, Hx) is the cyclic subgroup $H \cap x^{-1}Hx$, which is trivial since G is simple. Thus Γ has arc-type m.

It remains to show that Γ is prime. For the moment, suppose that $\Gamma \cong X \Box Y$ where X and Y are relatively prime non-trivial graphs. Then by Corollary 6.5, X and Y are vertex-transitive, and so by Theorem 6.6 we have $m = \operatorname{at}(\Gamma) = \operatorname{at}(X) + \operatorname{at}(Y)$, which is impossible. Hence the prime factors of Γ must be all the same, and so Γ is the Cartesian product of (say) k copies of a single prime graph X. But then the order of Γ is $|V(X)|^k$, which is impossible unless k = 1, since the prime p divides $|V(\Gamma)| = p(p-1)(p+1)/(2m)$ but p^2 does not. Hence Γ itself is prime.

At this point we remark that there are several other ways to produce infinitely many m-valent arc-transitive graphs for all $m \ge 3$. For example, another construction uses homological covers: start with a given m-valent arc-transitive graph X (such as the complete graph on m + 1 vertices), and then for every sufficiently large prime p, construct a homological p-cover Γ_p over X with no 4-cycles. Then Γ_p is also an m-valent arc-transitive graph, and is prime since it contains no 4-cycles; see [17].

Next, we consider half-arc-transitive graphs.

Lemma 8.2. For every integer $m \ge 2$, there exist infinitely many VT graphs that have arc-type (m + m) and are prime with respect to the Cartesian product.

Proof. In 1970, Bouwer [3] constructed an infinite family of vertex- and edge-transitive graphs of even valency, indexed by triples (m, k, n) of integers such that $m, k, n \ge 2$ and $2^k \equiv 1 \mod n$. Each such graph, which we will call B(m, k, n), has order kn^{m-1} and valency 2m. The construction is easy, using only modular arithmetic. Bouwer proved that the graphs B(m, 6, 9) are half-arc-transitive, thereby showing that for every even integer

2m > 2, there exists a half-arc-transitive graph with valency 2m. Recently the first and third authors of this paper adapted Bouwer's approach to prove that almost all the graphs B(m, k, n) are half-arc-transitive [7]. In particular, they showed that if n > 7 and k > 6 (and $2^k \equiv 1 \mod n$), then X(m, k, n) is a half-arc-transitive graph of girth 6, for every $m \ge 2$. This gives infinitely many prime graphs of type (m + m), for every $m \ge 2$.

Here we note that there are several constructions for half-arc transitive graphs. In particular, Li and Sim used properties of projective special linear groups to construct infinitely many half-arc transitive graphs of every even valency greater than 2 in [15]. A census of 4-valent half-arc transitive graphs up to 1000 vertices is given in [20].

Lemma 8.3. For every integer $m \ge 2$ there exist infinitely many prime VT graphs with arc-type m + 1.

Proof. By Theorem 7.5, for every $m \ge 2$ and every even n > 4, the thickened *m*-cover of C_n over a 1-factor F (of C_n) is a prime VT graph with arc-type m + 1.

In fact we will need only one prime VT graph with arc-type m + 1 for each m in the proof of Theorem 9.1, as we do for the next two arc-types, m + (1 + 1) and 1 + (m + m), as well.

Lemma 8.4. For every integer $m \ge 2$ there exists a prime VT graph with arc-type m + (1+1).

Proof. Let X be the graph with arc-type 1 + (1 + 1) given in Figure 3. Before proceeding, we describe some additional properties of X. First, $\operatorname{Aut}(X)$ is generated by the involutory automorphism α that takes $v \mapsto 21 - v$ for all $v \in V(X)$, and the automorphism β of order 4 that acts as (1, 7, 8, 2)(3, 20, 6, 9)(4, 14, 5, 15)(10, 17, 19, 12)(11, 16, 18, 13) on vertices. In fact $\operatorname{Aut}(X)$ is isomorphic to the semi-direct product $C_5 \rtimes_3 C_4$, with normal subgroup of order 5 generated by $\gamma = \alpha \beta^2$ (= $[\beta, \alpha]$), and $\beta^{-1} \gamma \beta = \gamma^3$. In particular, X is a Cayley graph (and a GRR) for this group.

The graph X has two edge-orbits: one of size 20 containing the edges $\{1, 2\}$ and $\{1, 7\}$, and one of size 10 containing the edge $\{1, 20\}$. Edges in the first orbit lie in quadrangles, while those in the second do not. The arc (1, 20) is reversed by the automorphism α , so it lies in a self-paired arc-orbit, of size 20. On the other hand, the arcs (1, 2) and (1, 7) lie in distinct paired arc-orbits, also of size 20. (This can be seen by either considering the images of (1, 20) under the 20 automorphisms $\beta^i \gamma^j$ (for $i \in \mathbb{Z}_4$ and $j \in \mathbb{Z}_5$), or by using the effect on 7-cycles to show there is no automorphism that takes (1, 2) to (1, 7).)

Now let F be the smaller edge-orbit, containing the edges of the form $\{2i, 2i+1\}$ (with the vertices considered mod 20, so we treat 20 as 0), and let Y be the thickened m-cover X(F,m) of X over F. Then Y is vertex-transitive, by Corollary 7.3, and its valency is m+2.

The edges from (1,0) to (2,0) and (1,0) to (7,0) both lie in a single quadrangle, namely the one with vertices (1,0), (2,0), (8,0) and (7,0), while the edge from (1,0) to (20,0) lies in exactly $(m-1)^2$ quadrangles, namely the ones with third and fourth vertices (1,i) and (20,j) for any $i,j \in \mathbb{Z}_m \setminus \{0\}$. Hence if m > 2, then the edges from (1,0) to (2,0) and (1,0) to (7,0) cannot lie in the same edge-orbit as the edge from (1,0) to (20,0). This is also true when m = 2, because (for example) the edges from (1,0) to (2,0) and (1,0) to (7,0) both lie in 16 different 7-cycles, while the edge from (1,0) to (20,0) lies in only 12 different 7-cycles. (This can be checked by hand or by use of MAGMA.) Also $X \setminus F$ is a disjoint union of quadrangles (on vertex-sets $\{4i + 1, 4i + 2, 4i + 7, 4i + 8\}$ for $i \in \mathbb{Z}_5$), and so Theorem 7.6 applies. By part (b) of Theorem 7.6, the edge-orbit F of X gives rise to a summand m for the arc-type of Y, and then by part (a), noting that (1, 2) and (7, 1) lie in the same arc-orbit of X, we find that Y = X(F, m) has arc-type m + (1 + 1) or m + 2.

To show that Y has arc-type m + (1 + 1), again we consider 7-cycles. It is an easy exercise to show that there are exactly $4m^2$ cycles of length 7 containing the edge from (1,0) to (2,0), namely those of the following forms:

- ((1,0), (2,0), (3,i), (4,i), (5,j), (6,j), (7,0)), for any $i, j \in \mathbb{Z}_m$,
- ((1,0), (2,0), (3,i), (4,i), (18,i), (19,j), (20,j)), for any $i, j \in \mathbb{Z}_m$,
- ((1,0),(2,0),(3,i),(17,i),(18,i),(19,j),(20,j)), for any $i,j \in \mathbb{Z}_m$,
- ((1,0), (2,0), (8,0), (9,i), (15,i), (14,j), (20,j)), for any $i, j \in \mathbb{Z}_m$.

Note that some of these can differ in only one vertex, namely in the 4th vertex of the second and third forms, for a given pair (i, j). Similarly, there are exactly $4m^2$ cycles of length 7 containing the edge from (1, 0) to (7, 0), namely those of the following forms:

- ((1,0), (7,0), (6,i), (12,i), (13,j), (14,j), (20,j)), for any $i, j \in \mathbb{Z}_m$,
- ((1,0),(7,0),(6,i),(12,i),(13,j),(19,j),(20,j)), for any $i,j \in \mathbb{Z}_m$,
- ((1,0), (7,0), (6,i), (5,i), (4,j), (3,j), (2,0)), for any $i, j \in \mathbb{Z}_m$,
- ((1,0), (7,0), (8,0), (9,i), (15,i), (14,j), (20,j)), for any $i, j \in \mathbb{Z}_m$.

But in these cases, when two such 7-cycles differ in only one vertex, they differ in the 6th vertex (of the first and second form, for a given pair (i, j)). It follows that there can be no automorphism of Y taking the arc ((1,0), (2,0)) to the arc ((1,0), (7,0)), and so the arc-type of Y must be m + (1 + 1).

It remains to show that Y = X(F, m) is prime. For this, we consider any decomposition of Y into Cartesian factors, which are connected by Proposition 6.1, and we apply Lemma 6.9. The edge $\{(1,0), (2,0)\}$ lies in no quadrangle with any of the edges of the form $\{(1,0), (20,i)\}$, for $i \neq 0$, and it follows from part (c) of Lemma 6.9 that all those edges must lie in the same factor of Y as $\{(1,0), (2,0)\}$, say U. The same argument holds for the edge $\{(1,0), (7,0)\}$, and so this lies in U as well. Hence U contains all m+2 edges incident with the vertex (1,0). By vertex-transitivity and connectivity, all edges of Y lie in U, and so U = Y. Thus X(F, m) is prime.

Lemma 8.5. For every integer $m \ge 2$ there exists a prime VT graph with arc-type 1 + (m+m).

Proof. This is very similar to the proof of Lemma 8.4. Again, let X be the graph with arctype 1 + (1+1) given in Figure 3, but this time take F to be the edge-orbit of X containing the edge $\{1,2\}$ (and the edge $\{1,7\}$). Then the thickened m-cover Z = X(F,m) of X over F is vertex-transitive, with valency 1 + 2m. Also the edge from (1,0) to (20,0) lies in no quadrangles, which implies immediately that Z is prime. On the other hand, the edge from (1,0) to (2,0) lies in $(2m - 1)^2$ quadrangles, and so again the edge from (1,0) to (2,0) cannot lie in the same edge-orbit as the edge from (1,0) to (20,0). Next, $X \setminus F$ is a union of 10 non-incident edges, and hence by part (a) of Theorem 7.6, we find that Z = X(F, m) has arc-type 1 + (m + m) or 2m + 1. Finally, as before, there are $4m^2$ cycles of length 7 containing the edge from (1,0) to (2,0), and $4m^2$ containing the edge from (1,0) to (7,0), but when two of these cycles differ in only one vertex, it is in the 4th vertex in the former case, but in the 6th vertex in the latter case, and so there can be no automorphism of Z taking the arc ((1,0), (2,0)) to the arc ((1,0), (7,0)). Hence the arc-type of Z is 1 + (m + m).

Now we consider the marked partition (1 + 1) + (1 + 1) of 4. For this one, we use a quite different construction.

Lemma 8.6. There are infinitely many prime VT graphs with arc-type (1 + 1) + (1 + 1).

Proof. For any prime number $p \equiv 1 \mod 6$, let G be the group $C_p \rtimes_k C_6$, generated by two elements a and b of orders 6 and p such that $a^{-1}ba = b^k$, where k is a primitive 6th root of 1 mod p. Also take $S = \{x, y, x^{-1}, y^{-1}\}$ where x = a and $y = ba^2$, and let X be the Cayley graph Cay(G, S).

Then X is a 4-valent VT graph, and from the natural action of G by right multiplication, it is easy to see that all edges of the form $\{g, xg\}$ or $\{g, x^{-1}g\}$ lie in a single edge-orbit, as do all edges of the form $\{g, yg\}$ or $\{g, y^{-1}g\}$. We now show that these edge-orbits are distinct, and that each gives rise to two distinct arc-orbits, by proving that the stabiliser in Aut(X) of vertex 1 is trivial.

First, we observe that $0 \equiv 1 - (k^2)^3 \equiv (1 - k^2)(1 + k^2 + k^4) \mod p$, and then since $k^2 \not\equiv 1 \mod p$, we have $1 + k^2 + k^4 \equiv 0 \mod p$. It follows that

$$y^{3} = (ba^{2})^{3} = b(a^{-4}ba^{4})(a^{-2}ba^{2}) = bb^{k^{4}}b^{k^{2}} = b^{1+k^{4}+k^{2}} = b^{0} = 1.$$

In particular, every edge of the form $\{g, yg\}$ or $\{g, y^{-1}g\}$ lies in a 3-cycle (associated with the relation $y^3 = 1$). On the other hand, it is easy to see that no edge of the form $\{g, xg\}$ or $\{g, x^{-1}g\}$ lies in a 3-cycle, and so X has two distinct edge-orbits, and its edge-type is 2+2.

Similarly, we note that $0 \equiv 1 - (k^3)^2 \equiv (1 - k^3)(1 + k^3) \mod p$ but $k^3 \not\equiv 1 \mod p$, so $k^3 \equiv -1 \mod p$, and therefore $yx = ba^3 = a^3b^{-1} = a^{-3}b^{-1} = x^{-1}y^{-1}$. Hence the two vertices x and y^{-1} have two common neighbours, namely 1 and yx. Also $xy = x(yx)x^{-1} = x(x^{-1}y^{-1})x^{-1} = y^{-1}x^{-1}$, and therefore x^{-1} and y have two common neighbours, namely 1 and xy. Furthermore, it is an easy exercise to verify that no other two neighbours of 1 have a second common neighbour.

It follows that every automorphism α of X that fixes the vertex 1 must either fix or swap its two neighbours y and y^{-1} , and similarly, must fix or swap its two neighbours x and x^{-1} . Also if α swaps one pair, then it must also swap the other pair. Hence α either fixes all four neighbours of 1, or induces a double transposition on them. By vertex-transitivity, the same holds for any automorphism fixing a vertex v. Moreover, if the automorphism α fixes one of the arcs incident with the vertex 1, then it fixes every neighbour s of 1, and then since it fixes the arc (s, 1), it must act trivially on the neighbourhood of s. Then by induction and connectedness, α fixes every vertex of X.

Now suppose $\operatorname{Aut}(X) \neq G$, or equivalently, that the stabiliser in $\operatorname{Aut}(X)$ of each vertex is non-trivial. Now if β and γ are non-trivial automorphisms of X that fix the vertex 1, then they induce the same permutation $(x, x^{-1})(y, y^{-1})$ on the four neighbours of 1, so $\beta\gamma^{-1}$ acts trivially on the neighbourhood of 1 and hence is trivial, giving $\beta = \gamma$. Hence the stabiliser of vertex 1 contains a unique non-trivial automorphism, which must have

order 2. In particular, $|\operatorname{Aut}(X)| = 2|V(X)| = 2|G|$, and so *G* is a normal subgroup of index 2 in $\operatorname{Aut}(X)$. Moreover, the element of $\operatorname{Aut}(X)$ of order 2 stabilising the vertex 1 must normalise *G*, and hence induces an automorphism θ of *G*, and from what we saw earlier, θ swaps x with x^{-1} , and y with y^{-1} . Now θ takes a = x to $x^{-1} = a^{-1}$, and $b = ya^{-2} = yx^{-2}$ to $y^{-1}x^2 = (ba^2)^{-1}a^2 = a^{-2}b^{-1}a^2 = b^{-k^2}$, and so θ takes b^k to $(b^k)^{-k^2} = b^{-k^3} = b^{-(-1)} = b$. But on the other hand, $b^k = a^{-1}ba$, and so θ takes b^k to $ab^{-k^2}a^{-1} = b^{-k}$ (since $a^{-1}b^{-k}a = (b^k)^{-k} = b^{-k^2}$). Thus $b^{-k} = (b^k)^{\theta} = b$, and it follows that $k \equiv -1 \mod p$, a contradiction.

Hence no such automorphism θ of G exists, and we find that Aut(X) = G, and that X has arc-type (1 + 1) + (1 + 1), as required.

Finally, we show that X is prime, using a similar argument to the one in the proof of Lemma 8.1. If $X \cong X_1 \square X_2$ where X_1 and X_2 are relatively prime non-trivial graphs, then by Theorem 6.6 we have $(1 + 1) + (1 + 1) = \operatorname{at}(X) = \operatorname{at}(X_1) + \operatorname{at}(X_1)$, which is impossible, since no VT graph has arc-type (1 + 1). Hence the prime factors of X must be all the same, and so X is a Cartesian product of (say) k copies of a single prime graph Y. But then $6p = |V(X)| = |V(Y)|^k$, which is impossible unless k = 1, since p is a prime number congruent to 1 mod 6. Thus X itself is prime.

Next, we use the first of these graphs (the one with p = 7) to prove the following.

Lemma 8.7. For every integer $m \ge 2$, there exists a prime VT graph with arc-type (m + m) + (1 + 1).

Proof. Let X be the graph with arc-type (1 + 1) + (1 + 1) in Figure 7, which is also the graph constructed in Lemma 8.6 for p = 7, and let F be the edge-orbit of X consisting of all the edges that are not contained in a triangle. (These are the edges corresponding to multiplication by the generator x for $G = C_7 \rtimes C_6$.) Now let Y = X(F, m), the thickened m-cover of X over F. Then Y is vertex-transitive, by Corollary 7.3, and its valency is 2m + 2. Also $X \setminus F$ is a disjoint union of triangles, so Theorem 7.6 applies, and tells us that all the edges of Y associated with edges of F lie in the same edge-orbit, and all the edges of Y associated with edges of $E(X) \setminus F$ lie in the same edge-orbit. We will show that Y has arc-type (m + m) + (1 + 1), by proving that these edge-orbits are distinct, and that each gives rise to two arc-orbits.

We do this by showing that every automorphism of Y = X(F, m) induces a permutation of the fibres over X, and therefore projects to an automorphism of X. It then follows that any automorphism of Y taking an arc ((v, i), (w, j)) to an arc ((v', i'), (w', j')) gives rise to an automorphism of X taking (v, w) to (v', w'). Hence if (v, w) and (v', w') lie in different arc-orbits of X, then ((v, i), (w, j)) and ((v', i'), (w', j')) lie in different arcorbits of Y, for all $i, j, i', j' \in \mathbb{Z}_m$.

Observe that the graph $X \setminus F$ is a disjoint union of 14 triangles in X, and that there are no other triangles in X. Also it is quite easy to see that every triangle in Y is one of the 14m triangles of the form $T_i = \{(u, i), (v, i), (w, i)\}$ for some triangle $T = \{u, v, w\}$ in X and some $i \in \mathbb{Z}_m$, and that these 14m triangles are pairwise disjoint. In particular, since every automorphism takes triangles to triangles, we find that every automorphism of Y preserves the set of edges of Y the form $\{(u, i), (v, i)\}$ with $i \in \mathbb{Z}_m$ and $\{u, v\} \in E(X) \setminus F$, and hence also preserves the set of edges of Y of the form $\{(u, i), (v, j)\}$ with $\{u, v\} \in F$. (This also implies that Y is not edge-transitive, so its edge-type is m + 2.) Next, consider what happens locally around a vertex (u, i) of Y. This vertex lies in a unique triangle $T_i = \{(u, i), (v, i), (w, i)\}$, where v = yu and $w = y^{-1}u$, and also lies in m edges of the form (r, j) and m edges of the form (s, j), for $j \in \mathbb{Z}_m$, where r = xu and $s = x^{-1}u$. The other vertices in the fibre over the vertex u have the form (u, ℓ) for some $\ell \in \mathbb{Z}_m$, and each of these lies at distance 2 from (u, i).

In fact, there are 2m paths of length 2 from each such (u, ℓ) to the given vertex (u, i), namely the *m* paths of the form $((u, \ell), (r, j), (u, i))$ for $j \in \mathbb{Z}_m$, and the *m* paths of the form $((u, \ell), (s, j), (u, i))$, for $j \in \mathbb{Z}_m$. On the other hand, from every other vertex at distance 2 from the given vertex (u, i) there are only 1, 2 or *m* paths of length 2 to (u, i). It follows that the stabiliser in Aut(Y) of the vertex (u, i) preserves the fibre over the vertex (u, i), and therefore Aut(Y) permutes the fibres over vertices of X.

Thus X(F, m) has arc-type (m + m) + (1 + 1).

Finally, we show that Y = X(F, m) is prime. If $Y \cong Y_1 \square Y_2$ where Y_1 and Y_2 are relatively prime non-trivial graphs, then each Y_i is vertex-transitive, and by Theorem 6.6 the arc-type of Y_1 or Y_2 is (1+1), which is impossible. Hence the prime factors of Y must be all the same, and so Y is a Cartesian product of (say) k copies of a single prime graph Z. Also by part (a) of Lemma 6.9, all the edges of a given triangle lie in the same factor, so Z contains a triangle. But now if k > 1 then some subgraph of Y is a Cartesian product of two triangles, and in the latter, every vertex lies in two distinct triangles, which does not happen in Y. Hence k = 1, and Y itself is prime.

We use yet another construction in the next case, to produce zero-symmetric graphs with arc-type 1 + 1 + 1. Many examples of such graphs are already well known, but we need an infinite family of examples that are prime. A sub-family of the family we use below appears in [8, p. 66].

Lemma 8.8. There are infinitely many prime VT graphs with arc-type 1 + 1 + 1.

Proof. Let G be the dihedral group D_n of order 2n, where n is any integer of the form 2m-1 where $m \ge 6$ (so that n is odd and $n \ge 11$). Then G is generated by two elements x and y satisfying $x^2 = y^n = 1$ and $xyx = y^{-1}$, and the elements of G are uniquely expressible in the form $x^i y^j$ where $i \in \mathbb{Z}_2$ and $j \in \mathbb{Z}_n$. (In fact G is the symmetry group of a regular n-gon, with the powers of y being rotations and elements of the form xy^j being reflections.)

Now define X as the Cayley graph $Cay(G, \{x_1, x_2, x_3\})$, where $x_1 = x$, $x_2 = xy$ and $x_3 = xy^3$. This graph is vertex-transitive, and since the x_i are involutions, it is 3-valent and bipartite. We show that X is prime and has arc-type 1 + 1 + 1.

The vertices at distance 2 from the identity element are the products of two of the x_i , which are all distinct: $x_1x_2 = y$, $x_1x_3 = y^3$, $x_2x_1 = y^{-1}$, $x_2x_3 = y^2$, $x_3x_1 = y^{-3}$ and $x_3x_2 = y^{-2}$. In particular, X has no 4-cycles, and hence is prime. Since X is bipartite, it also follows that the girth of X is 6.

Next, there are 12 paths of length 3 starting from the identity element, but only 7 vertices at distance 3 from the identity element. Indeed it is an easy exercise to show that the coincidences are precisely the following:

$$\begin{array}{ll} x_1x_2x_1 \,=\, x_2x_3x_2 \,=\, xy^{n-1}, & x_1x_2x_3 \,=\, x_2x_1x_2 \,=\, x_3x_2x_1 \,=\, xy^2, \\ x_1x_3x_2 \,=\, x_2x_3x_1 \,=\, xy^{n-2}, & \text{and} & x_2x_1x_3 \,=\, x_3x_1x_2 \,=\, xy^4. \end{array}$$

In particular, the edge $\{1, x_1\}$ lies in exactly four cycles of length 6, namely $(1, x_1, x_2x_1, x_1x_2x_1, x_3x_2, x_2)$, $(1, x_1, x_2x_1, x_3x_2x_1, x_2x_3, x_3)$, $(1, x_1, x_2x_1, x_3x_2x_1, x_1x_2, x_2)$ and $(1, x_1, x_3x_1, x_2x_3x_1, x_3x_2, x_2)$. Similarly, the edge $\{1, x_2\}$ lies in exactly five 6-cycles, and the edge $\{1, x_3\}$ lies in only three. These numbers are different, and it follows that the edges $\{1, x_1\}$, $\{1, x_2\}$ and $\{1, x_3\}$ lie in distinct arc-orbits.

Hence the arc-type of X is 1 + 1 + 1, as claimed.

The next four lemmas deals with the remaining basic arc-types we need.

Lemma 8.9. There exist more than one prime VT graphs with arc-type 1 + (1 + 1).

Proof. We have already observed that the zero-symmetric graph on 20 vertices given in Figure 3 has arc-type 1 + (1 + 1), and because not every edge is contained in a 4-cycle, it is prime by Corollary 6.8. Some other examples of graphs of arc-type 1 + (1 + 1) appear in [8, p. 39]; these can be described with LCF-codes $[2k, 2k, -2k, -2k]^m$ for $(m, k) \in \{(13, 5), (17, 13), (25, 7), (29, 17)\}$, and they are all prime, since they all have edges that are not contained in 4-cycles.

Lemma 8.10. There exists a prime VT graph with arc-type 1 + 1 + (1 + 1).

Proof. The graph on 20 vertices given in Figure 9 has arc-type 1+1+(1+1). Now suppose that this graph is not prime. Then since 20 is not a non-trivial power of any integer, the graph must be the Cartesian product of two smaller connected VT graphs that are relatively prime. Then since there are no VT graphs with arc-type 1 + 1 or (1 + 1), it must be a Cartesian product of two connected VT graphs with arc-types 1 and 1 + (1 + 1). The former has to be K_2 , and so the other is a VT graph of order 10 with arc-type 1 + (1 + 1). But no such graph exists — in fact, the smallest VT graph with arc-type 1 + (1 + 1) has 20 vertices. Hence the given graph is prime.

Lemma 8.11. There exists a prime VT graph with arc-type 1 + 1 + 1 + 1.

Proof. The graph on 16 vertices given in Figure 10 has arc-type 1+1+1+1. Also this graph cannot be the Cartesian product of two smaller connected VT graphs that are relatively prime, by a similar argument to the one given in the proof of Lemma 8.10, because there is no VT graph of order 8 with arc-type 1 + 1 + 1. (The smallest VT graph with arc-type 1 + 1 + 1 has order 18.) Finally, if it is the Cartesian power of some smaller graph, then it has to be the Cartesian square of C_4 (or the Cartesian 4th power of K_2 , which is isomorphic to $C_4 \square C_4$), but this graph is arc-transitive, with arc-type 4. Hence the given graph is prime.

Lemma 8.12. There exists a prime VT graph with arc-type (1 + 1) + (1 + 1) + (1 + 1).

Proof. Let X be the Cayley graph Cay(G, S) for the group G = SL(2,3) of all 2×2 matrices of determinant 1 over \mathbb{Z}_3 , given by the set $S = \{x, x^{-1}, y, y^{-1}, xy, (xy)^{-1}\}$, where

$$x = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$
 and $y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

These two elements generate G and satisfy the relations $x^3 = y^4 = 1$ and $yx^{-1} = (xy)^2$, which are defining relations for G. This Cayley graph X is 6-valent, with girth 3, and it is not difficult to show that its diameter is 3.

In the neighbourhood of the identity element 1 in X, there is an edge between y and xy, and a path of length 3 from y^{-1} to $(xy)^{-1}$ via x and x^{-1} , but there are no other edges (between vertices of that neighbourhood). Also the vertices y and y^{-1} have another common neighbour, namely y^2 , and the vertices xy and $(xy)^{-1}$ have another common neighbour, namely $y^{-1}xy$ (= $(xyx)^{-1}$), but y and $(xy)^{-1}$ have no other common neighbour, and y^{-1} and xy have no other common neighbour. It follows that the stabiliser in Aut(X) of the vertex 1 either fixes all its neighbours, or interchanges y with xy, and y^{-1} with $(xy)^{-1}$, and x with x^{-1} . But the number of neighbours of the vertex y that are at distance 2 from x is 4, while the number of neighbours of the vertex xy that are at distance 2 from x^{-1} is only 3, so the latter cannot happen, and hence the stabiliser in Aut(X) of 1 acts trivially on the neighbourhood of 1. By vertex-transitivity, the same holds at every vertex, and then by induction and connectedness, it follows that the stabiliser of every vertex is trivial.

Thus Aut(X) = G, making X a GRR. Then since the edges $\{1, s\}$ and $\{1, s^{-1}\}$ lie in the same edge-orbit for each $s \in S$, we find that X has type (1 + 1) + (1 + 1) + (1 + 1).

Finally, X cannot be the Cartesian product of two smaller connected VT graphs that are relatively prime, since there are no VT graphs with arc-type (1+1). Also X cannot be a Cartesian power of some smaller VT graph, since its order 24 is not a non-trivial power of any integer. Hence X is prime.

The graph used in the proof of Lemma 8.12 is shown in Figure 12.



Figure 12: A VT graph with arc-type (1+1) + (1+1) + (1+1), on 24 vertices

9 Realisability

We say that a marked partition Π is *realisable* if there exist a vertex-transitive graph with arc-type Π . Recall that the marked partitions 1 + 1 and (1 + 1) are not realisable (as we explained in the introductory section), and on the other hand, some other marked partitions with few summands are realisable by infinitely many vertex-transitive graphs (as we showed in Section 8).

In this final section we prove that all other marked partitions are realisable. We then find (as a corollary) that all standard partitions except 1 + 1 are realisable as the edge-type of a vertex-transitive graph.

Theorem 9.1. Every marked partition other than (1 + 1) and 1 + 1 is realisable as the arc-type of a vertex-transitive graph.

Proof. Let $\Pi = n_1 + \cdots + n_t + (m_1 + m_1) + \cdots + (m_s + m_s)$ be a marked partition of an integer $d \ge 2$, different from 1 + 1 and (1 + 1). We may assume that $n_1 \ge \cdots \ge n_t$ and $m_1 \ge \cdots \ge m_s$. If $d \le 4$, then we know from the examples given in Section 5 that Π is realisable, and therefore we may assume that $d \ge 5$ when necessary.

We will show how to find a VT graph with arc-type Π , by taking the Cartesian product of prime graphs with smaller degrees and simpler arc-types, chosen so that the sum of their arc-types is Π . To do this, we consider separately the two cases where s = 0 and t = 0, with a focus on the number of n_i or m_j that are equal to 1, respectively, and then we combine these two cases in order to show how to handle all possibilities.

Case (A): s = 0, with $\Pi = n_1 + \cdots + n_t$.

Let k be the number of n_i that are equal to 1, so that $n_i > 1$ for $1 \le i \le t - k$, and $n_t = 1$ for $t - k + 1 \le i \le t$.

If k = 0, then by Lemma 8.1 we can find t pairwise non-isomorphic prime VT graphs with arc-types n_1, \ldots, n_t , and by Theorem 6.6, their Cartesian product is a VT graph with arc-type Π .

If k = 1, we can take the Cartesian product of t - 2 pairwise non-isomorphic prime VT graphs with arc-types n_1, \ldots, n_{t-2} , and one prime VT graph with arc-type $n_{t-1} + 1$, as given by Lemma 8.3, and again, this is a VT graph with arc-type Π .

If k = 2, we can take the Cartesian product of t - 3 pairwise non-isomorphic prime VT graphs with arc-types n_1, \ldots, n_{t-3} , one prime VT graph with arc-type $n_{t-2} + 1$, and the graph K_2 .

Finally, if $k \ge 3$, we can take the Cartesian product of t - k pairwise non-isomorphic prime VT graphs with arc-types n_1, \ldots, n_{t-k} , plus

- (i) k/3 pairwise non-isomorphic prime VT graphs with arc-type 1 + 1 + 1 taken from Lemma 8.8, when $k \equiv 0 \mod 3$, or
- (ii) one prime VT graph of type 1+1+1+1 from Lemma 8.11, and (k-4)/3 pairwise non-isomorphic prime VT graphs with arc-type 1+1+1, when $k \equiv 1 \mod 3$, or
- (iii) one copy of K_2 , and one prime VT graph of type 1 + 1 + 1 + 1, and (k 5)/3 pairwise non-isomorphic prime VT graphs with arc-type 1 + 1 + 1, when $k \equiv 2 \mod 3$.

Case (B): t = 0, with $\Pi = (m_1 + m_1) + \dots + (m_s + m_s)$.

Let ℓ be the number of m_j that are equal to 1, so that $m_j > 1$ for $1 \le i \le s - \ell$, and $m_j = 1$ for $s - \ell + 1 \le i \le s$.

If $\ell = 0$, then by Lemma 8.2 we can find s pairwise non-isomorphic VT graphs with arc-types $(m_1 + m_1), \ldots, (m_s + m_s)$, and then their Cartesian product is a VT graph with arc-type Π .

If $\ell = 1$, we can take the Cartesian product of s - 2 pairwise non-isomorphic VT graphs with arc-types $(m_1 + m_1), \ldots, (m_{s-2} + m_{s-2})$, and one prime VT graph with arc-type $(m_{s-1} + m_{s-1}) + (1 + 1)$ from Lemma 8.7.

Finally, if $\ell \ge 2$, we can take the Cartesian product of $s - \ell$ pairwise non-isomorphic prime VT graphs with arc-types $(m_1 + m_1), \ldots, (m_{s-\ell} + m_{s-\ell})$, plus

- (i) ℓ/2 pairwise non-isomorphic prime VT graphs with arc-type (1+1) + (1+1) from Lemma 8.6, when ℓ is even, or
- (ii) one prime VT graph of type (1 + 1) + (1 + 1) + (1 + 1) from Lemma 8.12, and $(\ell 3)/2$ pairwise non-isomorphic prime VT graphs with arc-type (1+1) + (1+1), when ℓ is odd.

Case (C): s > 0 and t > 0.

In this case, we can write Π as the sum of the marked partitions $\Pi_1 = n_1 + \cdots + n_t$ and $\Pi_2 = (m_1 + m_1) + \cdots + (m_s + m_s)$, and we can deal with most possibilities by simply taking a Cartesian product of a VT graph X_1 with arc-type Π_1 and a VT graph X_2 with arc-type Π_2 . Note that case (A) uses the prime VT graphs produced by Lemmas 8.1, 8.3, 8.8 and 8.11, plus the graph K_2 , while case (B) uses the prime VT graphs produced by Lemmas 8.2, 8.7, 8.6 and 8.12. These prime graphs can be chosen to be pairwise nonisomorphic, and hence pairwise relatively prime, in which case X_1 and X_2 are relatively prime, and therefore $X_1 \Box X_2$ has arc-type $\Pi_1 + \Pi_2 = \Pi$.

All that remains for us to do is to deal with the exceptional situations, namely those where the sum of the n_i or the sum of the m_j is so small that no suitable candidate can be found for X_1 or X_2 . There are two exceptional possibilities for Π_1 not covered in case (A), namely 1 and 1 + 1, and just one for Π_2 in case (B), namely (1 + 1).

If $\Pi_1 = 1$, then we can take a Cartesian product of K_2 with a VT graph produced in case (B), since we are assuming that $d \ge 5$.

If $\Pi_1 = 1 + 1$, then there are two sub-cases to consider, depending on the number ℓ of terms m_j that are equal to 1. If $\ell < s$, then we can adapt the approach taken in case (B) by replacing the prime VT graph of type $(m_1 + m_1)$ by a prime VT graph of type $1 + (m_1 + m_1)$ from Lemma 8.5, and then also add a single copy of K_2 as above. On the other hand, if $\ell = s$, so that Π_2 is the sum of s terms of the form (1 + 1), then we take

- (i) two non-isomorphic prime VT graphs with arc-type 1 + (1 + 1) from Lemma 8.9, when s = 2, or
- (ii) a prime VT graph of type 1 + 1 + (1 + 1) from Lemma 8.10, and a 2(s 1)-valent VT graph of type $(1 + 1) + \cdots + (1 + 1)$ as found in case (B) when $s \ge 3$.

Finally, if $\Pi_2 = (1 + 1)$, again there are two sub-cases to consider, this time depending on the number k of terms n_i that are equal to 1. If k < t, then we can adapt the approach taken in case (A) by replacing the prime VT graph of type n_1 by a prime VT graph of type $n_1 + (1 + 1)$ from Lemma 8.4. On the other hand, if k = t, so that Π_1 is the sum of t terms all equal to 1, then we take

- (i) a single copy of K_2 and a prime VT graph with arc-type 1+1+(1+1) from Lemma 8.10, when t = 3, or
- (ii) a prime VT graph of type 1+(1+1) and a (t-1)-valent VT graph of type $1+\cdots+1$ as found in case (A) when $t \ge 4$.

This completes the proof.

Corollary 9.2. With the exception of 1 + 1 (for the integer 2), every standard partition of a positive integer is realisable as the edge-type of a vertex-transitive graph.

Proof. This follows easily from Theorem 9.1. In fact, every such partition $n_1 + \cdots + n_t$ (except 1 + 1) occurs as both the edge-type and the arc-type of some VT graph with the property that all of its arc-orbits are self-paired.

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Spherical quadrangles with three equal sides and rational angles

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Abstract

When the condition of having three equal sides is imposed upon a (convex) spherical quadrangle, the four angles of that quadrangle cannot longer be freely chosen but must satisfy an identity. We derive two simple identities of this kind, one involving ratios of sines, and one involving ratios of tangents, and improve upon an earlier identity by Ueno and Agaoka.

The simple form of these identities enable us to further investigate the case in which all of the angles are rational multiples of π and produce a full classification, consisting of 7 infinite classes and 29 sporadic examples. Apart from being interesting in its own right, these quadrangles play an important role in the study of spherical tilings by congruent quadrangles.

Keywords: Spherical quadrangle, rational angle, spherical tiling. Math. Subj. Class.: 51M09, 52C20, 11Y50

1 Introduction

In general there will be an infinite number of non-congruent spherical quadrangles with given (ordered) quadruple of angles $\alpha, \beta, \gamma, \delta$, provided that $2\pi < \alpha + \beta + \gamma + \delta < 6\pi$. By imposing restrictions on the sides of a quadrangle this is reduced to a finite number. In this paper we shall investigate the case of a convex quadrangle ABCD with (at least) three equal sides, say |AB| = |BC| = |CD| = a and derive two simple identities which must be satisfied by the angles of that quadrangle as a consequence of this restriction (cf. Theorem 2.1).

A similar, but more complicated identity for this case was already published by Ueno and Agaoka in [3]. We shall show that our identities are stronger (cf. Section 2) in a sense to be made clear below.

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The identity of Ueno and Agaoka arose in the search for tilings of the sphere by congruent quadrangles. In that context it is particularly relevant to consider quadrangles all of whose angles are rational multiples of π (henceforth simply called *rational angles*).

Indeed, consider a vertex P of such a tiling. P belongs to a certain number (say N_A) of quadrangles in the tiling for which P corresponds to vertex A of the quadrangle. Likewise there will be N_B quadrangles for which P corresponds to B, and similar numbers N_C, N_D for C and D. Because the sum of all angles in P must be 2π , we find

$$N_A \alpha + N_B \beta + N_C \gamma + N_D \delta = 2\pi, \tag{1.1}$$

where $\alpha, \beta, \gamma, \delta$ are the corresponding angles of the quadrangle (see Figure 1 for naming conventions). A different vertex P' of the tiling will lead to a similar identity, but generally with different values of N_A, N_B, N_C, N_D .

We may treat the set of identities (1.1) that arise from all vertices of a given tiling as a system of equations with unknowns $\alpha, \beta, \gamma, \delta$. Note that all coefficients in these equations are integers, while every right hand side is equal to 2π . In particular, if this system has rank 4, there will be exactly one solution and it will consist entirely of rational angles.

In Theorem 3.2 we give a full classification of all convex spherical quadrangles with three equal sides whose angles are rational. There turn out to be 7 infinite families of such quadrangles and 29 sporadic examples. The proof of Theorem 3.2 hinges on the fact that our identity (3.2) can be rewritten as an equality between two products of two sines and that instances of such identities with rational angles were already classified by Myerson [2] (cf. Theorem 3.1).



Figure 1: Naming conventions for a spherical quadrangle ABCD with three equal sides.

2 **Relations between the angles**

In what follows we shall consider a spherical quadrangle ABCD with corresponding angles $\alpha, \beta, \gamma, \delta$, sides a, a, a, b and diagonals x, y as indicated in Figure 1. The spherical quadrangle will be called *convex* if it satisfies $0 < a, b, x, y, \alpha, \beta, \gamma, \delta < \pi$. In particular this means that all constituent spherical triangles ABC, ABD, ACD and BCD are 'proper' and satisfy the classical laws of spherical trigonometry.

We take the following inequalities for such quadrangles from [1, Lemma 2.1]:

$$\begin{array}{lll}
\alpha + \delta &< \pi + \beta, \\
\alpha + \delta &< \pi + \gamma, \\
\alpha + \beta &< \pi + \delta, \\
\gamma + \delta &< \pi + \alpha.
\end{array}$$
(2.1)

As mentioned in the introduction, we also have

$$E = \alpha + \beta + \gamma + \delta - 2\pi > 0, \qquad (2.2)$$

where E denotes the *spherical excess* of the quadrangle, which is equal to the area of the quadrangle on a unit sphere.

Finally, we note that $\alpha = \delta$ if and only if $\beta = \gamma$, cf. [1, Lemma 2.3].

Theorem 2.1. In a convex spherical quadrangle ABCD with three equal sides, the following identities hold:

$$\frac{\sin(\alpha - \frac{\gamma}{2})}{\sin\frac{\gamma}{2}} = \frac{\sin(\delta - \frac{\beta}{2})}{\sin\frac{\beta}{2}},\tag{2.3}$$

or equivalently,

$$\frac{\tan\left(\frac{\delta}{2} - \frac{\beta}{2}\right)}{\tan\frac{\delta}{2}} = \frac{\tan\left(\frac{\alpha}{2} - \frac{\gamma}{2}\right)}{\tan\frac{\alpha}{2}}.$$
(2.4)

Proof. Consider the equilateral spherical triangle ABC. The (polar) cosine rule for side BC yields

$$\cos a = \frac{\cos \phi + \cos \phi \cos \beta}{\sin \phi \sin \beta} = \cot \phi \cdot \frac{1 + \cos \beta}{\sin \beta} = \cot \phi \cot \frac{\beta}{2}, \quad (2.5)$$

where $\phi = \angle BAC = \angle ACB$ as indicated in Figure 2. The sine rules for side AC in both



Figure 2: The spherical triangles ABC and ACD.

ABC and ACD, yield

$$\frac{\sin\beta}{\sin x} = \frac{\sin\phi}{\sin a}, \quad \frac{\sin\delta}{\sin x} = \frac{\sin(\alpha-\phi)}{\sin a},$$

and hence

$$\frac{\sin \delta}{\sin \beta} = \frac{\sin(\alpha - \phi)}{\sin \phi} = \sin \alpha \cot \phi - \cos \alpha.$$

Multiplying by $\cot \frac{\beta}{2}$ and using $\sin \beta = 2 \cos \frac{\beta}{2} \sin \frac{\beta}{2}$ and (2.5), yields

$$\frac{\sin \delta}{2\sin^2 \frac{\beta}{2}} = \sin \alpha \cos a - \cos \alpha \cot \frac{\beta}{2},$$

whence

$$\cos a = \frac{\sin \delta + \cos \alpha \sin \beta}{2 \sin \alpha \sin^2 \frac{\beta}{2}}.$$
(2.6)

By repeating the argument above for triangles ABD and BCD, or equivalently, by interchanging $\alpha \leftrightarrow \delta$ and $\beta \leftrightarrow \gamma$, we find

$$\cos a = \frac{\sin \alpha + \cos \delta \sin \gamma}{2 \sin \delta \sin^2 \frac{\gamma}{2}}.$$
(2.7)

We shall now use (2.6-2.7) to compute

$$\Delta \stackrel{\text{def}}{=} 2\cos a\sin\alpha\sin\delta - \sin^2\alpha + \cos^2\delta = 2\cos a\sin\alpha\sin\delta + \cos^2\alpha - \sin^2\delta$$

in two ways. From (2.6) we obtain

$$\begin{split} \Delta &= \csc^2 \frac{\beta}{2} \sin^2 \delta + \csc^2 \frac{\beta}{2} \cos \alpha \sin \beta \sin \delta + \cos^2 \alpha - \sin^2 \delta \\ &= \left(\csc^2 \frac{\beta}{2} - 1\right) \sin^2 \delta + 2 \cot \frac{\beta}{2} \cos \alpha \sin \delta + \cos^2 \alpha \\ &= \cot^2 \frac{\beta}{2} \sin^2 \delta + 2 \cot \frac{\beta}{2} \cos \alpha \sin \delta + \cos^2 \alpha = \left(\cot \frac{\beta}{2} \sin \delta + \cos \alpha\right)^2. \end{split}$$

By symmetry, from (2.7) we obtain

$$\Delta = \left(\cot\frac{\gamma}{2}\sin\alpha + \cos\delta\right)^2.$$

(Note that the original definition of Δ remains unchanged when interchanging α and δ .) Combining both values of Δ we end up with two possibilities:

$$\cot\frac{\beta}{2}\sin\delta + \cos\alpha = \pm\left(\cot\frac{\gamma}{2}\sin\alpha + \cos\delta\right).$$
(2.8)

We consider both cases separately. The second case will turn out to be impossible.

Case 1. Assume there is a plus sign in the right hand side of (2.8). Then (2.8) rewrites to

$$\cot\frac{\beta}{2}\sin\delta - \cos\delta = \cot\frac{\gamma}{2}\sin\alpha - \cos\alpha,$$
(2.9)

which is equivalent to (2.3).

In general, if $x_1/y_1 = x_2/y_2$, then also $(x_1 - y_1)/(x_1 + y_1) = (x_2 - y_2)/(x_2 + y_2)$. Applying this to (2.3) yields

$$\frac{\sin(\delta - \frac{\beta}{2}) - \sin\frac{\beta}{2}}{\sin(\delta - \frac{\beta}{2}) + \sin\frac{\beta}{2}} = \frac{\sin(\alpha - \frac{\gamma}{2}) - \sin\frac{\gamma}{2}}{\sin(\alpha - \frac{\gamma}{2}) + \sin\frac{\gamma}{2}},$$

which transforms to

$$\frac{\cos\frac{\delta}{2}\sin(\frac{\delta}{2}-\frac{\beta}{2})}{\sin\frac{\delta}{2}\cos(\frac{\delta}{2}-\frac{\beta}{2})} = \frac{\cos\frac{\alpha}{2}\sin(\frac{\alpha}{2}-\frac{\gamma}{2})}{\sin\frac{\alpha}{2}\cos(\frac{\alpha}{2}-\frac{\gamma}{2})},$$

and hence

$$\frac{\tan\left(\frac{\delta}{2} - \frac{\beta}{2}\right)}{\tan\frac{\delta}{2}} = \frac{\tan\left(\frac{\alpha}{2} - \frac{\gamma}{2}\right)}{\tan\frac{\alpha}{2}}.$$

Case 2. Assume there is a minus sign in the right hand side of (2.8), i.e., $\cot \frac{\beta}{2} \sin \delta + \cos \alpha = -\cot \frac{\gamma}{2} \sin \alpha - \cos \delta$. This formula can be obtained from the formula for the first case by replacing α by $-\alpha$ and δ by $\pi - \delta$. As a consequence, we now have the following identities:

$$\frac{\sin(\pi-\delta-\frac{\beta}{2})}{\sin\frac{\beta}{2}} = \frac{\sin(-\alpha-\frac{\gamma}{2})}{\sin\frac{\gamma}{2}}, \qquad \frac{\tan\left(\frac{\pi}{2}-\frac{\delta}{2}-\frac{\beta}{2}\right)}{\tan\left(\frac{\pi}{2}-\frac{\delta}{2}\right)} = \frac{\tan\left(-\frac{\alpha}{2}-\frac{\gamma}{2}\right)}{-\tan\frac{\alpha}{2}},$$

equivalent to

$$\frac{\sin(\delta + \frac{\beta}{2})}{\sin\frac{\beta}{2}} = -\frac{\sin(\alpha + \frac{\gamma}{2})}{\sin\frac{\gamma}{2}}, \qquad \frac{\tan\frac{\delta}{2}}{\tan\left(\frac{\delta}{2} + \frac{\beta}{2}\right)} = \frac{\tan\left(\frac{\alpha}{2} + \frac{\gamma}{2}\right)}{\tan\frac{\alpha}{2}}$$

Because the tangent function is monotonous in the interval $[0, \pi/2[$, the latter is only possible if $\beta = \gamma = 0$ or if one of $\frac{1}{2}(\delta + \beta), \frac{1}{2}(\alpha + \gamma)$ lies outside that interval. And because of the signs, this implies that both values must belong to the interval $]\frac{1}{2}\pi, \pi[$. Hence $\pi < \alpha + \gamma, \beta + \delta$. Now $\alpha + \beta < \pi + \delta$ by (2.1). Hence $\alpha + \beta < \beta + 2\delta$ and hence $\alpha < 2\delta$. By symmetry, also $\delta < 2\alpha$, a contradiction.

In [3] Ueno and Agaoka derived the following identity for spherical quadrangles with three equal sides:

$$(1 - \cos\beta)\cos^2\alpha - (1 - \cos\beta)(1 - \cos\gamma)\cos\alpha\cos\delta + (1 - \cos\gamma)\cos^2\delta + \cos\beta\cos\gamma + \sin\alpha\sin\beta\sin\gamma\sin\delta - 1 = 0.$$
(2.10)

We have

Lemma 2.2. Formula (2.10) is equivalent to

$$\cot\frac{\beta}{2}\sin\delta - \cot\frac{\gamma}{2}\sin\alpha = \pm(\cos\alpha - \cos\delta). \tag{2.11}$$

Proof. We express $\cos \beta$ and $\sin \beta$ in terms of $\cot \frac{\beta}{2}$ as follows:

$$\sin\beta = \frac{2\cot^2\frac{\beta}{2}}{\cot^2\frac{\beta}{2}+1}, \quad \cos\beta = \frac{\cot^2\frac{\beta}{2}-1}{\cot^2\frac{\beta}{2}+1}, \quad 1-\cos\beta = \frac{2}{\cot^2\frac{\beta}{2}+1}$$
(2.12)

and similar for $\cos \gamma$ and $\sin \gamma$. Also note that

$$\cos\beta\cos\gamma - 1 = \frac{(\cot^2\frac{\beta}{2} - 1)(\cot^2\frac{\gamma}{2} - 1)}{(\cot^2\frac{\beta}{2} + 1)(\cot^2\frac{\gamma}{2} + 1)} - 1 = \frac{-2\cot^2\frac{\beta}{2} - 2\cot^2\frac{\gamma}{2}}{(\cot^2\frac{\beta}{2} + 1)(\cot^2\frac{\gamma}{2} + 1)}.$$
 (2.13)

Applying (2.12-2.13) to the left hand side of (2.10) transforms it into

$$\frac{2\cos^2\alpha}{\cot^2\frac{\beta}{2}+1} - \frac{4\cos\alpha\cos\delta}{(\cot^2\frac{\beta}{2}+1)(\cot^2\frac{\gamma}{2}+1)} + \frac{2\cos^2\delta}{\cot^2\frac{\gamma}{2}+1} \\ - \frac{2\cot^2\frac{\beta}{2}+2\cot^2\frac{\gamma}{2}}{(\cot^2\frac{\beta}{2}+1)(\cot^2\frac{\gamma}{2}+1)} + \frac{4\sin\alpha\cot\frac{\beta}{2}\cot\frac{\gamma}{2}\sin\delta}{(\cot^2\frac{\beta}{2}+1)(\cot^2\frac{\gamma}{2}+1)}$$

which after multiplying by the common denominator and dividing by 2, reduces to

$$\cos^{2} \alpha \left(\cot^{2} \frac{\gamma}{2} + 1 \right) - 2 \cos \alpha \cos \delta + \cos^{2} \delta \left(\cot^{2} \frac{\beta}{2} + 1 \right)$$
$$- \cot^{2} \frac{\beta}{2} - \cot^{2} \frac{\gamma}{2} + 2 \sin \alpha \cot \frac{\beta}{2} \cot \frac{\gamma}{2} \sin \delta$$
$$= \cos^{2} \alpha - 2 \cos \alpha \cos \delta + \cos^{2} \delta$$
$$+ \cos^{2} \alpha \cot^{2} \frac{\gamma}{2} + \cos^{2} \delta \cot^{2} \frac{\beta}{2} - \cot^{2} \frac{\beta}{2} - \cot^{2} \frac{\gamma}{2}$$
$$+ 2 \sin \alpha \cot \frac{\beta}{2} \cot \frac{\gamma}{2} \sin \delta$$
$$= (\cos \alpha - \cos \delta)^{2} - \left(\cot \frac{\beta}{2} \sin \delta - \cot \frac{\gamma}{2} \sin \alpha \right)^{2}.$$

Remark that choosing the minus sign in (2.11) yields our formula (2.9) from the proof of Theorem 2.1. This shows that Theorem 2.1 is stronger than the result of Ueno and Agaka, as they also allow solutions with a plus sign in the right hand side of (2.11).

3 Rational angles

In what follows we shall investigate spherical quadrangles with three equal sides with the additional property that the four angles α , β , γ , δ are rational. Our main tool is the following theorem from [2].

Theorem 3.1 (Myerson). For all θ we have

$$\sin\frac{\pi}{6}\sin\theta = \sin\frac{\theta}{2}\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right).$$
(3.1)

All other solutions of

$$\sin \pi x_1 \sin \pi x_2 = \sin \pi x_3 \sin \pi x_4 \tag{3.2}$$

with rational numbers x_1, x_2, x_3, x_4 such that $0 < x_1 < x_3 \le x_4 < x_2 \le 1/2$, are given in Table 1.

x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
1/21	8/21	1/14	3/14	4/15	7/15	3/10	11/30
1/14	5/14	2/21	5/21	1/30	11/30	1/10	1/10
4/21	10/21	3/14	5/14	7/30	13/30	3/10	3/10
1/20	9/20	1/15	4/15	1/15	4/15	1/10	1/6
2/15	7/15	3/20	7/20	2/15	8/15	1/6	3/10
1/30	3/10	1/15	2/15	1/12	5/12	1/10	3/10
1/15	7/15	1/10	7/30	1/10	3/10	1/6	1/6
1/10	13/30	2/15	4/15				

Table 1: Nongeneric solutions to (3.2).

Althought our condition (2.3) is almost a direct match with equations (3.1) and (3.2) of the theorem, there are some additional complications that must be taken into account. Most importantly, Theorem 3.1 imposes extra conditions on the angles $\pi x_1, \ldots, \pi x_4$ which are too stringent for the angles $\alpha - \frac{\gamma}{2}, \frac{\beta}{2}, \frac{\gamma}{2}, \delta - \frac{\beta}{2}$ of (2.3). First, all angles in Theorem 3.1 must lie in the interval $]0, \pi/2[$ while of the four angles

First, all angles in Theorem 3.1 must lie in the interval $]0, \pi/2[$ while of the four angles in (2.3) only $\frac{\beta}{2}$ and $\frac{\gamma}{2}$ satisfy this restriction, while the other two $(\alpha - \frac{\gamma}{2}, \delta - \frac{\beta}{2})$ are only known to lie in the interval $] - \pi/2, \pi[$. This means that we have to 'renormalize' these angles by using the identities

$$\sin(\pi - \pi x_i) = \sin \pi x_i, \quad \sin(-\pi x_i) = -\sin \pi x_i.$$

As a consequence, we shall always need to consider the following five cases:

$$\{\pi x_1, \pi x_2, \pi x_3, \pi x_4\} = \begin{cases} \{\alpha - \frac{\gamma}{2}, \frac{\beta}{2}, \frac{\gamma}{2}, \delta - \frac{\beta}{2}\}, \\ \{\pi - \alpha + \frac{\gamma}{2}, \frac{\beta}{2}, \frac{\gamma}{2}, \delta - \frac{\beta}{2}\}, \\ \{\alpha - \frac{\gamma}{2}, \frac{\beta}{2}, \frac{\gamma}{2}, \pi - \delta + \frac{\beta}{2}\}, \\ \{\pi - \alpha + \frac{\gamma}{2}, \frac{\beta}{2}, \frac{\gamma}{2}, \pi - \delta + \frac{\beta}{2}\}, \\ \{\frac{\gamma}{2} - \alpha, \frac{\beta}{2}, \frac{\gamma}{2}, \frac{\beta}{2} - \delta\}. \end{cases}$$
(3.3)

(Note that $\alpha - \frac{\gamma}{2} < 0$ automatically implies $\delta - \frac{\beta}{2} < 0$ because the signs of both sides of (2.3) must be the same.)

Furthermore Theorem 3.1 assumes a specific ordering of the variables x_1, x_2, x_3, x_4 , which again we cannot guarantee. In principle we must therefore consider *eight* different ways to assign the angles on the right hand side of (3.3) to the angles of the left hand side, yielding 40 possibilities in total. We can reduce this amount by half by taking into account the symmetry $\alpha \leftrightarrow \delta, \beta \leftrightarrow \gamma$.

Finally, Theorem 3.1 does not consider the 'trivial' cases where one (and then at least two) of the angles is zero, or where $\{\sin \pi x_1, \sin \pi x_2\} = \{\sin \pi x_3, \sin \pi x_4\}$.

Taking all of this into consideration leads to

Theorem 3.2. Consider a convex spherical quadrangle with three equal sides, with angles and sides as indicated in Figure 1.

If the angles $\alpha, \beta, \gamma, \delta$ are rational multiples of π , then they must satisfy one of the following properties, or a property derived from these by interchanging $\alpha \leftrightarrow \delta$ and $\beta \leftrightarrow \gamma$:

1. $\alpha = \gamma$ and $\beta = \delta$ (and all four sides are equal),

2.
$$\alpha = \delta$$
 and $\beta = \gamma$

- 3. $\alpha = \frac{\gamma}{2}$ and $\delta = \frac{\beta}{2}$, with $\alpha + \delta < \pi$,
- 4. $\alpha = \frac{3\gamma}{2}$, $\beta = \frac{\pi}{3}$ and $\delta = \frac{2\pi}{3} \frac{\gamma}{2}$, with $\frac{\pi}{2} < \gamma < \frac{2\pi}{3}$.
- 5. $\alpha = \frac{\pi}{6} + \frac{\gamma}{2}, \beta = 2\gamma \text{ and } \delta = \frac{\pi}{2} + \frac{\gamma}{2}, \text{ with } \frac{\pi}{3} < \gamma < \frac{\pi}{2},$
- 6. $\alpha = \frac{\pi}{6} + \frac{\gamma}{2}$, $\beta = 2\gamma$ and $\delta = \frac{\pi}{2} + \frac{3\gamma}{2}$ (= 3 α), with $\frac{4\pi}{15} < \gamma < \frac{\pi}{3}$,
- 7. $\alpha = \frac{\pi}{6} + \frac{\gamma}{2}$, $\beta = 2\pi 2\gamma$ and $\delta = \frac{3\pi}{2} \frac{3\gamma}{2}$, with $\frac{\pi}{2} < \gamma < \frac{5\pi}{6}$,
- 8. (sporadic cases) α/π , β/π , γ/π , δ/π are as listed in Table 2.

$lpha/\pi$	β/π	γ/π	δ/π	$lpha/\pi$	β/π	γ/π	δ/π
29/42	8/21	3/7	23/42	5/6	8/15	3/5	19/30
31/42	8/21	3/7	23/42	23/30	8/15	3/5	19/30
5/6	8/21	5/7	17/42	5/6	8/15	11/15	17/30
37/42	8/21	5/7	17/42	9/10	8/15	11/15	17/30
5/6	3/7	20/21	17/42	23/60	8/15	9/10	13/60
11/42	5/7	20/21	1/6	31/60	8/15	9/10	19/60
29/42	5/7	20/21	23/42	17/30	8/15	13/15	11/30
49/60	4/15	7/10	17/60	31/60	3/5	5/6	23/60
53/60	4/15	7/10	17/60	11/15	3/5	13/15	8/15
7/10	4/15	13/15	7/30	19/30	3/5	14/15	13/30
49/60	3/10	14/15	17/60	5/6	3/5	14/15	17/30
23/30	1/3	14/15	3/10	19/60	7/10	14/15	13/60
11/15	7/15	3/5	8/15	37/60	7/10	14/15	29/60
13/15	7/15	3/5	8/15	23/30	11/15	14/15	19/30
17/30	7/15	14/15	3/10				

Table 2: Sporadic cases of Theorem 3.2.

Proof. (The proofs of the inequalities in the statement of the Theorem are left to the reader. They are immediate consequences of (2.1-2.2).)

We split the proof into three parts.

Part 1. We first consider the 'trivial' cases. The only angles in (2.3) which are allowed to be zero, are $\alpha - \frac{\gamma}{2}$ and $\delta - \frac{\beta}{2}$. This corresponds to case 3 in the statement of this theorem. Next, $\{\sin \pi x_1, \sin \pi x_2\} = \{\sin \pi x_3, \sin \pi x_4\}$ corresponds to either

$$\sin\left(\alpha - \frac{\gamma}{2}\right) = \sin\frac{\gamma}{2} \quad \text{and} \quad \sin\left(\beta - \frac{\delta}{2}\right) = \sin\frac{\beta}{2},$$
 (3.4)

or

$$\sin\left(\alpha - \frac{\gamma}{2}\right) = \sin\left(\delta - \frac{\beta}{2}\right) \quad \text{and} \quad \sin\frac{\beta}{2} = \sin\frac{\gamma}{2}.$$
 (3.5)

Equation (3.4) further splits into 4 different cases:

$$\begin{aligned} \alpha - \frac{\gamma}{2} &= \frac{\gamma}{2} & \text{and} \quad \delta - \frac{\beta}{2} &= \frac{\beta}{2}, \\ \alpha - \frac{\gamma}{2} &= \pm \pi - \frac{\gamma}{2} & \text{and} \quad \delta - \frac{\beta}{2} &= \frac{\beta}{2}, \\ \alpha - \frac{\gamma}{2} &= \frac{\gamma}{2} & \text{and} \quad \delta - \frac{\beta}{2} &= \pm \pi - \frac{\beta}{2}, \\ \alpha - \frac{\gamma}{2} &= \pm \pi - \frac{\gamma}{2} & \text{and} \quad \delta - \frac{\beta}{2} &= \pm \pi - \frac{\beta}{2}. \end{aligned}$$

The first case corresponds to case 1 in the statement of this theorem, the other three are not allowed because then $\alpha = \pm \pi$ or $\beta = \pm \pi$.

Similarly, equation (3.5) splits into the following cases:

$$\begin{aligned} \alpha - \frac{\gamma}{2} &= \delta - \frac{\beta}{2} & \text{and} \quad \frac{\beta}{2} &= \frac{\gamma}{2}, \\ \alpha - \frac{\gamma}{2} &= \pm \pi - \delta + \frac{\beta}{2} & \text{and} \quad \frac{\beta}{2} &= \frac{\gamma}{2}, \\ \alpha - \frac{\gamma}{2} &= \delta - \frac{\beta}{2} & \text{and} \quad \frac{\beta}{2} &= \pi - \frac{\gamma}{2}, \\ \alpha - \frac{\gamma}{2} &= \pm \pi - \delta + \frac{\beta}{2} & \text{and} \quad \frac{\beta}{2} &= \pi - \frac{\gamma}{2}. \end{aligned}$$

The first of these reduces to $\alpha = \delta$ and $\beta = \gamma$, i.e., case 2 in the statement of this theorem. The second implies $\beta = \gamma$, $\alpha + \delta = \pi + \gamma$ which is disallowed by (2.1). The third leads to $\alpha + \pi = \gamma + \delta$, again forbidden by (2.1). The last yields either $\alpha = 2\pi - \delta$ or $\alpha = -\delta$, which again is not allowed.

Part 2. Let us now consider formula (3.1). As mentioned above, this formula must be applied to our problem in 20 different ways, 4 permutations of the angles in (3.1) each time matched to the 5 cases listed in (3.3).

In Table 3 we list each of these 20 possibilities (columns 1–4), and the corresponding values of α , β , γ , δ (columns 5–8). In each of the four tables, columns 1–4 contain the same values but correspond to different angles of (3.1), as indicated in the column headers.

θ	$\frac{\pi}{6}$	$\frac{\theta}{2}$ $\frac{\pi}{2}$	$\frac{1}{2} - \frac{\theta}{2}$	α	β	γ	δ		
$\alpha - \frac{\gamma}{2}$	$\frac{\beta}{2}$	$\frac{\gamma}{2}$ δ	$b - \frac{\beta}{2}$	$\frac{3\theta}{2}$	$\frac{\pi}{3}$	$\theta \frac{2\pi}{3}$	$\frac{\pi}{2} - \frac{\theta}{2}$	$\alpha + \cdots +$	$-\delta < 2\pi$
$\alpha - \frac{\gamma}{2}$	$\frac{p}{2}$	$\frac{\gamma}{2}$ π -	$-\delta + \frac{p}{2}$	$\frac{30}{2}$	$\frac{\pi}{3}$	$\theta \frac{2\pi}{3}$	$\frac{1}{2} + \frac{9}{2}$	$\alpha + \delta <$	$\beta + \pi \Rightarrow \theta < \frac{\pi}{3}$ but
$\pi - \alpha + \frac{\gamma}{2}$	<u>β</u>	<u>2</u>	_ <u>β</u>	$\pi - $	<u>θ</u> <u>π</u>	A 21	<u>τ_θ</u>	$\alpha + \cdots + \alpha + \cdots + \alpha + \cdots + \alpha + \cdots + \alpha$	$\cdot + \delta > 2\pi \Rightarrow \theta > \frac{\pi}{3}$ $- \delta = 2\pi$
$\pi - \alpha + \frac{\gamma}{2}$	$\frac{2}{\beta}$	$\frac{2}{\gamma}$ π -	$-\delta + \frac{\beta}{2}$	$\pi - $	$\frac{2}{\theta} = \frac{3}{\pi}$	$\theta \frac{3}{2}$	$\frac{1}{\tau} + \frac{2}{\theta}$	$\alpha + \delta >$	$\pi + \beta$
$\frac{\gamma}{2} - \alpha$	$\frac{\beta}{2}$	$\frac{\gamma}{2}$	$\frac{3}{2} - \delta$	$-\frac{\theta}{2}$	$\frac{2}{\frac{\pi}{3}}$	$\theta - \theta$	$\frac{\pi}{3} + \frac{\theta}{2}$	$\alpha < 0$	
θ	$\frac{\pi}{6}$	$\frac{\pi}{2} - \frac{\theta}{2}$	$\frac{\theta}{2}$		α	β	γ	δ	
$\alpha - \frac{\gamma}{2}$	$\frac{\beta}{2}_{\beta}$	$\frac{\gamma}{2}$	$\delta -$	$\frac{\beta}{2}_{\beta}$	$\frac{\pi}{2} + \frac{\theta}{2}$	$\frac{\pi}{3}$	$\pi - \theta$	$\frac{\pi}{6} + \frac{\theta}{2}$	$\alpha + \dots + \delta = 2\pi$
$\alpha - \frac{1}{2}$	$\frac{\beta}{2}_{\beta}$	$\frac{1}{2}$	$\pi - \delta$	$\frac{+\frac{\beta}{2}}{\beta}$	$\frac{\pi}{2} + \frac{5}{2}$ $3\pi - 36$	$\frac{\pi}{3}$	$\pi - \theta$	$\frac{\pi}{6} - \frac{\theta}{2}$	$\alpha + \delta = \pi + \beta$
$\pi - \alpha + \frac{\gamma}{2}$ $\pi - \alpha + \frac{\gamma}{2}$	$\frac{\overline{2}}{\beta}$	$\frac{\overline{2}}{\gamma}$	$\pi - \delta$	$\frac{\overline{2}}{+\frac{\beta}{2}}$	$\frac{\overline{2}}{3\pi} = \frac{\overline{2}}{36}$	$\frac{3}{\pi}$	$\pi = 0$ $\pi = \theta$	$\overline{6} \pm \overline{2}$ $\underline{7\pi} - \underline{\theta}$	$\alpha + \delta > \pi + \beta$
$\frac{\gamma}{2} - \alpha$	$\frac{\frac{2}{\beta}}{2}$	$\frac{2}{\frac{\gamma}{2}}$	$\frac{\beta}{2}$ –	δ^2	$\frac{2}{\frac{\pi}{2}} - \frac{3\theta}{2}$	$\frac{3}{\frac{\pi}{3}}$	$\pi - \theta$	$\frac{6}{\frac{\pi}{6}} - \frac{2}{\frac{\theta}{2}}$	$\alpha + \dots + \delta < 2\pi$
π		ρ θ	πθ	9	0	ß	<i></i>	s	
$\frac{\overline{6}}{\alpha - \underline{\gamma}}$		$\frac{b}{\underline{\beta}}$ $\underline{\gamma}$	$\frac{\overline{2}}{\delta - \beta}$	2	$\frac{\pi}{\pi} + \frac{\theta}{2}$	р 2.0	$\frac{\gamma}{\theta}$ $\frac{\pi}{\pi}$	$\frac{\theta}{\theta}$	
$\alpha - \frac{\gamma}{2}$		$\frac{2}{\beta}$ $\frac{2}{\gamma}$	$\pi - \delta +$	$\frac{\beta}{2}$	$\frac{6}{\frac{\pi}{6}} + \frac{2}{\frac{\theta}{2}}$	$\frac{2\theta}{2\theta}$	$\theta \frac{\pi}{2}$	$+\frac{3\theta}{2}$	
$\pi - \alpha +$	$\frac{\gamma}{2}$	$\frac{\frac{2}{\beta}}{\frac{2}{2}}$ $\frac{\frac{2}{\gamma}}{\frac{2}{2}}$	$\delta - \frac{\beta}{2}$		$\frac{5\pi}{6} + \frac{\theta}{2}$	2θ	$\theta \frac{\pi}{2}$	$+\frac{\tilde{\theta}}{2}$ c	$\alpha + \delta > \pi + \gamma$
$\pi - \alpha +$	$\frac{\gamma}{2}$	$\frac{\beta}{2}$ $\frac{\gamma}{2}$	$\pi - \delta +$	$\frac{\beta}{2}$	$\frac{5\pi}{6} + \frac{\theta}{2}$	2θ	$\theta = \frac{\pi}{2}$	$+\frac{3\theta}{2}$ ϵ	$\alpha + \delta > \pi + \beta$
$\frac{\gamma}{2} - \alpha$		$\frac{\beta}{2}$ $\frac{\gamma}{2}$	$\frac{\beta}{2} - \delta$	5 -	$-\frac{\pi}{6}+\frac{\theta}{2}$	2θ	$\theta - \frac{\pi}{2}$	$\frac{1}{2} + \frac{3\theta}{2} \mid \alpha$	$\alpha + \dots + \delta < 2\pi$
<u>π</u>	θ	$\frac{\pi}{2}$	<u>)</u>	2	α	в	γ	δ	
$\frac{6}{\alpha - \frac{\gamma}{2}}$	$\frac{\beta}{2}$	$\frac{2}{\frac{\gamma}{2}}$	<u>2</u> 2 δ –	$-\frac{\beta}{2}$	$\frac{2\pi}{3} - \frac{6}{3}$	$\frac{1}{2\theta}$	$\pi - \theta$	$\frac{3\theta}{2}$	
$\alpha - \frac{\gamma}{2}$	$\frac{\beta}{2}$	$\frac{\dot{\gamma}}{2}$	$\pi - \delta$	$\tilde{b} + \frac{\beta}{2}$	$\frac{2\pi}{3} - \frac{6}{2}$	2θ	$\pi - heta$	$\pi + \frac{\theta}{2}$	$\gamma + \delta > \pi + \alpha$
$\pi - \alpha + \frac{\gamma}{2}$	$\frac{\beta}{2}$	$\frac{\gamma}{2}$	δ –	$-\frac{\beta}{2}$	$\frac{4\pi}{3} - \frac{6}{2}$	2θ	$\pi - \theta$	$\frac{3\theta}{2}$	$\alpha+\beta>\pi+\delta$
$\pi - \alpha + \frac{\gamma}{2}$	$\frac{\beta}{2}$	$\frac{\gamma}{2}$	$\pi - \delta$	$5 + \frac{\beta}{2}$	$\frac{4\pi}{3} - \frac{6}{2}$	2θ	$\pi - \theta$	$\pi + \frac{\theta}{2}$	$\alpha + \delta > \pi + \gamma$
$\frac{1}{2} - \alpha$	$\frac{p}{2}$	$\frac{1}{2}$	$\frac{p}{2}$ -	$-\delta$	$\left \frac{\pi}{3} - \frac{\pi}{2} \right $	2θ	$\pi - \theta$	$\frac{v}{2}$	$ \alpha + \dots + \delta < 2\pi$

Table 3: The generic case of Theorem 3.2.

It turns out that 16 of these options are disallowed by the inequalities (2.1–2.2). We list the corresponding details in the right hand column of each table. The four possibilities that remain are listed as cases 4–7 in the statement of the theorem.

Part 3. For the sporadic examples from Table 1 we could proceed in the same manner as in part 2 of this proof. Although there are some shortcuts which could be taken to avoid to have to consider each of the $20 \times 15 = 300$ cases separately, we thought it less error prone to enlist the help of a computer.

Recall that $i \sin \frac{2m\pi}{n}$ belongs to the cyclotomic field $\mathbf{Q}(\zeta_n)$ where ζ_n is a primitive *n*-th root of unity. Modern computer algebra systems can do exact arithmetic over such cyclotomic fields, hence we may use such a system to directly check all instances of equation (2.3) in which $\alpha, \beta/2, \gamma/2, \delta$ are integral multiples of $\frac{2\pi}{n}$ and are in the required range. From Table 1 we may derive all values of *n* which we are required to try: for each row let *n* denote twice the least common multiple of the four denominators. In fact, many rows will yield the same value of *n* and it turns out to be sufficient to do the computations only for n = 84 and n = 120. We used this method to obtain the values in Table 2. (The source code for these computations is available from http://caagt.ugent.be/ratguad/.)

The same method, with n = 12p, p a prime > 7, was used to verify the results of part 2 of this proof.

Note that in case 3 of Theorem 3.2 the quadrangle is a union of three disjoint congruent triangles with angles α , δ and $\pi/3$ — cf. Figure 3.



Figure 3: The special case $\alpha = \frac{\gamma}{2}, \delta = \frac{\beta}{2}$.

References

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Petra Šparl Award 2018: Call for nominations

The Petra Šparl Award has been established to recognise (in each even-numbered year) the best paper published recently by a young woman mathematician in one of the two journals *Ars Mathematica Contemporanea* (AMC) and *The Art of Discrete and Applied Mathematics* (ADAM).

The award is named in memory of Dr Petra Šparl, a talented woman mathematician with a promising future who worked in graph theory and combinatorics, but died mid-career in 2016 after a battle with cancer.

This award consists of a certificate with the recipient's name, and an invitation to give a lecture at the Mathematics Colloquium at the University of Primorska, and to give lectures at the University of Maribor and University of Ljubljana.

The Petra Šparl Award Committee is now calling for nominations for the first award.

ELIGIBILITY: Each nominee must be a woman author or co-author of a paper published either in AMC or ADAM in the last five years, who was at most 40 years old at the time of the paper's first submission.

NOMINATION FORMAT: Each nomination should specify the following:

- (a) the name, birth-date and affiliation of the candidate;
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PROCEDURE: Nominations should be submitted by email to any one of the three members of the Petra Šparl Award Committee (see below), by 31 August 2017.

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