Discussiones Mathematicae Graph Theory 42 (2022) 1351–1382 https://doi.org/10.7151/dmgt.2436

ON SINGULAR SIGNED GRAPHS WITH NULLSPACE SPANNED BY A FULL VECTOR: SIGNED NUT GRAPHS

Nino Bašić

 FAMNIT, University of Primorska, Koper, Slovenia, and IAM, University of Primorska, Koper, Slovenia, and
 Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

e-mail: nino.basic@upr.si

PATRICK W. FOWLER

Department of Chemistry University of Sheffield, Sheffield S3 7HF, UK e-mail: p.w.fowler@sheffield.ac.uk

Tomaž Pisanski

FAMNIT, University of Primorska, Koper, Slovenia, and IAM, University of Primorska, Koper, Slovenia, and Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia, and Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia

e-mail: tomaz.pisanski@upr.si

AND

IRENE SCIRIHA

Department of Mathematics, Faculty of Science University of Malta, Msida, Malta

e-mail: irene.sciriha-aquilina@um.edu.mt

Abstract

A signed graph has edge weights drawn from the set $\{+1, -1\}$, and is *sign-balanced* if it is equivalent to an unsigned graph under the operation of sign switching; otherwise it is *sign-unbalanced*. A nut graph has a one dimensional kernel of the 0-1 adjacency matrix with a corresponding eigenvector that is full. In this paper we generalise the notion of nut graphs to signed graphs. Orders for which regular nut graphs with all edge weights +1

exist have been determined recently for the degrees up to 12. By extending the definition to signed graphs, we here find all pairs (ρ, n) for which a ρ -regular nut graph (sign-balanced or sign-unbalanced) of order n exists with $\rho \leq 11$. We devise a construction for signed nut graphs based on a smaller 'seed' graph, giving infinite series of both sign-balanced and signunbalanced ρ -regular nut graphs. Orders for which a regular nut graph with $\rho = n - 1$ exists are characterised; they are sign-unbalanced with an underlying graph K_n for which $n \equiv 1 \pmod{4}$. Orders for which a regular sign-unbalanced nut graph with $\rho = n - 2$ exists are also characterised; they have an underlying cocktail-party graph CP(n) with even order $n \geq 8$.

Keywords: signed graph, nut graph, singular graph, graph spectrum, Fowler construction, sign-balanced graph, sign-unbalanced graph, cocktail-party graph.

2010 Mathematics Subject Classification: 05C50, 15A18, 05C22, 05C92.

1. INTRODUCTION AND MOTIVATION

Spectral graph theory is an important branch of discrete mathematics that links graphs to linear algebra [8,9,12–14]. Singular graphs have a zero eigenvalue of the 0-1 adjacency matrix. A special class of singular graphs consists of the core graphs, graphs of which the kernel of the adjacency matrix contains a full vector (i.e., a vector that has no zero entry). One subclass of core graphs, known as nut graphs, is of particular interest. A nut graph is a singular graph in which every non-zero vector in the kernel of the 0-1 adjacency matrix is full. A necessary condition is that for a nut graph, the dimension of the kernel (i.e., the nullity η) is one. In this sense, a nut graph is a maximally-extended core graph of nullity 1 [34, 37]. Some properties of nut graphs are easily proved. For instance, nut graphs are connected, non-bipartite, and have no vertices of degree one [37]. It is conventional to require that a nut graph has $n \geq 2$ vertices, although some authors consider K_1 as the trivial nut graph. There exist numerous construction rules for making larger nut graphs from a smaller 'seed' nut graph [33, 37].

In this contribution we will consider signed graphs, i.e., graphs with edge weights drawn from $\{-1, 1\}$ and ask whether they can also be nut graphs. Although the problem may appear to be purely mathematical, we were driven to study it by the chemical interest arising from the specific properties expected of conjugated π systems whose molecular graphs are nut graphs. The Hückel molecular orbital theory of conjugated π systems [39] is essentially an exercise in applied spectral graph theory [40]. In this electronic structure theory, systems based on nut graphs have distributed radical reactivity, since occupation by a single electron of the molecular orbital corresponding to the kernel eigenvector leads to spin density on all carbon centres [36]. In the context of theories of molecular conduction, nut graphs have a unique status as the strong omniconductors of nullity 1 [19]. Extension of our considerations to signed graphs allows the study of twisted carbon networks. Möbius carbon networks, where the carbon framework is embedded on a surface with a half twist are representable by signed graphs. Such molecules have been synthesised [26,30,41,42], and they obey different electron counting rules from those of the standard unweighted Hückel networks [17, 25]. The distinct electronic structure and unusual steric interactions of Möbius systems suggest potential for applications in functional materials of various types [16].

The notion of signed graphs goes back to at least the 1950s and is documented in two dynamic-survey papers [44, 45]. The fundamentals of this theory and its standard notation were developed by Zaslavsky in 1982 in [43] and in a series of other papers. For general discussion of signed graphs the reader is referred to recent papers [5, 22] which set out notation and basic properties. For nut graphs, several useful papers are available, for instance [20, 31–33]. Recently the problem of existence of regular nut graphs was posed, and solved for cubic and quartic graphs [21]. Later, it was solved for degrees ρ , $\rho \leq 11$ [18] and $\rho = 12$ [4]. A recent study explored cases where the class of circulant graphs provides nut graphs [15].

In this paper we carry the problem of the existence of regular nut graphs over from ordinary graphs to signed graphs. We characterise all orders n and degrees $\rho \leq 11$ for which a ρ -regular nut graph of order n (either signed or unsigned) exists. This depends on a construction based on work on unsigned nut graphs [18,21]. In the new formulation, it produces larger signed nut graphs from smaller, whether regular or not (though it is used here only for regular graphs). Cases where a sign-unbalanced nut graph exists with $\rho = n - 1$ or $\rho = n - 2$ are also fully characterised. We finish the paper with two questions for the open cases (i.e., $\rho \geq 12$).

We note that our investigation is a special case of the spectral theory of finitedimensional symmetric linear operators with nullspace spanned by a full vector. The case where a fixed matrix A with eigenvalue λ has a part-full eigenvector has also attracted attention [27, 28].

2. Signed Graphs and Nut Graphs

2.1. Signed graphs

In this section we start with formal definitions. A signed graph $\Gamma = (G, \Sigma)$ is a graph G = (V, E) with a distinguished subset of edges $\Sigma \subseteq E$ that we shall call negative edges. Equivalently, we may consider the signed graph (G, σ) to be a graph endowed with a mapping $\sigma \colon E \to \{-1, +1\}$ where $\Sigma = \{e \in E \mid$ $\sigma(e) = -1$. The adjacency matrix $A(\Gamma)$ of a signed graph is a symmetric matrix obtained from the adjacency matrix A(G) of the underlying graph G by replacing 1 by -1 for entries where the vertices are connected by a negative edge. In this context, an unweighted graph can be regarded as a signed graph without negative edges. Symmetries (automorphisms) of a signed graph $\Gamma = (G, \Sigma)$ are also symmetries of the underlying graph G. They preserve edge weights (1)

$$\operatorname{Aut} \Gamma = \{ \alpha \in \operatorname{Aut} G \mid \forall e = uv \in E(G), \ e \in \Sigma \iff \alpha(e) = \alpha(u)\alpha(v) \in \Sigma \}.$$

Hence, the automorphism group Aut Γ of a signed graph Γ is a subgroup of the automorphism group $\operatorname{Aut} G$ of the underlying graph G.

2.2. Singular graphs, core graphs and nut graphs

A graph that has zero as an eigenvalue is called a *singular graph*, i.e., a graph is singular if and only if its adjacency matrix has a non-trivial kernel. The dimension of the kernel is the *nullity*. An eigenvector \mathbf{x} can be viewed as a weighting of vertices, i.e., a mapping $\mathbf{x}: V \to \mathbb{R}$. A vector \mathbf{x} belongs to the kernel, ker A, i.e., $\mathbf{x} \in \ker A$, if and only if for each vertex v the sum of entries on the neighbours $N_G(v)$ equals 0, i.e.

(2)
$$\sum_{u \in N_G(v)} \mathbf{x}(u) = 0.$$

We call equation (2) the *local condition*. The support, $supp \mathbf{x}$, of a kernel eigenvector $\mathbf{x} \in \ker A$ is the subset of V at which \mathbf{x} attains non-zero values, i.e.

(3)
$$\operatorname{supp} \mathbf{x} = \{ v \in V \mid \mathbf{x}(v) \neq 0 \}$$

If supp $\mathbf{x} = V$, then the vector \mathbf{x} is *full*. Define supp ker A as follows

(4)
$$\operatorname{supp} \ker A = \bigcup_{\mathbf{x} \in \ker A} \operatorname{supp} \mathbf{x}$$

A singular graph G is a core graph if supp ker A = V. A core graph of nullity 1 is called a *nut graph*. Although the kernel of a core graph may have a basis that has no full vectors, there exists a basis with all vectors full.

Proposition 1. Each core graph admits a kernel basis that contains only full vectors.

Proof. Let $V(G) = \{1, \ldots, n\}$ and let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be an arbitrary kernel basis. Let ι be the smallest integer (i.e., vertex label), such that at least one of the entries $\mathbf{x}_1(\iota), \ldots, \mathbf{x}_\eta(\iota)$ is zero, and let $\mathbf{x}_\ell(\iota)$ be one of those entries. As G is a

1354

core graph, at least one of the entries $\mathbf{x}_1(\iota), \ldots, \mathbf{x}_\eta(\iota)$ is non-zero; let us denote the first such entry that is encountered by $\mathbf{x}_k(\iota)$. We can replace vector \mathbf{x}_ℓ by $\mathbf{x}_\ell + \alpha \mathbf{x}_k$, where $\alpha > 0$. If we pick α large enough, i.e., if

(5)
$$\alpha > \max\left\{\frac{|\mathbf{x}_{\ell}(i)|}{|\mathbf{x}_{k}(i)|} \mid i \neq \iota, \mathbf{x}_{k}(i) \neq 0\right\},$$

then $\mathbf{x}_{\ell}(i) + \alpha \mathbf{x}_k(i)$ will be non-zero for all *i*. No new zero entries were created in the replacement process and at least one zero was eliminated. We repeat this process until no more zeros remain.

Corollary 2. Each core graph admits a kernel basis that contains only full vectors with integer entries.

Proof. An integer basis always exists for an integer eigenvalue, as can be seen from the following argument. Let M be a matrix with rational entries. Let λ be any of its rational eigenvalues and \mathbf{x} any eigenvector corresponding to λ . The eigenvector \mathbf{x} can be obtained by Gaussian elimination (i.e., row reduction to echelon form) and thus contains only rational entries. Hence, there exists a constant k, such that the eigenvector $k\mathbf{x}$ has all entries integer.

An integer basis (vectors may contain 0 entries) can then be transformed to a basis where all vectors are full by using the replacement process described in the proof of Proposition 1. If we choose an integer for the value of α at each step, the process will keep all entries integer.

2.3. Switching equivalence of signed graphs

Let $\Gamma = (G, \Sigma)$ be a signed graph over G = (V, E) and let $U \subseteq V(G)$ be a set of its vertices. A *switching* at U is an operation that transforms $\Gamma = (G, \Sigma)$ to a signed graph $\Gamma^U = (G, \Sigma \nabla \partial U)$ where ∇ denotes symmetric difference of sets and

(6)
$$\partial U = \{ uv \in E \mid u \in U, v \notin U \}.$$

Note that $\partial U = \partial(V(G) \setminus U)$, $\Gamma^U = \Gamma^{V(G) \setminus U}$ and $(\Gamma^U)^U = \Gamma$. In fact, switching is an equivalence relation on the signed graphs with the same underlying graph. Any graph G can be regarded as a signed graph $\Gamma = (G, \emptyset)$. We will want to emphasise a useful distinction. Any signed graph is a *sign-balanced* graph if it is switching equivalent to $\Gamma = (G, \emptyset)$, otherwise it is called *sign-unbalanced* [43, 44]. There is precedent for these terms [44], though the shorter 'balanced' and 'unbalanced' are more often used [45]. However, the term 'balanced' has also been used in a different context, where it denotes 3-regular nut graphs with the property that the entries of the kernel vector on the neighbours of every vertex are in ratio 2:-1:-1 [36]. Hence, to avoid potential confusion, we adopt the more explicit terms here.

As observed, for instance in [5], switching has an obvious linear algebraic description.

Proposition 3 [5]. Let $A(\Gamma)$ be the adjacency matrix of signed graph Γ and $A(\Gamma^U)$ be the corresponding adjacency matrix of the signed graph switched at U. Let $S = \text{diag}(s_1, s_2, \ldots, s_n)$ be the diagonal matrix with $s_i = -1$ if $v_i \in U$ and $s_i = 1$ elsewhere. Then

(7)
$$A(\Gamma^U) = SA(\Gamma)S$$

Since $S^T = S^{-1} = S$ we also have

(8)
$$A(\Gamma) = SA(\Gamma^U)S.$$

Clearly, switching-equivalent signed graphs with the same underlying graph G are cospectral. In particular, all sign-balanced graphs with the same underlying graph G are cospectral. The following lemma will be useful.

Lemma 4. Let G be a labelled connected graph on n vertices and m edges and let T be a spanning tree of G. Every switching equivalence class of signed graphs over G contains exactly one signed graph with all edges of the tree T positive.

Proof. Recall that in any tree there is a unique path between any two vertices. Choose any vertex w from V. Let U be the set of vertices v in T that have an even number of negative edges on the unique (w, v)-path of T. Then $V \setminus U$ contains the vertices v that have an odd number of negative edges on the path from w to v along T. The sign switching $(U, V \setminus U)$ will make T all positive. Hence, each switching class has at least one signed graph that makes T all positive.

Let Γ and Γ' be two switching equivalent signed graphs over G with edges of T all positive. Then there exists $W \subseteq V$ such that Γ' can be obtained by switching Γ at W. Let e = uv be an edge of T. Since the edge e has to remain positive, $u \in W$ if and only if $v \in W$. Because T is a spanning tree, it follows that W = V or $W = \emptyset$. In either case, $\Gamma = \Gamma'$.

The essential idea of using a spanning tree is present in the earlier literature, e.g. Lemma 3.1 in [43]. Here we use it to find cardinalities of the switching classes, which in turn is needed for the analysis of Algorithm 1.

Proposition 5. Let G be a labelled connected graph on n vertices and m edges. There are 2^m signed graphs over G, there are 2^{m-n+1} switching equivalence classes, and each class has 2^{n-1} signed graphs. **Proof.** At the beginning we choose a fixed but arbitrary spanning tree T in G. We divide the argument into three steps.

Step (a). For a. given connected graph G (and the spanning tree T) there are 2^m different signed graphs. Indeed, we may choose any subset Σ of edges E and make all edges in Σ negative. Some of the signed graphs will have all edges of T positive, while others will have some edges of T negative.

Step (b). Among the 2^m signed graphs over G exactly 2^{m-n+1} will have all edges of T positive. Indeed, while fixing (n-1) edges of T positive, any selection of the remaining (m-n+1) non-tree edges determines Σ . Such a selection can be done in 2^{m-n+1} ways.

Hence, Step (a) gives the total number of signed graphs while Step (b) gives the number of signed graphs having all edges of T positive. Using Lemma 4, we deduce that there are 2^{m-n+1} switching equivalence classes.

Step (c). There are 2^{n-1} switchings available. Namely, any switching is determined by a pair $(U, V \setminus U)$, but $(U, V \setminus U)$ is the same switching as $(V \setminus U, U)$. Hence we have to divide 2^n , the number of subsets of V, by 2. Thus, each switching equivalence class contains 2^{n-1} signed graphs.

Note that a part of Proposition 5, and the idea to use spanning trees to obtain switching classes (used in Algorithm 1) can also be found in [38].

Proposition 5 is cast in terms of labelled graphs. If we consider unlabelled graphs, the number of classes may be reduced by symmetry. For example, consider a graph G consisting of two copies of a cycle and a path between them, then there are four switching classes on G, but only three non-switching-isomorphic signed graphs: one with both cycles sign-balanced, one with both cycles sign-unbalanced, and a third with one cycle sign-balanced and the other sign-unbalanced. The third possibility corresponds to two distinct switching classes of labelled graphs: it does not matter which cycle is taken to be sign-balanced, up to isomorphism.

2.4. Singular, Core and Nut Signed Graphs

One may consider the kernel of the adjacency matrix of a *signed* graph. The local condition (2) generalises to

(9)
$$\sum_{u \sim v} x_u \sigma(uv) = 0$$

for each choice of a pivot vertex v, where $\sigma(uv)$ is the weight (± 1) of the edge between u and v, $\mathbf{x}(u)$ has been written as x_u for brevity and $u \sim v$ denotes $u \in N_G(v)$. These conventions for vectors and edges will be used in the rest of the paper. Note that definitions (3) and (4) can be extended to a signed graph in a natural way. A signed graph is a singular signed graph if it has a zero as an eigenvalue. A signed graph is a core signed graph if supp ker $A(\Gamma) = V(G)$. A signed graph is a signed nut graph¹ if its adjacency matrix $A(\Gamma)$ has nullity one and ker $A(\Gamma)$ contains a full kernel eigenvector. It follows that a signed nut graph is a core signed graph of nullity one.

A graph G on n vertices and m edges gives rise to 2^m distinct signed graphs. If we are interested in non-isomorphic signed graphs only, this number may be reduced by the symmetries that preserve signs. However, there is also an equivalence relation, to be described in the next section, among the signed graphs $\Gamma = (G, \sigma)$ over a given underlying graph that is very convenient, as it preserves several important signed invariants and reduces the number of graphs to be considered.

2.5. Switching equivalence and singular signed graphs

Proposition 3 has the following immediate consequence.

Proposition 6. Let Γ be a signed graph and let $U \subseteq V(G)$. If Γ is singular and if \mathbf{x} is any of its kernel vectors, then Γ^U is singular and the vector \mathbf{x}^U defined as

(10)
$$\mathbf{x}^{U}(v) = \begin{cases} \mathbf{x}(v), & \text{if } v \in V(G) \setminus U, \\ -\mathbf{x}(v), & \text{if } v \in U, \end{cases}$$

is a kernel eigenvector for Γ^U .

This proposition is helpful in the study of singular graphs. Namely, it follows that many properties of signed graphs concerning singularity hold for the whole switching equivalence class.

Corollary 7. Let Γ and Γ' be two switching-equivalent signed graphs. The following holds.

- (1) If one of the pair is singular, then the other is also singular. In addition, Γ and Γ' have the same nullity.
- (2) If one of the pair is a core graph, then the other is also a core graph.
- (3) If one of the pair is a nut graph, then the other is also a nut graph.

In particular, this reduces the search for nut graphs to a search over distinct switching equivalence classes. Note that Corollary 7 holds also in the case

¹In this case we are conscious that the logical word order would be 'nut signed graph', as we have started with signed graphs and looked for those that have the extra property of being a nut graph, but using 'nut' as an adjective strikes the ear very oddly, so for euphony we retain the term 'signed nut graph'.

when Γ and Γ' are switching isomorphic (i.e., signed graphs such that up to vertex labelling, each of them belongs to the switching class of the other). This observation could reduce the search even more. The following fact is also useful.

Corollary 8. Every switching equivalence class of signed nut graphs has exactly one representative that has kernel eigenvector with all entries positive.

Proof. Let Γ be a signed nut graph and **x** be its kernel eigenvector. Let

(11)
$$U = \{ v \in V \mid \mathbf{x}(v) < 0 \}.$$

The switching at U gives rise to the switching-equivalent signed graph Γ^U with an all-positive kernel eigenvector, i.e., a nut graph.

The above corollary enables us to select for any signed nut graph $\Gamma = (G, \Sigma)$ a unique switching-equivalent graph $\Gamma' = (G, \Sigma')$ such that the kernel eigenvector \mathbf{x}' relative to Γ' is given by $\mathbf{x}'(v) = |\mathbf{x}(v)|$. This canonical choice of switching can be viewed in the more general setting of signed graphs.

Using the idea of the proof of Proposition 5 and a database of regular connected graphs of a given order [29], we may search for signed nut graphs of that order. Let $F(n, \rho)$ be the number of regular connected graphs of order n and degree ρ . In the worst case, Algorithm 1 has to check 2^{m-n+1} sign structures on each graph. Since $2m = n\rho$ this implies a maximum of $F(n, \rho)2^{m-n+1}$ tests.

Algorithm 1 Given the class of graphs $\mathcal{G}_{n,\rho}$, i.e., the class of connected ρ -regular graphs of order n, find a signed nut graph in this class.

Input: $\mathcal{G}_{n,\rho}$, the class of all connected ρ -regular graphs of order n.

Output: A signed nut graph in $\mathcal{G}_{n,\rho}$ (or report that there is none).

```
1: for all G \in \mathcal{G}_{n,\rho} do
```

- 2: $T \leftarrow \text{spanning tree of } G$
- 3: for all $\Sigma \subseteq E(G) \setminus T$ do
- 4: $\Gamma \leftarrow (G, \Sigma)$
- 5: **if** Γ is a signed nut graph **then**
- 6: return Γ
- 7: end if
- 8: end for
- 9: **end for**

10: **report** there is no signed nut graph in class $\mathcal{G}_{n,\rho}$

3. EXISTENCE OF REGULAR SIGNED GRAPHS THAT ARE NUT GRAPHS

In what follows we will use the fact that there are no regular graphs of odd degree and odd order. This is an obvious consequence of the Handshaking Lemma. In this section, we provide sufficient conditions for the existence of regular signed nut graphs of order n and degree $\rho = n - 1$ or $\rho = n - 2$. For $\rho \leq 11$, we also establish the orders for which there exist nut graphs that are sign-unbalanced but none that are sign-balanced. Our contribution was prompted by recent interest in the study of families of nut graphs. An efficient strategy for generating nut graphs of small order was published in 2018 [10, 11] and the collection of nut graphs found there for orders up to 20 was reported in the House of Graphs [7]. For arbitrary simple graphs, the list is complete for orders up to 12, and counts are given for degrees up to 13. A list of regular nut graphs for orders from 3 to 8 was deposited in the same place. This list covers orders up to 22 and is complete up to order 14. More recently, the orders for which regular nut graphs of degree ρ exist have been established for $\rho \in \{3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$ [4, 18]. In [21] the set $N(\rho)$ was defined as the set consisting of all integers n for which a ρ -regular nut graph of order n exists. There it was shown that

(12)

$$N(1) = N(2) = \emptyset,$$

$$N(3) = \{12\} \cup \{2k \mid k \ge 9\},$$

$$N(4) = \{8, 10, 12\} \cup \{k \mid k \ge 14\}.$$

In [18], $N(\rho)$ was determined for every ρ , $5 \le \rho \le 11$. In [4], these results were extended to $\rho = 12$. Combining these results, we obtain the following.

Theorem 9 [18, Theorems 2, 3 and 7], [4, Theorem 1.3]. The following holds.

1. $N(1) = \emptyset$, 2. $N(2) = \emptyset$, 3. $N(3) = \{12\} \cup \{2k \mid k \ge 9\}$, 4. $N(4) = \{8, 10, 12\} \cup \{k \mid k \ge 14\}$, 5. $N(5) = \{2k \mid k \ge 5\}$, 6. $N(6) = \{k \mid k \ge 12\}$, 7. $N(7) = \{2k \mid k \ge 6\}$, 8. $N(8) = \{12\} \cup \{k \mid k \ge 14\}$, 9. $N(9) = \{2k \mid k \ge 8\}$, 10. $N(10) = \{k \mid k \ge 15\}$, 11. $N(11) = \{2k \mid k \ge 16\}$.

SIGNED NUT GRAPHS

Note that, for each ρ in the range $3 \leq \rho \leq 12$, the set N(d) misses only a finite number of integer values. The question we tackle here is: which of the missing numbers can be covered by extending the search for regular nut graphs to include regular signed graphs? Here, we take the search as far as $\rho = 11$. The main result of this paper is summarised in Table 1 which embodies the results from Theorem 9 above and the two new Theorems 10 and 18 below.

$n \\ \rho$	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	
3		∄		∄		∄		√*		*		*		√*		\Rightarrow
4	*	∄	*	√*	*	√*	*	√*	*	√*	√*	√*	√*	√*	√*	\Rightarrow
5		∄		∄		√*		√*		√*		√*		√*		\Rightarrow
6			∄	*	*	*	*	√*	√*	√*	√*	√*	√*	√*	√*	\Rightarrow
7				∄		*		√*		√*		√*		√*		\Rightarrow
8					*	*	*	√*	*	√*	√*	√*	√*	√*	√*	\Rightarrow
9						∄		*		*		√*		√*		\Rightarrow
10							∄	*	*	*	√*	√*	√*	√*	√*	\Rightarrow
11								∄		*		√*		√*		\Rightarrow

Table 1. Existence of regular nut graphs of order n and degree ρ . Notation: \checkmark ... there exists a sign-balanced nut graph; \nexists ... there exists a sign-unbalanced nut graph; \nexists ... there exists no nut graph, signed or unsigned. Shaded squares denote parameters for which no simple graph exists, as in these cases either ρ and n would both be odd, or ρ would exceed n-1. Arrows \Rightarrow indicate that the table continues to infinity to the right: regular nut graphs, both sign-balanced and sign-unbalanced, with the given degree ρ exist for all higher values of n (even ρ), or all higher even values of n (odd ρ). Examples for all cases marked with \bigstar are given in [3]. Some small examples are illustrated in Figure 1.

Theorem 10. Let $N_s(\rho)$ denote the set of orders n for which there exists no ρ -regular sign-balanced nut graph but there exists a ρ -regular sign-unbalanced nut graph.

- 1. $N_s(1) = \emptyset$,
- 2. $N_s(2) = \emptyset$,
- 3. $N_s(3) = \{14, 16\},\$
- 4. $N_s(4) = \{5, 7, 9, 11, 13\},\$
- 5. $N_s(5) = \emptyset$,
- 6. $N_s(6) = \{8, 9, 10, 11\},\$
- 7. $N_s(7) = \{10\},\$

- 8. $N_s(8) = \{9, 10, 11, 13\},\$
- 9. $N_s(9) = \{12, 14\},\$
- 10. $N_s(10) = \{12, 13, 14\},\$
- 11. $N_s(11) = \{14\}.$

Proof. Case $N_s(1) = \emptyset$ is trivial. The only possible graph is switching-equivalent to K_2 which is not a nut graph. Case $N_s(2) = \emptyset$ is also straightforward. The only possible graphs are switching equivalent to the cycle C_n or the Möbius cycle M_n (a cycle where exactly one edge carries weight -1). It is well known that $\{\eta(C_n), \eta(M_n)\} = \{0, 2\}$ (see, e.g. [17]) and hence neither is a nut graph.

From Theorem 9 we have only a finite number of further cases to check (all those pairs (n, ρ) that do not correspond to \checkmark in Table 1) in order to establish the theorem. For some sets of parameters (n, ρ) , we were immediately able to prove existence/non-existence by search using the straightforward Algorithm 1. For some parameter combinations, exhaustive search was unfeasible, but in these cases an example was generated by various computer-aided heuristic approaches. For some cases this involved planting a small number of negative edges in a general graph. For others, a negative Hamiltonian cycle or perfect matching was added to an unsigned nut graph.

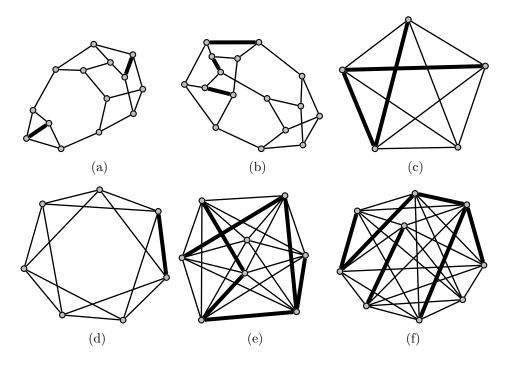


Figure 1. Some small examples of regular signed nut graphs. (a) cubic, n = 14; (b)

cubic, n = 16; (c) quartic, n = 5; (d) quartic, n = 7; (e) sextic, n = 8; (f) sextic, n = 9. Thick lines denote edges with negative weight.

All signed graphs mentioned in the proof can be found in [3].

4. A Construction for Signed Nut Graphs

Theorem 10 has answered our initial question, in that if we consider ordinary graphs as special cases of signed graphs, we need only to perform a computer search for existence of signed nut graphs for all values of n for which no ordinary nut graph exists. However, if we want to search for sign-unbalanced nut graphs with the intention of determining those orders for which a sign-unbalanced nut graph exists, then methods are needed for generating larger signed nut graphs. There are several known constructions that take a nut graph and produce a larger nut graph [33, 37]. We will revisit one such here and extend it to signed graphs. This is the so-called *Fowler Construction* for enlarging unweighted nut graphs.

Let G be a graph and v a vertex of degree ρ . Let $N(v) = \{u_1, u_2, \dots, u_{\rho}\}$. Recall [18,21] that the Fowler construction, denoted F(G, v), is a graph with

(13)
$$V(F(G, v)) = V(G) \sqcup \{q_1, \dots, q_\rho\} \sqcup \{p_1, \dots, p_\rho\}$$

and

$$E(F(G, v)) = (E(G) \setminus \{vu_i \mid 1 \le i \le \rho\}) \cup \{q_i p_j \mid 1 \le i, j \le \rho, i \ne j\}$$

(14)
$$\cup \{vq_i \mid 1 \le i \le \rho\} \cup \{p_i u_i \mid 1 \le i \le \rho\}.$$

Here, we generalise this construction to signed graphs.

Definition. Let $\Gamma = (G, \sigma)$ be a signed graph and v a vertex of G that has degree ρ . Then $F(\Gamma, v) = (F(G, v), \sigma')$, where for $1 \leq i, j \leq \rho$,

(15)
$$\sigma'(e) = \begin{cases} 1 & \text{if } e = vq_i, \\ 1 & \text{if } e = q_ip_j, \\ \sigma(vu_i) & \text{if } e = p_iu_i, \\ \sigma(e) & \text{otherwise,} \end{cases}$$

is the Fowler construction for signed graphs.

Lemma 11. Let $\Gamma = (G, \sigma)$ be a signed graph and v a vertex of G that has degree ρ and let \mathbf{x} be a kernel eigenvector for Γ . Then \mathbf{x}' , defined as

(16)
$$\mathbf{x}'(w) = \begin{cases} -(\rho - 1)\mathbf{x}(v) & \text{if } w = v, \\ \sigma(vu_i)\mathbf{x}(u_i) & \text{if } w = q_i, \\ \mathbf{x}(v) & \text{if } w = p_i, \\ \mathbf{x}(w) & \text{otherwise}. \end{cases}$$

for $w \in V(F(\Gamma, v))$, is a kernel eigenvector for $F(\Gamma, v)$.

The local structures in the signed graphs Γ and $F(\Gamma, v)$ are shown in Figure 2, which also indicates the relationships between kernel eigenvectors in these graphs.

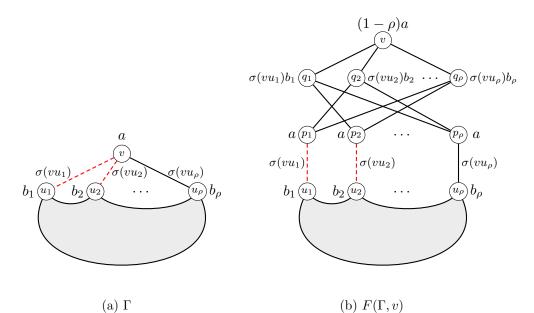


Figure 2. A construction for expansion of a signed nut graph Γ about vertex v of degree ρ , to give $F(\Gamma, v)$. The labelling of vertices in Γ and $F(\Gamma, v)$ is shown within the circles that represent vertices. Shown beside each vertex is the corresponding entry of the (unique) kernel eigenvector with integer entries for the respective graph. Panel (a) shows the neighbourhood of vertex v in Γ . Edges from vertex v to its neighbours have weights $\sigma(vu_i)$ which are either +1 or -1. In the figure, edges with weight -1 are dashed, as an illustration. Edges of the remainder of the graph, indicated by the shaded bubble, may take arbitrary signs. Panel (b) shows additional vertices and edges in $F(\Gamma, v)$. Vertices q_i inherit their entries from Γ as described in Equation (16). Edges p_iu_i inherit their weights (signs) from Γ . All other new edges in Panel (b) have weights +1.

Lemma 12. Let Γ be a singular signed graph, and let \mathbf{x} be a kernel eigenvector. Let $u, v \in V$ be any two non-adjacent vertices, having the same degree, say ρ , and sharing $\rho - 1$ neighbours. Let u' denote the neighbour of u that is not a neighbour of v, and let v' denote the neighbour of v that is not a neighbour of u. If $\sigma(uw) = \sigma(wv)$ for all $w \in N(u) \setminus \{u'\}$, then $|\mathbf{x}(u')| = |\mathbf{x}(v')|$. Moreover, $\mathbf{x}(u') = \mathbf{x}(v')$ if and only if $\sigma(vv') = \sigma(uu')$.

Proof. Let $N(u) \setminus \{u'\} = N(v) \setminus \{v'\} = \{w_2, \ldots, w_{\rho}\}$ (see Figure 3). The respective local conditions at vertices u and v are

(17)
$$\sigma(uu')\mathbf{x}(u') + \sum_{i=2}^{\rho} \sigma(uw_i)\mathbf{x}(w_i) = 0,$$

(18)
$$\sigma(vv')\mathbf{x}(v') + \sum_{i=2}^{\rho} \sigma(w_i v)\mathbf{x}(w_i) = 0.$$

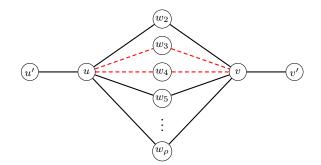


Figure 3. The neighbourhood of vertices u and v in Lemma 12. The dashed edges indicate a possible selection of edges with weight -1.

Since $\sigma(uw_i) = \sigma(w_iv)$ for all $2 \le i \le \rho$, we get that

(19)
$$\sigma(uu')\mathbf{x}(u') = \sigma(vv')\mathbf{x}(v'),$$

by taking the difference of Equations (17) and (18). Clearly,

(20)
$$|\mathbf{x}(u')| = |\sigma(uu')\mathbf{x}(u')| = |\sigma(vv')\mathbf{x}(v')| = |\mathbf{x}(v')|.$$

If $\sigma(uu') = \sigma(vv')$, then Equation (19) implies $\mathbf{x}(u') = \mathbf{x}(v')$. Similarly, if $\mathbf{x}(u') = \mathbf{x}(v')$, then Equation (19) implies $\sigma(uu') = \sigma(vv')$.

Lemma 13. Let Γ and Γ' be signed graphs over the same underlying graph G, i.e., $\Gamma = (G, \sigma)$ and $\Gamma' = (G, \sigma')$. Let v be a vertex of G. Then Γ is switching equivalent to Γ' if and only if $F(\Gamma, v)$ is switching equivalent to $F(\Gamma', v)$.

Proof. Let Γ and Γ' be two signed graphs over graph G, say $\Gamma = (G, \Sigma)$ and $\Gamma' = (G, \Sigma')$. Let $v \in V(G)$ and let $F(\Gamma, v)$ and $F(\Gamma', v)$ be the corresponding Fowler constructions. Let Γ and Γ' be switching equivalent. This means that there exists $S \subset V(G)$, such that $\Gamma' = \Gamma^S$. We know that $\Gamma^S = \Gamma^{V(G) \setminus S}$. Without loss of generality we may assume that $v \notin S$. Let the vertex labelling of $F(\Gamma, v)$, $F(\Gamma', v)$ and F(G, v) be the same as in Figure 2. In particular, this means that all vertices of G belong also to F(G, v). Since $v \notin S$, we have

(21)
$$F(\Gamma', v) = F(\Gamma^S, v) = F(\Gamma, v)^S$$

Hence it follows

(22)
$$\Gamma \sim \Gamma' \Rightarrow F(\Gamma, v) \sim F(\Gamma', v).$$

To prove the converse, assume the following: $F(\Gamma, v) \sim F(\Gamma', v)$, where $\Gamma = (G, \Sigma)$ and $\Gamma' = (G, \Sigma')$. Let $S \subset V(F(G, v))$ such that $v \notin S$. Since all edges above u_1, u_2, \ldots, u_s in Figure 2(b) are positive in both signed graphs, it is clear that $S \subset V(G)$ and the result follows.

Theorem 14. Let Γ be a signed graph and v any one of its vertices. Then the nullities of Γ and $F(\Gamma, v)$ are equal, i.e., $\eta(\Gamma) = \eta(F(\Gamma, v))$. Moreover, ker Γ admits a full eigenvector if and only if ker $F(\Gamma, v)$ admits a full eigenvector.

Proof. Let u_1, \ldots, u_ρ be the neighbours of vertex v in G. Assume first that G is a core graph and that \mathbf{x} is an admissible eigenvector. Let $\mathbf{x}(w)$ denote the entry of \mathbf{x} at vertex w. Let $a = \mathbf{x}(v)$ and let $b_i = \mathbf{x}(u_i)$. We now produce a vertex labelling \mathbf{x}' of $F(\Gamma, v)$ as above. It follows that if \mathbf{x} is a valid assignment of G, then \mathbf{x}' is a valid assignment on $F(\Gamma, v)$. Thus $\eta(F(\Gamma, v)) \ge \eta(\Gamma)$.

On the other hand, apply Lemma 12 to $F(\Gamma, v)$ and an admissible assignment \mathbf{x}' . First consider vertices q_i and q_j and their neighbourhoods. Lemma 12 implies that $\mathbf{x}'(p_i) = \mathbf{x}'(p_j)$. Hence \mathbf{x}' is constant on p_i , say $\mathbf{x}'(p_i) = a$. Thus, it follows that $\mathbf{x}'(v) = -(\rho - 1)a$. The second application of the lemma goes to vertices v and p_i . It implies that for each i the values $\mathbf{x}'(q_i)$ and $\mathbf{x}'(u_i)$ are equal, namely $\mathbf{x}'(q_i) = \mathbf{x}'(u_i)$. Finally, let $\mathbf{x}(w) = \mathbf{x}'(w)$ for every $w \in V(G) \setminus \{v\}$ and let $\mathbf{x}(v) = a$. Hence, the existence of an admissible \mathbf{x}' on $F(\Gamma, v)$ implies the existence of an admissible \mathbf{x} on Γ . Thus $\eta(F(\Gamma, v)) \leq \eta(\Gamma)$.

Corollary 15. Let $\Gamma = (G, \sigma)$ be a signed graph and $v \in V(G)$ any one of its vertices. The following statements hold.

- (1) $F(\Gamma, v)$ is a signed nut graph if and only if Γ is a signed nut graph.
- (2) $F(\Gamma, v)$ is a sign-balanced nut graph if and only if Γ is a sign-balanced nut graph.

Proof. Follows directly from Lemma 13 and Theorem 14. Namely, if Γ is signbalanced, then it is switching equivalent to the all-positive signed nut graph $\Gamma' = (G, \emptyset)$. However, in this case $F(\Gamma', v) = F((G, \emptyset), v) = (F(G, v), \emptyset)$. Virtually the same argument can be used in the opposite direction.

The question answered by Table 1 and the associated theorems was about finding graph orders where *only* sign-unbalanced nut graphs would exist. The above construction allows us to say something about the cases where both signbalanced and sign-unbalanced nut graphs exist. A useful observation is the following. **Observation 16.** Whenever there is a parameter pair (n, ρ) marked with a * inTable 1, there is an infinite series of values $n, n + 2\rho, n + 4\rho, n + 6\rho, \ldots$ at which a ρ -regular sign-unbalanced nut graph exists.

Theorem 17. Let $U(\rho)$ be the set consisting of all integers n for which a ρ -regular sign-unbalanced nut graph of order n exists. The following holds.

1. $U(1) = \emptyset$, 2. $U(2) = \emptyset$, 3. $U(3) = \{2k \mid k \ge 6\}$, 4. $U(4) = \{5\} \cup \{k \mid k \ge 7\}$, 5. $U(5) = \{2k \mid k \ge 5\}$, 6. $U(6) = \{k \mid k \ge 8\}$, 7. $U(7) = \{2k \mid k \ge 5\}$, 8. $U(8) = \{k \mid k \ge 9\}$, 9. $U(9) = \{2k \mid k \ge 6\}$, 10. $U(10) = \{k \mid k \ge 12\}$, 11. $U(11) = \{2k \mid k \ge 7\}$.

Proof. Cases $U(1) = \emptyset$ and $U(2) = \emptyset$ follow from the proof of Theorem 10. For the remaining cases Table 1 suggests a conjecture for each row, which is proved by identifying at least one sign-unbalanced nut graph for key small values of n, and applying the construction.

Case U(3). A check for n = 12 yielded an example of a sign-unbalanced nut graph. Hence by use of Theorem 10 and Observation 16, sign-unbalanced nut graphs exist for all even $n \ge 12$.

Case U(4). Checking that a sign-unbalanced nut graph exists for orders 8, 10, 12 and 14 gives a run of cases from which the result follows by use of the construction.

Case U(5). From Table 1, 5-regular sign-balanced nut graphs exist for all even $n \ge 10$. Checking the cases $n = 10, 12, \ldots, 18$ shows that 5-regular sign-unbalanced nut graphs also exist, and the result follows by use of the construction.

Case U(6). Checking cases $n = 12, 13, \ldots, 19$ is sufficient.

Case U(7). Checking cases $n = 12, 14, \ldots, 22$ is sufficient.

Case U(8). Checking cases n = 12 and $n = 14, 15, \ldots, 24$ is sufficient.

Case U(9). Checking cases $n = 16, 18, \ldots, 28$ is sufficient.

Case U(10). Checking cases $n = 15, 16, \ldots, 31$ is sufficient.

Case U(11). Checking cases $n = 16, 18, \ldots, 34$ is sufficient.

Note that $N_s(\rho) = U(\rho) \setminus N(\rho)$. Clearly, $N(\rho) \subseteq U(\rho)$ for all $1 \le \rho \le 11$.

5. Signed Nut Graphs with $\rho = n - 1$ and $\rho = n - 2$

Further theorems extend the results of Theorem 10 to infinity along the leading diagonals of the table.

Theorem 18. Let Γ be a signed graph whose underlying graph is K_n . If Γ is a signed nut graph, then $n \equiv 1 \pmod{4}$. Moreover, for each $n \equiv 1 \pmod{4}$, there exists a signed nut graph with underlying graph K_n .

Proof. Graphs on the leading diagonal are regular of degree $\rho = n-1$ and hence all have underlying graph K_n . Note that there are no unsigned nut graphs on this diagonal, as K_n is non-singular.

Let n = 4k + q, where $0 \le q \le 3$. We divide the proof into three parts: (a) $q \in \{0, 2\}$, (b) q = 3, and (c) q = 1.

Assume that Γ is singular. Let **x** be a full kernel eigenvector (existence established by Proposition 1). We may assume that **x** is a non-zero integer vector. If **x** has no odd coordinate, we may multiply **x** by an appropriate power of $\frac{1}{2}$ so that at least one coordinate becomes odd. We call vertex *s* even if $x_s \equiv 0 \pmod{2}$ and odd if $x_s \equiv 1 \pmod{2}$. The local condition (9) at *r* implies that there is an even number of odd vertices around *r* and hence, together with *r*, an odd number of odd vertices in total for a presumed K_n nut graph.

Case (a). $q \in \{0,2\}$. This means that n is even. The signed graph Γ must have an even vertex t. The local condition at t implies that there is an even number of odd vertices around t, and hence an even number of odd vertices in total, a contradiction. This rules out the existence of signed nut graphs whose underlying graph is the complete graph for $q \in \{0,2\}$.

Case (b). $q \in 3$. In this case all entries x_s are odd: the parity of the sum in (9) is opposite for even and odd vertices.

Let m_+ denote the number of edges in Γ with positive sign. For each vertex s, let $\rho_+(s)$ and $\rho_-(s)$, respectively, denote the number of edges with positive sign and negative sign that are incident with s. Note that $\rho_+(s) + \rho_-(s) = n - 1$. Summing local conditions over pivots r, we have

(23)
$$0 = \sum_{r} \rho_{+}(r) x_{r} - \sum_{r} \rho_{-}(r) x_{r}.$$

Hence,

(24)
$$0 = \sum_{r} \{\rho_{+}(r) - \rho_{-}(r)\} x_{r} = \sum_{r} \{2\rho_{+}(r) - n + 1\} x_{r},$$

1368

and

(25)
$$\sum_{r} \rho_{+}(r) x_{r} = \frac{n-1}{2} \sum_{r} x_{r} = \{2k+1\} \sum_{r} x_{r}.$$

The RHS of (25) is an odd number as it is a product of two odd numbers, hence $\sum_r \rho_+(r)x_r$ is odd. Therefore, the subgraph with only positive edges has an odd number of vertices with odd degree. By the Handshaking Lemma this is impossible.

Case (c). q = 1 is the only remaining possibility and the first part of the theorem follows, provided such nut graphs exist. Now we construct a signed nut graph for each n of the form n = 4k + 1. A signed graph Γ is constructed from K_{4k+1} as follows. Partition the vertex set of K_{4k+1} into a single vertex r = 0 and k subsets of 4 vertices for k copies of the path P_4 . Change the signs of all edges internal to each P_4 to -1. To construct a kernel eigenvector \mathbf{x} of Γ for $\lambda = 0$ place +1 on vertex 0, then entries -1, +1, +1, -1 on each P_4 . We denote by 1, 2, 3, 4 the vertices of the first P_4 , by 5, 6, 7, 8 the vertices of the second P_4 , etc. Owing to the symmetry of Γ (since automorphisms of Γ preserve edge-weights) there are only three vertex types to be considered.

1. For r = 0 all weights $\sigma(rs) = 1$ and exactly half of the x_s are equal to 1 and the other half are equal to -1. Hence, (9) is true in this case.

2. The vertex r may be an end-vertex of any of the k paths P_4 . The net contribution of the three remaining vertices of P_4 is -1, and all contributions of other paths cancel out. Taking into account the edge to vertex 0, the weighted sum in (9) is equal to 0.

3. The vertex r may be an inner vertex of any of the k paths P_4 . Again, the net contribution of the three remaining vertices of P_4 is -1, and by the same argument, the weighted sum in (9) is equal to 0.

As **x** is a full kernel eigenvector, Γ is a *core* signed graph.

It remains to prove that Γ is a signed nut graph, i.e., with nullity $\eta(\Gamma) = 1$. This is done by showing that the constructed full kernel eigenvector \mathbf{x} is the only eigenvector for $\lambda = 0$ (up to a scalar multiple). First, note that all edges incident with vertex 0 have weight +1. Hence for r = 0, (9) becomes

(26)
$$\sum_{s\neq 0} x_s = 0.$$

It follows that

(27)
$$\sum_{s=0}^{n} x_s = x_0.$$

Now consider any path P_4 with vertices, say, 1, 2, 3, 4. Note that vertices 1 and 4 fall into one symmetry class while vertices 2 and 3 are in the other. The local conditions are the following.

(28)
$$0 = x_0 - x_2 + \sum_{s \neq 0, 1, 2} x_s = x_0 - x_1 - 2x_2,$$

(29)
$$0 = x_0 - x_1 - x_3 + \sum_{s \neq 0, 1, 2, 3} x_s = x_0 - 2x_1 - x_2 - 2x_3,$$

(30)
$$0 = x_0 - x_2 - x_4 + \sum_{s \neq 0, 2, 3, 4} x_s = x_0 - 2x_2 - x_3 - 2x_4,$$

(31)
$$0 = x_0 - x_3 + \sum_{s \neq 0, 3, 4} x_s = x_0 - 2x_3 - x_4.$$

It is straightforward to show that x_1, \ldots, x_4 are related to x_0 as

$$(32) x_1 = x_4 = -x_0, x_2 = x_3 = x_0.$$

Since this holds for all k path graphs P_4 , it follows that Γ is a signed nut graph.

We can also prove a theorem that accounts for the next diagonal of Table 1. The graphs on this diagonal are ρ -regular $\rho \geq 3$ and $\rho = n - 2$, implying even order $n \geq 6$. They are therefore the cocktail-party graphs, CP(n) (also known as hyperoctahedral graphs [6, p. 17], as they are 1-skeletons of the cross-polytope duals of hypercubes). Exhaustive search shows that there is no nut graph for the case CP(6).

Lemma 19. Let $\Gamma = (G, \Sigma)$ be a signed graph whose underlying graph G is the cocktail-party graph of order 2p, $CP(2p) \cong \overline{p K_2}$, p > 1. Then Γ is not a sign-balanced nut graph.

Proof. The spectrum of CP(2p) is $\sigma(CP(2p)) = \{2p - 2, 0^{(p)}, -2^{(p-1)}\}$ [6, p. 17] and so $\eta(CP(2p)) = p > 1$. Therefore, G is not a nut graph, and Γ is not switching-equivalent to a sign-balanced nut graph.

Theorem 20. Let $\Gamma = (G, \Sigma)$ be a signed graph whose underlying graph G is the cocktail-party graph of order 2p, $\operatorname{CP}(2p) \cong \overline{p K_2}$. For each even $p, p \ge 4$, there exists at least one sign-unbalanced nut graph Γ .

Proof. Construct $\Gamma(G, \Sigma)$ with G = CP(2p) and Σ defined as follows. Let K_{2p} be the complete graph with $V(K_{2p}) = \{0, 1, \ldots, 2p - 1\}$. Take the Hamiltonian cycle $[0, 1, 2, \ldots, 2p - 1, 0]$ and assign weights 0 and -1 to alternate edges. All edges not in the cycle have weight 1. To obtain the signed graph Γ , remove from K_{2p} all edges that were given weight 0. Note that $\Sigma = \{(1, 2), (3, 4), \ldots, (2p - 3, N)\}$

(2p-2), (2p-1, 0) and that every vertex has a unique antipodal partner in Γ ; the partner pairs are the non-edges $\{(0, 1), (2, 3), \dots, (2p-2, 2p-1)\}$.

With this assignment of Σ , the local condition for an eigenvector **x** corresponding to an eigenvalue λ of Γ is

(33)
$$\lambda x_u = \left(\sum_{v \notin \{u, \overline{u}, u'\}} x_v\right) - x_{u'}$$

for all $u \in V(G)$, where \overline{u} is the antipodal partner of u, and u' is the (unique) vertex connected to u by a negative edge. Condition (33) can be rewritten as

(34)
$$\lambda x_u = \left(\sum_{v \in V(G)} x_v\right) - x_u - x_{\overline{u}} - 2x_{u'},$$

and summing over all $u \in V(G)$ gives

(35)
$$(\lambda - 2p + 4) \sum_{u \in V(G)} x_u = 0$$

Hence, if $\lambda = 0$, the desired vector has $S = \sum_{v \in V(G)} x_v = 0$ and (34) reduces to

(36)
$$x_u + x_{\overline{u}} = -2x_{u'} = -2x_{\overline{u}'} = -(x_{u'} + x_{\overline{u}'}),$$

where the second equality follows by substituting u for \overline{u} in the first (with the labelling convention $\overline{u}' = (\overline{u})'$).

Note that the vector \mathbf{y} with entries specified by

(37)
$$y_u = \begin{cases} +1, & \text{if } u \equiv 0 \text{ or } 1 \pmod{4}, \\ -1, & \text{otherwise,} \end{cases}$$

is both full and a kernel eigenvector of Γ . Therefore, Γ is a core signed graph. We now show that the nullity $\eta(\Gamma)$ is not greater than 1.

Uniqueness of the kernel vector follows from a symmetry argument. The dihedral group \mathcal{D}_p is a subgroup of Aut |G| and Aut $|\Gamma|$. This fact is given a spatial realisation by identifying the vertices of Γ with those of a regular [p]gonal prism, so that edges in Σ correspond to consistently oriented diagonals on vertical quadrilateral faces, pairs of antipodal partners in Γ lie on vertical edges of the prism, and positively weighted edges of Γ are symmetrically distributed on faces and in the prism interior. The group \mathcal{D}_p with even p has two classes of two-fold rotational axis perpendicular to the principal (C_p) axis, passing through midpoints of vertical edges, and centres of vertical faces, respectively. These generate C'_2 and C''_2 rotations, respectively. Figure 4 illustrates the case of n = 2p = 12.

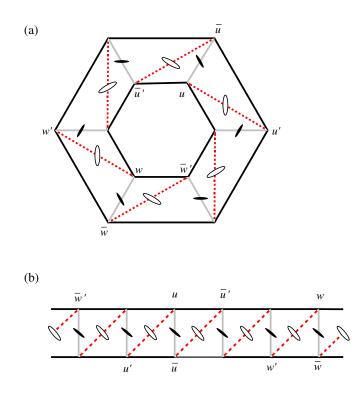


Figure 4. Construction of sign-unbalanced regular nut graphs with degree n - 2. The graphs $\Gamma(G, \Sigma)$ are based on cocktail-party graphs $G = \operatorname{CP}(2p)$ where 2p is divisible by 4. (a) Schlegel and (b) unfolded-net representations of the graph $\Gamma = (\operatorname{CP}(12), \Sigma)$ in a prism setting of the chiral point group \mathcal{D}_6 . Black- and white-filled symbols indicate points where two-fold rotational axes enter and leave the prism. Axis $C'_2(u)$ enters the prism midway between vertex u and its graph-antipodal partner \overline{w} . Axis $C''_2(u)$ enters the prism between vertex u and its graph-antipodal partner \overline{w} . Axis $C''_2(u)$ enters the prism between vertex u and its neighbour on a negative edge u', to emerge between vertices w and w'. Dashed lines denote the edges with weight -1, chosen as described in the proof of Theorem 20. Grey lines denote the 'missing edges' deleted from the complete graph K_{2p} . Solid black lines denote edges of weight +1, though not all are shown: the graph has an edge of weight +1 connecting each vertex w with all vertices other than \overline{w} , w' and w itself.

Consider the local rotation $C'_2(u)$. This exchanges u with \overline{u} and u' with \overline{u}' . As the operation is an involution partitioning the vertices into orbits of size 2, the eigenspace for any given eigenvalue λ of Γ can be partitioned such that each eigenvector is either symmetric or antisymmetric under the action of $C'_2(u)$. In particular, for kernel vector \mathbf{x} , we have

(38)
$$C_2'(u)\mathbf{x} = \chi(C_2'(u))\mathbf{x}$$

with character $\chi(C'_2(u)) = \pm 1$. From the local condition (36) we know that $x_{u'} = x_{\overline{u}'}$ for every kernel vector of Γ , and so $\chi(C'_2(u)) = +1$, and $x_u = x_{\overline{u}}$. Also from (36), we have $x_{u'} = x_{\overline{u}'} = -x_{u'} = -x_{\overline{u}'}$ for every kernel vector of Γ . As $C''_2(u)$ exchanges u and u', this relation implies $\chi(C''_2(u)) = -1$. Operations $C'_2(u)$ (respectively, $C''_2(u)$) for u form a class within the group \mathcal{D}_p , and hence have the same character $\chi(C'_2)$ (respectively, $\chi(C''_2)$).

We may propagate the vector \mathbf{x} starting from the entry $x_u = a$, using consecutive $C'_2(u)$ and $C''_2(u)$ operations, shifting the axis each time by a rotation of π/p about the principal axis. This process covers every vertex with an entry $|x_v| = a$ and returns consistently to u. The resulting vector \mathbf{x} is $a\mathbf{y}$, where \mathbf{y} is the kernel vector given by (37); it has equal entries on antipodal partners in G, but equal and opposite entries on pairs of vertices linked by a negative edge in Γ . The underlying graph G is not a nut graph.

Theorem 21. Let $\Gamma = (G, \Sigma)$ be a signed graph whose underlying graph G is the cocktail-party graph of order 2p, $CP(2p) \cong \overline{p K_2}$. For each odd p, $p \ge 5$, there exists at least one sign-unbalanced nut graph Γ .

Proof. Let p = 2q + 1. The proof separates into Case 1, where q is even, and Case 2, where q is odd. In both cases we construct Γ to have p + 1 edges in Σ . In both, a symmetry argument is used to split the cases further according to the character (± 1) of a candidate kernel vector under a two-fold rotation.

Case 1. n = 2p = 4q + 2, q is even. The candidate graph Γ_a for this case is illustrated in Figure 5(a). The signed graph retains only one axis of two-fold rotational symmetry, which exchanges vertex u with its antipodal partner \overline{u} ; every vertex w has a unique rotational partner \widetilde{w} , but only for u is $\overline{w} = \widetilde{w}$.

The graph Γ can be divided into two 'halves' H and H related by the $C_2(u)$ rotation (see Figure 5(a)). Fragment H contains a path of three negative edges (2 - 0 - u - t), a set of q - 2 isolated negative edges (with lower endpoints $3, 5, \ldots, s$), and exactly one vertex that is on no negative edge.

A full kernel vector of Γ_a is easily found. The vector \mathbf{z} is defined to have entries in $H z_0 = -z_1 = -z_2 = 1$, and $z_{2w+1} = -z_{2w+2} = (-1)^w$ for $1 \le w \le q-1$, and entries in \widetilde{H} given by $z_{\widetilde{v}} = -z_v$. The vector \mathbf{z} constructed in this way is full, with eigenvalue 0 and character -1 under the rotation $C_2(u)$.

To check whether other kernel vectors with this character exist, consider a putative kernel vector \mathbf{x} . All kernel vectors of Γ_a obey the local condition (pivoting on vertex w)

(39)
$$0 = \left(\sum_{v \in V(G)} x_v\right) - x_w - x_{\overline{w}} - 2\sum_{\sigma(vw) = -1} x_v.$$

Note that vertex 1 (and $\tilde{1} \equiv 2p - 2$) have no incident negative edges. As the kernel vector **x** has character -1 under $C_2(u)$, $x_{\tilde{w}} = -x_w$ for all w. The sum $S = \sum_{v \in V(G)} x_v$ vanishes by symmetry for vectors with $\chi(C_2(u)) = -1$.

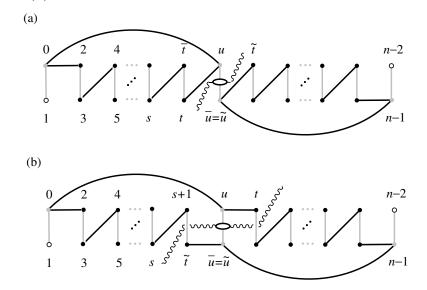


Figure 5. Construction of sign-unbalanced regular nut graphs with degree n-2 (continued). The graphs $\Gamma(G, \Sigma)$ are based on cocktail-party graphs $G = \operatorname{CP}(2p)$ where 2p is not divisible by 4. (a) Signed graph Γ_a for the case n = 2p = 4q + 2, with q even. (b) Signed graph Γ_b for the case n = 2p = 4q + 2, with q odd. In each case, the graph is shown in a shorthand ribbon format where each vertex lies directly above its antipodal partner. Solid black lines denote the edges with weight -1. Grey lines denote the 'missing edges' deleted from the complete graph K_{2p} . Vertices are colour coded by the number of incident edges of weight -1: white for 0, black for 1 and grey for 2. The elliptical symbol indicates the axis of the unique two-fold rotation $C_2(u)$ that swaps vertices $u \equiv (n/2) - 1$ and $\overline{u} \equiv (n/2)$. (The notation \overline{w} indicates the antipodal partner of vertex w, and \widetilde{w} its image under the rotation.) The wavy lines show the different splitting of Γ_a and Γ_b into fragments H (to the left) and \widetilde{H} (to the right). Constructions (a) and (b) differ in the position of t, the end vertex of the path of negative edges: t is at position u - 1 in Γ_a , but u + 2 in Γ_b .

Entries on vertices 0 and u = n/2 - 1 = 2q are assigned variables $b = x_0$ and $a = x_u = x_{\overline{u}}$. From the local condition it is apparent that all entries in **x** are linear combinations of a and b. Pivoting on $1, 0, 2, \ldots$ and on $u, t, \overline{t}, \ldots$ gives

(40)
$$\begin{aligned} x_0 &= b, & x_1 &= -b, & x_2 &= -a, \\ x_3 &= a - 2b, & x_4 &= b, & \dots \\ x_u &= a, & x_{\overline{u}} &= -a, & x_t &= x_{u-1} &= -b, \\ x_{\overline{t}} &= x_{u-2} &= b - 2a, & x_s &= x_{u-3} &= a, & \dots \end{aligned}$$

Now we propagate vector \mathbf{x} starting from the left side of H and determine the relationship between parameters a and b by requiring consistency when the neighbourhood of u is reached. (NB For the smallest case, n = 10, q = 2, (40) with $x_t \equiv x_3$ already gives a = b and $\mathbf{x} = a\mathbf{z}$.)

The fragment H contains (q-2) independent negative edges. Consecutive application of the local condition to each vertex of this ladder of negative K_2 units, $(3, 4), (5, 6), \ldots, (u-3, u-1)$ gives a recurrence relation for the entries in **x** on top and bottom rows of Figure 5(a), with solution for $q \ge 4$.

(41)
$$\begin{aligned} x_{2w+1} &= (-1)^{w+1}(wa - (w+1)b) & (1 \le w \le q-2), \\ x_{2w+4} &= x_{2w+1} & (1 \le w \le q-2). \end{aligned}$$

Consistency of (40) and (41) for $x_{\overline{t}} \equiv x_{2w+4} = x_{2w+1}$ with w = q - 3, requires a = b and therefore $\mathbf{x} = a\mathbf{z}$. Hence, Γ_a is a core with exactly one kernel vector that has $\chi(C_2(u)) = -1$.

It remains to check that Γ_a has no kernel vector with $\chi(C_2(u)) = +1$, i.e., with $x_u = x_{\tilde{u}} = x_{\overline{u}}$. We assign three variables $a = x_u$, $b = x_0$ and $c = x_1$. The extra parameter caters for the fact that the sum S is not now guaranteed to vanish by symmetry. Pivoting on vertex 1 shows that S = b + c. Proceeding as before, local conditions fix entries with lowest and highest labels in H.

(42)
$$\begin{array}{c} x_0 = b, & x_1 = c, & x_2 = -a, \\ x_3 = a - b + c, & x_4 = b, & \dots \\ x_u = a, & x_{\overline{u}} = a, & x_t = -a - \frac{1}{2}b + \frac{1}{2}c, \\ x_{\overline{t}} = -a + \frac{3}{2}b + \frac{1}{2}c, & x_s = x_{u-3} = a, & \dots \end{array}$$

Working along the ladder of vertices in sequence from 3, recurrence relations are found.

(43)
$$\begin{aligned} x_{4w+1} &= -2wa + (w+1)b - wc & (1 \le w \le q/2 - 1), \\ x_{4w+3} &= (2w+1)a - (w+1)b + (w+1)c & (1 \le w \le q/2 - 2), \\ x_{4w} &= x_{4w-3} = x_{4(w-1)+1} & (1 \le w \le q/2 - 1), \\ x_{4w+2} &= x_{4w-1} = x_{4(w-1)+3} & (0 \le w \le q/2 - 2). \end{aligned}$$

There are three consistency conditions to be applied to reduce the number of free parameters. Entries $x_{\bar{t}}$ and x_s must match general relation (42), and the sum of all entries must be consistent with S as obtained from the local condition at vertex 1. The first two conditions are

(C1)
$$q(2a - b + c) = 2a + 2c,$$

(C2)
$$q(2a - b + c) = 4a + b + 3c.$$

The third follows by summing the local condition for $\lambda = 0$ (39) over all vertices of Γ_b , to give

(44)
$$0 = (n-2)S - 2\sum_{v \in V(G)} \rho_{-}(v)x_{v},$$

where ρ_{-} is as introduced in the proof of Theorem 18; see (23). Noting that $x_w = x_{\tilde{w}}$ for character +1, S = b + c, and that apart from vertices 0, u and 1, all vertices w and their rotational partners have $\rho_{-}(w) = 1$, the result is

(C3)
$$(2q-3)(b+c) = 2a - 4c.$$

It is straightforward to show that conditions (C1) to (C3) admit only the trivial solution a = b = c = 0, as the determinant of the coefficients in the 3×3 set of linear equation vanishes only for q = 0, therefore **x** is the null vector and Γ_a is a sign-unbalanced nut graph.

Case 2. n = 2p = 4q + 2, q is odd. The candidate graph Γ_b for this case is illustrated in Figure 5(b). The signed graph retains the two-fold rotational symmetry exchanging vertex u = 2q with its antipodal partner \overline{u} , but now the path of three negative edges has endpoint t at position u+2, leading to a different partition into fragments H and \widetilde{H} . The argument follows the same lines as Case 1. A full kernel vector is readily constructed for Γ_b . Here, this is \mathbf{z}' , with entries in H defined by $z'_0 = -z'_1 = -z'_2 = z'_u = -z'_t = 1$, and $z'_{2w+1} = -z'_{2w+2} = (-1)^w$ for $1 \le w \le n/2 - 4$, and entries in \widetilde{H} found from $z'_v = -z'_{\widetilde{v}}$. By construction, this vector is antisymmetric under the reflection $C_2(u)$.

As in Case 1, we construct a general kernel vector \mathbf{x} with $\chi(C_2(u)) = -1$, working outwards from vertex 0.

(45)
$$\begin{aligned} x_0 &= b, & x_1 = -b, & x_2 = -a, \\ x_3 &= a - 2b, & x_4 = b, & \dots \\ x_u &= a, & x_{\overline{u}} = -a, & x_t = -b, \\ x_{\widetilde{t}} &= b, & x_{s+1} = 2a - b, & x_s = -a, & \dots \end{aligned}$$

Here s + 1 labels the final vertex of the ladder of (q - 2) disjoint negative edges, s + 1 = u - 2 = 2q - 2 (see Figure 5(b)).

The recurrence relation for vertices in H is

(46)
$$\begin{aligned} x_{2w} &= (-1)^{w+1}(wa - (w+1)b) & (1 \le w \le q-2), \\ x_{2w+2} &= x_{2w11} & (1 \le w \le q-2). \end{aligned}$$

Consistency with the expression for x_{s+1} requires a = b and $\mathbf{x} = a\mathbf{z}'$. Hence, Γ_b is a core and has exactly one kernel vector that has $\chi(C_2(u)) = -1$.

SIGNED NUT GRAPHS

It remains to check that Γ_b has no kernel vector with $\chi(C_2(u)) = +1$. Constructing a general kernel vector **x** with character +1, assigning parameters a, b, cas in Case 1 gives the same entries as in (42) and the same recurrence relations for the forward direction in H as in (43), if we note that the entry for \bar{t} for Γ_a now applies to s + 1. Consistency conditions (C1) and (C3) also apply here. Condition (C2) is replaced by (C2'), as the offset of vertex s + 1 from u is 2 rather than 4

(C2')
$$q(2a - b + c) = 8a - 4b + 2c'.$$

Again, it is straightforward to show that the three conditions admit only the trivial solution a = b = c = 0, and **x** is the null vector. Hence, Γ_b is a sign-unbalanced nut graph.

Taken together, Theorems 20 and 21 fully characterise the sub-diagonal $(\rho, n) = (n - 2, n)$ of Table 1. This diagonal is populated for all $n \ge 8$ with sign-unbalanced nut graphs. The following theorem summarises Theorems 18, 20 and 21.

Theorem 22. Let Γ be a signed nut graph on $n \ge 2$ vertices with the underlying ρ -regular graph G.

- (a) If $\rho = n 1$ (i.e., $G = K_n$), then $n \equiv 1 \pmod{4}$ and Γ is sign-unbalanced. Moreover, for each $n \equiv 1 \pmod{4}$ there exists such a signed nut graph.
- (b) If $\rho = n 2$ (i.e., $G = CP(2p) \cong \overline{p K_2}$ for some p), then n is even, $n \ge 8$, n = 2p and Γ is sign-unbalanced. Moreover, for each even $n \ge 8$ there exists such a signed nut graph.

6. CONCLUSION

Invocation of signed graphs as candidates for nut graphs allows extension of the orders at which a nut graph exists, and leads to a proof of all cases for regular nut graphs (either sign-balanced or sign-unbalanced) with degree at most 11. As with unweighted nut graphs, signed nut graphs can be generated by a generic construction in which the order of a smaller signed nut graph increases from n to $n + 2\rho$, where ρ is the degree of the vertex chosen as the focus of this vertex-expansion construction. This was used to establish Theorem 17, which specifies infinite series of orders n for which both sign-balanced and sign-unbalanced regular nut graphs exist. Two natural questions arise.

Question 23. Does there exist a degree ρ and order n such that there is at least one ρ -regular nut graph of order n that is sign-balanced, but no nut graph with the same parameters ρ and n that is sign-unbalanced?

Current data collected in Table 1 are compatible with the existence of three patterns for $U(\rho)$ based on divisibility by 4. These give the basis for the following question for ρ large enough.

Question 24. For all $\rho \geq 6$, prove or find a counterexample to

(47)
$$U(\rho) = \begin{cases} \{k \mid k \in \mathbb{Z}, k \ge \rho + 1\} & \text{if } \rho \equiv 0 \pmod{4}, \\ \{k \mid k \in \mathbb{Z}, k \ge \rho + 2\} & \text{if } \rho \equiv 2 \pmod{4}, \\ \{2k \mid k \in \mathbb{Z}, 2k \ge \rho + 3\} & \text{otherwise.} \end{cases}$$

Clearly, Equation (47) would not hold for $\rho < 6$ (see Theorem 18).

A connection with other work can be made via the concepts of two-graphs, equiangular lines and Seidel matrices [1, 2, 23, 24, 35]. The theory of two-graphs and Seidel matrices is equivalent to the theory of signed graphs with the underlying graph the complete graph K_n . The two-graphs are thus special cases of the signed graphs considered in Table 1 (those on the main diagonal, covered by Theorem 18). After completing our manuscript, it came to our attention that a result that covers one direction of Theorem 18 is given already in [23]. Recently, an independent proof covering the other direction of Theorem 18 was published in [1]; this work also gives results for the possible entries in the kernel eigenvector. Table 1 includes this interesting case of the first diagonal, but also gives a complete treatment of the next (where G is the cocktail-party graph), and characterises regular signed nut graphs of degrees 3 to 11 to all order.

In previous work [11,36] the question of which entries appear in the integer form of the kernel eigenvector has been considered. Haemers had raised this question for complete signed graphs in 2011 (see [5, Problem 3.26]) asking in effect whether all signed nut graphs with $G = K_n$ have kernel eigenvectors with entries ± 1 only. We have not specifically searched for (signed) nut graphs with constraints on the entries of the kernel eigenvector, but the data in [3] give some information on the values that can occur. It is interesting to note that the Fowler construction has a specific effect on the ratio of largest to smallest magnitudes that appear in the kernel eigenvector. Application of the construction to any vertex of degree greater than 2 increases the magnitude of its entry; iteration of the construction on the vertex carrying the largest entry can therefore be used to increase the ratio indefinitely.

SUPPLEMENTARY MATERIAL

The GitHub repository [3] currently contains examples of sign-unbalanced nut graphs that were used in the paper for verification of Table 1 and Theorems 10 and 17. Each entry gives an adjacency list, together with the pattern of

positive and negative weights and the kernel eigenvector as a list of integer entries. This data can also be found in the arXiv version of the present paper (https://arxiv.org/abs/2009.09018 [math.CO]).

Acknowledgements

We thank Thomas Zaslavsky and two anonymous referees for helpful comments on earlier drafts of this paper. The work of Tomaž Pisanski is supported in part by the Slovenian Research Agency (research program P1-0294 and research projects N1-0032, J1-9187, J1-1690, N1-0140 and J1-2481), and in part by H2020 Teaming InnoRenew CoE. The work of Nino Bašić is supported in part by the Slovenian Research Agency (research program P1-0294 and research projects J1-9187, J1-1691, N1-0140 and J1-2481). The work of Irene Sciriha and Patrick Fowler is supported by The University of Malta under the project Graph Spectra, Computer Network Design and Electrical Conductivity in Nano-Structures MATRP01-20.

References

- S. Akbari, S.M. Cioabă, S. Goudarzi, A. Niaparast and A. Tajdini, On a question of Haemers regarding vectors in the nullspace of Seidel matrices, Linear Algebra Appl. 615 (2021) 194–206. https://doi.org/10.1016/j.laa.2021.01.003
- I. Balla, F. Dräxler, P. Keevash and B. Sudakov, Equiangular lines and spherical codes in Euclidean space, Invent. Math. 211 (2018) 179-212. https://doi.org/10.1007/s00222-017-0746-0
- [3] N. Bašić, P.W. Fowler, T. Pisanski and I. Sciriha, Signed nut graphs (2021). https://github.com/UP-LaTeR/signed-nut-graphs
- [4] N. Bašić, M. Knor and R.Škrekovski, On 12-regular nut graphs, Art Discrete Appl. Math. (2021), in-press. https://doi.org/10.26493/2590-9770.1403.1b1
- [5] F. Belardo, S.M. Cioabă, J. Koolen and J. Wang, Open problems in the spectral theory of signed graphs, Art Discrete Appl. Math. 1 (2018) #P2.10. https://doi.org/10.26493/2590-9770.1286.d7b
- [6] N. Biggs, Algebraic Graph Theory, 2nd Edition (Cambridge University Press, Cambridge, 1993). https://doi.org/10.1017/CBO9780511608704
- G. Brinkmann, K. Coolsaet, J. Goedgebeur and H. Mélot, House of Graphs: A database of interesting graphs, Discrete Appl. Math. 161 (2013) 311–314. https://doi.org/10.1016/j.dam.2012.07.018
- [8] A.E. Brouwer and W.H. Haemers, Spectra of Graphs (Springer, New York, 2012). https://doi.org/10.1007/978-1-4614-1939-6

- F.R.K. Chung, Spectral Graph Theory (American Mathematical Society, Providence, RI, 1997). https://doi.org/10.1090/cbms/092
- [10] K. Coolsaet, P.W. Fowler and J. Goedgebeur, Nut graphs (2018). http://caagt.ugent.be/nutgen/
- [11] K. Coolsaet, P.W. Fowler and J. Goedgebeur, Generation and properties of nut graphs, MATCH Commun. Math. Comput. Chem. 80 (2018) 423–444.
- [12] D.M. Cvetković, M. Doob and H. Sachs, Spectra of Graphs: Theory and Applications, 3rd Edition (Johann Ambrosius Barth, Heidelberg, 1995).
- [13] D.M. Cvetković, P. Rowlinson and S. Simić, Eigenspaces of Graphs (Cambridge University Press, Cambridge, 1997). https://doi.org/10.1017/cbo9781139086547
- [14] D.M. Cvetković, P. Rowlinson and S. Simić, An Introduction to the Theory of Graph Spectra (Cambridge University Press, Cambridge, 2010). https://doi.org/10.1017/CBO9780511801518
- [15] I. Damnjanović and D. Stevanović, On circulant nut graphs, Linear Algebra Appl.
 633 (2022) 127–151. https://doi.org/10.1016/j.laa.2021.10.006
- [16] F. Ema, M. Tanabe, S. Saito, T. Yoneda, K. Sugisaki, T. Tachikawa, S. Akimoto, S. Yamauchi, K. Sato, A. Osuka, T. Takui and Y. Kobori, *Charge-transfer character* drives Möbius antiaromaticity in the excited triplet state of twisted [28] hexaphyrin, J. Phys. Chem. Lett. 9 (2018) 2685–2690. https://doi.org/10.1021/acs.jpclett.8b00740
- [17] P.W. Fowler, Hückel spectra of Möbius π systems, Phys. Chem. Chem. Phys. 4 (2002) 2878–2883. https://doi.org/10.1039/b201850k
- [18] P.W. Fowler, J.B. Gauci, J. Goedgebeur, T. Pisanski and I. Sciriha, Existence of regular nut graphs for degree at most 11, Discuss. Math. Graph Theory 40 (2020) 533–557. https://doi.org/10.7151/dmgt.2283
- [19] P.W. Fowler, B.T. Pickup, T.Z. Todorova, M. Borg and I. Sciriha, Omni-conducting and omni-insulating molecules, J. Chem. Phys. 140 (2014) 054115. https://doi.org/10.1063/1.4863559
- [20] P.W. Fowler, T. Pisanski and N. Bašić, *Charting the space of chemical nut graphs*, MATCH Commun. Math. Comput. Chem. **86** (2021) 519–538.
- [21] J.B. Gauci, T. Pisanski and I. Sciriha, Existence of regular nut graphs and the Fowler construction, Appl. Anal. Discrete Math. (2021), in-press. https://doi.org/10.2298/aadm190517028g
- [22] E. Ghorbani, W.H. Haemers, H.R. Maimani and L.P. Majd, On sign-symmetric signed graphs, Ars Math. Contemp. 19 (2020) 83–93. https://doi.org/10.26493/1855-3974.2161.f55

- [23] G. Greaves, J.H. Koolen, A. Munemasa and F. Szöllősi, Equiangular lines in Euclidean spaces, J. Combin. Theory Ser. A 138 (2016) 208–235. https://doi.org/10.1016/j.jcta.2015.09.008
- [24] W.H. Haemers, Seidel switching and graph energy, MATCH Commun. Math. Comput. Chem. 68 (2012) 653–659.
- [25] E. Heilbronner, Hückel molecular orbitals of Möbius-type conformations of annulenes, Tetrahedron Lett. 5 (1964) 1923–1928. https://doi.org/10.1016/s0040-4039(01)89474-0
- R. Herges, Topology in chemistry: Designing Möbius molecules, Chem. Rev. 106 (2006) 4820-4842. https://doi.org/10.1021/cr0505425
- [27] J.S. Maybee, D.D. Olesky and P. van den Driessche, Partly zero eigenvectors, Linear Multilinear Algebra 28 (1990) 83–92. https://doi.org/10.1080/03081089008818033
- [28] J.J. McDonald, Partly zero eigenvectors and matrices that satisfy Au = b, Linear Multilinear Algebra 33 (1992) 163–170. https://doi.org/10.1080/03081089308818190
- [29] B.D. McKay and A. Piperno, Practical graph isomorphism, II, J. Symbolic Comput. 60 (2014) 94–112. https://doi.org/10.1016/j.jsc.2013.09.003
- [30] H.S. Rzepa, Möbius aromaticity and delocalization, Chem. Rev. 105 (2005) 3697– 3715. https://doi.org/10.1021/cr0300921
- [31] I. Sciriha, On the construction of graphs of nullity one, Discrete Math. 181 (1998) 193-211. https://doi.org/10.1016/s0012-365x(97)00036-8
- [32] I. Sciriha, A characterization of singular graphs, Electron. J. Linear Algebra 16 (2007) 451–462. https://doi.org/10.13001/1081-3810.1215
- [33] I. Sciriha, Coalesced and embedded nut graphs in singular graphs, Ars Math. Contemp. 1 (2008) 20–31. https://doi.org/10.26493/1855-3974.20.7cc
- [34] I. Sciriha, Maximal core size in singular graphs, Ars Math. Contemp. 2 (2009) 217–229. https://doi.org/10.26493/1855-3974.115.891
- [35] I. Sciriha and L. Collins, Two-graphs and NSSDs: An algebraic approach, Discrete Appl. Math. 266 (2019) 92–102. https://doi.org/10.1016/j.dam.2018.05.003
- [36] I. Sciriha and P.W. Fowler, Nonbonding orbitals in fullerenes: Nuts and cores in singular polyhedral graphs, J. Chem. Inf. Model. 47 (2007) 1763–1775. https://doi.org/10.1021/ci700097j

- [37] I. Sciriha and I. Gutman, Nut graphs: Maximally extending cores, Util. Math. 54 (1998) 257–272.
- [38] Z. Stanić, Perturbations in a signed graph and its index, Discuss. Math. Graph Theory 38 (2018) 841–852. https://doi.org/10.7151/dmgt.2035
- [39] A. Streitwieser, Molecular Orbital Theory for Organic Chemists (Wiley, New York, 1961).
- [40] N. Trinajstić, Chemical Graph Theory, 2nd Edition (CRC Press, Boca Raton, FL, 1992). https://doi.org/10.1201/9781315139111
- [41] T. Yoneda, Y.M. Sung, J.M. Lim, D. Kim and A. Osuka, Pd^{II} complexes of [44]and [46] decaphyrins: The largest Hückel aromatic and antiaromatic, and Möbius aromatic macrocycles, Angew. Chem. Int. Ed. 53 (2014) 13169–13173. https://doi.org/10.1002/anie.201408506
- [42] Z.S. Yoon, A. Osuka and D. Kim, Möbius aromaticity and antiaromaticity in expanded porphyrins, Nature Chemistry 1 (2009) 113–122. https://doi.org/10.1038/nchem.172
- [43] T. Zaslavsky, Signed graphs, Discrete Appl. Math. 4 (1982) 47–74. https://doi.org/10.1016/0166-218x(82)90033-6
- [44] T. Zaslavsky, Glossary of signed and gain graphs and allied areas, Electron. J. Combin., Dynamic Surveys (1998) #DS9. https://doi.org/10.37236/31
- [45] T. Zaslavsky, A mathematical bibliography of signed and gain graphs and allied areas, Electron. J. Combin., Dynamic Surveys (1998) #DS8. https://doi.org/10.37236/29

Received 27 January 2021 Revised 14 October 2021 Accepted 14 October 2021