

Coalesced and Embedded Nut Graphs in Singular Graphs

Irene Sciriha[†]

*Department of Mathematics, Faculty of Science
University of Malta, Msida MSD 06, Malta*

Received 1 August 2007, accepted 9 May 2008, published online 19 June 2008

Abstract

A nut graph has a non-invertible (singular) 0-1 adjacency matrix with non-zero entries in every kernel eigenvector. We investigate how the concept of nut graphs emerges as an underlying theme in the theory of singular graphs. It is known that minimal configurations (MCs) are necessarily found as subgraphs of singular graphs. We construct MCs having nut graphs as subgraphs. Nut graphs can be coalesced with singular graphs at particular vertices or grown into a family of core graphs of larger nullity by adding a vertex at a time. Moreover, we propose a local enlargement of nut fullerenes and tetravalent nut graphs.

Keywords: Adjacency matrix, nut graph, kernel eigenvector, singular graphs, core, periphery, nut fullerenes, line graphs of trees.

Math. Subj. Class.: 05C50, 05B20, 05C90, 92E10

1 Introduction

A graph G has vertex set $\mathcal{V}_G = \{1, 2, \dots, n\}$ and edge set \mathcal{E}_G joining distinct vertices of \mathcal{V}_G . The complement \overline{G} of G has $\mathcal{V}_{\overline{G}} = \mathcal{V}_G$ and $\mathcal{E}_{\overline{G}}$ is the set of non-edges of G . The adjacency matrix $\mathbf{A}_G (= \mathbf{A} \text{ or } \mathbf{G})$, of a graph G , is the matrix (a_{ij}) , where a_{ij} is one if $ij \in \mathcal{E}_G$ and zero otherwise. The graphs we consider are simple, i.e without loops or multiple edges; thus each entry on the main diagonal is zero. Since a graph is uniquely determined by its adjacency matrix, we use terminology for a graph and its adjacency matrix interchangeably. For different labellings of the vertices of a graph G , the corresponding adjacency matrices are similar. Thus the collection of eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, (with repetitions), which is said to be the spectrum $Sp(G)$ of G , is an invariant of G [1, 2].

[†]Research supported by the AWRF, University of MALTA.

E-mail address: irene.sciriha-aquilina@um.edu.mt (Irene Sciriha)

Singular graphs have the eigenvalue zero. In section 2, we survey properties of core graphs and nut graphs as particular singular graphs. Minimal configurations (MCs) and singular configurations (SCs) are subgraphs determined by the vectors in $\ker(\mathbf{A})$. A graph of nullity η has η independent MCs as subgraphs [17]. Catalogues of MCs of small order can be found in [11] and [13]. The simplest MCs are trees including paths on an odd number of vertices. A tree is a MC if and only if it is a subdivision of some tree [19]. In section 3, we survey the properties of MCs and proceed, in section 4, to explore possible ways of converting singular graphs to larger ones. If a graph G has an eigenvalue λ_0 of multiplicity k , then k vertices can be deleted to produce a star complement for λ_0 , that is, a maximal induced subgraph of G that does not have λ_0 as an eigenvalue. We show that a vertex deleted subgraph $Y - v$ of a nut graph Y is a star complement for $\lambda_0 = 0$. Nut graphs can be coalesced with singular graphs at particular vertices to obtain larger nut graphs or other particular types of singular graphs. Moreover, if to nut graphs, vertices are added to increase the nullity at each stage, a family of core graphs of increasing nullity, with a nut graph as an induced subgraph, is produced. The last section presents a local enlargement for trivalent polyhedra, cylindrical constructions for nut fullerenes and an extension of four-valent polyhedra to produce larger core graphs.

2 Nut Graphs

A graph G is singular if \mathbf{A} is singular, that is if \mathbf{A} is not injective. Hence, there exist linearly independent vectors \mathbf{x} , s.t. $\mathbf{A}\mathbf{x} = \mathbf{0}$, so that zero is an eigenvalue of \mathbf{A} . The multiplicity η of the eigenvalue zero is the dimension of the nullspace, $\ker(\mathbf{A})$ and is said to be the **nullity** $\eta(G)$ of G .

Definition 1. Let G be a singular graph. A non-zero vector \mathbf{x} satisfying $\mathbf{A}\mathbf{x} = \mathbf{0}$ is said to be a **kernel eigenvector** of G .

There exist singular graphs, called **core graphs**, of nullity one or more, with a kernel eigenvector having no zero entries. We say that a subgraph, F , of a singular graph G , is a **core of G** , if there exists a kernel eigenvector \mathbf{x} of G such that F is the subgraph induced by the vertices corresponding to the non-zero entries (or support) of \mathbf{x} . Hence a core F of G is a core graph, with a kernel eigenvector \mathbf{x}_F , the non-zero restriction of \mathbf{x} . The $|F|$ vertices of F are determined by the $|F|$ labels corresponding to \mathbf{x}_F . We label a graph G , of nullity one, so that a kernel eigenvector of the form $\mathbf{x} = (\mathbf{x}_F, \mathbf{0})^t$, generates the nullspace $\ker(\mathbf{G})$, where $\mathbf{x}_F \in \mathbb{R}^{|F|}$ is the non-zero part of \mathbf{x} with each of the $|F|$ entries being non-zero. For nullity greater than one, there are a number of cores, each corresponding to a non-trivial vector in $\ker(\mathbf{G})$. Note that each core of G is a core graph in its own right.

The set of **core vertices**, CV , of G , consists of those vertices that lie in some core of G . A vertex, not lying in any core, is said to be a **core-forbidden** vertex. Thus a core graph has no core-forbidden vertices. Moreover, core graphs are distinguished from other singular graphs, since the deletion of any vertex reduces the nullity (Corollaries 13 and 16).

Definition 2. A nut graph is a singular graph such that no kernel eigenvector has zero entries.

Proposition 3. A nut graph is a core graph of nullity one.

Proof. By definition, a nut graph has at least one kernel eigenvector with no zero entries. Since linear combinations of linearly independent kernel eigenvectors can produce a kernel eigenvector with a zero entry and this cannot be the case for nut graphs, it follows that all

kernel eigenvectors are linearly dependent. Hence, for a nut graph Y , the dimension of $\ker Y$ is one. □

Theorem 4. [10] *A nut graph*

- (i) *is connected;*
- (ii) *has no terminal vertex;*
- (iii) *is not bipartite.*

Remark 5. Nut graphs exist on seven or more vertices. The second and third graphs in Figure 1 are nut graphs. From Proposition 4(iii), it follows that all nut graphs have odd cycles. The girth of a graph is the size i of the smallest odd cycle C_i , on i vertices. It is given by the index i of the first non-vanishing odd coefficient, a_i , in the characteristic polynomial $\sum_{i=0}^n a_i \lambda^{n-i}$ of the adjacency matrix of the graph [8]. There exist nut graphs with girth three. Nut fullerenes are three-regular and have girth five.

Proposition 6. [10] *If a triangle $C_3 = \{v_1, v_2, v_3\}$ is a subgraph of the nut graph Y and the vertex v_1 is of degree two in Y , then v_2 and v_3 do not have the same neighbours. (Equivalently, v_2 and v_3 are not co-duplicate vertices.)*

3 Minimal Configurations

In [14], we show that a singular graph of nullity η has η subgraphs called minimal configurations (MCs). In [17], a stronger result is obtained for singular configurations (SCs), namely that a singular graph of nullity η has η SCs as *induced* subgraphs. MCs and SCs are singular graphs of nullity one, determined by the non-zero part of their kernel eigenvector as follows [11, 17]:

Definition 7. Let F be a core graph on at least two vertices, with nullity $s \geq 1$ and a kernel eigenvector \mathbf{x}_F having no zero entries. If a graph N , of nullity one, having \mathbf{x}_F as the non-zero part of a kernel eigenvector, is obtained, by adding $s - 1$ independent vertices, whose neighbours are vertices of F , then N is said to be a **minimal configuration** (MC).

The set of $s - 1$ independent vertices added to F to produce N is said to be the **periphery** $\mathcal{P}(N)$ of N . Figure 1 shows three MCs with $s = 2, 1, 1$ and $|\mathcal{P}(N)| = 1, 0, 0$ respectively.

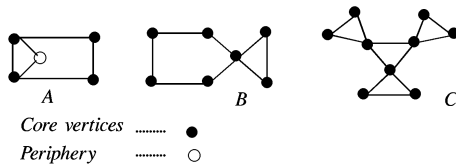


Figure 1: Three MCs

If the condition that the $(s - 1)$ vertices added are independent is dropped, then the singular graph S of nullity one obtained is said to be a SC. Various MCs may be constructed for the same F and \mathbf{x}_F . The MCs, shown in Figure 2, have the same core $N_5 = \overline{K_5}$ and $(1, 1, -2, -1, 2)$ or $(1, 1, -1, -1, 1)$ as the non-zero part of the kernel eigenvector.

We present properties of MCs.

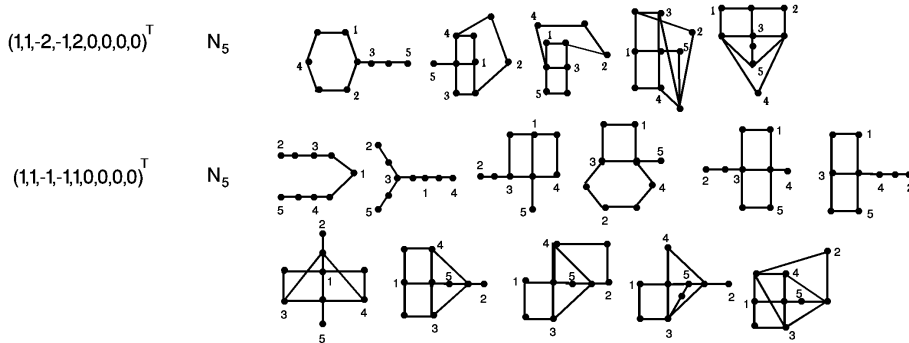


Figure 2: MCs with core $\overline{K_5}$ for two feasible 0-eigenvectors

Theorem 8. *A MC is connected.*

Proof. Suppose, for contradiction that a MC N is disconnected. Without loss of generality N has a connected component N_1 having a non-zero kernel eigenvector \mathbf{x}_1 . If the vertices of N_1 are labelled first, then $\mathbf{N} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$ and $\mathbf{N}_1 \mathbf{x}_1 = \mathbf{0}$. Since $\mathbf{x}_1 \neq \mathbf{0}$, then $\mathbf{x}_2 = \mathbf{0}$, otherwise $\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{0} \end{pmatrix}$ and $\begin{pmatrix} \mathbf{0} \\ \mathbf{x}_2 \end{pmatrix}$ would be linearly independent kernel eigenvectors of N , contradicting that the nullity of N is one. Thus \mathbf{x}_2 corresponds to vertices in the periphery and hence there are no edges among them. But then N has isolated vertices which contribute to the nullity, so that $\eta(N) > 1$, a contradiction. Thus $N = N_1$. \square

Theorem 9. [16] *Let N be a singular graph of order $n \geq 3$. The graph N is a MC having a core F with respect to the kernel eigenvector \mathbf{x} and periphery $\mathcal{P} := \mathcal{V}(N) - \mathcal{V}(F)$ if and only if the following conditions are all satisfied:*

- (i) $\eta(N) = 1$,
- (ii) $\mathcal{P} = \emptyset$ or \mathcal{P} induces a graph consisting of isolated vertices,
- (iii) $\eta(F) = |\mathcal{P}| + 1$.

Proof. Condition (i) follows from the definition of MC.

If the nullity of F is one, then $F = N$ and $\mathcal{P} = \emptyset$, so that both (ii) and (iii) are satisfied.

If the nullity s of F is more than one, then (ii) and (iii) follow from the construction of a MC in Definition 7.

Conversely, if the three conditions hold, then

- a. N has nullity one;
- b. if $\mathcal{P} \neq \emptyset$, then the neighbours of the vertices in \mathcal{P} are vertices of F ;
- c. by the Interlacing Theorem, condition (iii) requires that the nullity of the core F decreases successively by one with each addition of the $(s - 1)$ vertices in \mathcal{P} , in turn. \square

The above properties of MCs do not depend on the edges or non-edges among the vertices of the periphery, so that they hold also for SCs [17]. Note that a nut graph is a MC with $\mathcal{P} = \emptyset$. For $\eta(G) = 1$, a singular graph G has a unique core F and a unique periphery. For $\eta(G) > 1$, it is convenient to use a minimal basis B_{min} for the nullspace of G . The vectors

$\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_\eta$ in B_{min} are chosen so that the total number of non-zero entries in the vectors is a minimum. A somewhat surprising result is the following: if $|x_i|$ denotes the number of non-zero entries in \mathbf{x}_i , then, every possible B_{min} has a unique sequence $|x_1|, |x_2|, \dots, |x_\eta|$ [15, 17].

4 Extensions

In [10], we explored the possibilities of growing nut graphs into larger nut graphs by adding vertices and modifying the kernel eigenvector. This prompts us to explore other ways of constructing singular graphs that have a nut graph embedded as an induced subgraph.

4.1 Coalescence with Nut Graphs

Definition 10. [9] If a vertex v_1 of a graph G_1 is identified with a vertex v_2 of a graph G_2 , then the graph $G_1.G_2$ obtained, of order $|G_1| + |G_2| - 1$, is said to be the **coalescence** of G_1 and G_2 .

We shall consider coalescence of singular graphs with nut graphs. The following theorem [9], which we shall have occasion to use, gives an expression for the characteristic polynomial $\phi(G, \lambda)$ of a graph $G = K.H$ in terms of characteristic polynomials of K and H , and of their vertex-deleted subgraphs.

Theorem 11. *The characteristic polynomial of the coalescence $K.H$ of two rooted graphs (K, u) , (H, w) obtained by identifying the vertices u , and w so that this vertex $v = u = w$ becomes a cut-vertex of $K.H$ is given by:*

$$\phi(K.H) = \phi(K)\phi(H - w) + \phi(K - u)\phi(H) - \lambda\phi(K - u)\phi(H - w). \quad (1)$$

Proposition 12. *If G is a graph of nullity η , there exists a subset X of η vertices of $\mathcal{V}(G)$, whose deletion yields a non-singular graph¹.*

Proof. Let G be labelled so that the vertices in CV are labelled first. If $B = \{\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_\eta\}$ is a basis for the nullspace of $\mathbf{A}(G)$, then the $\eta \times n$ matrix \mathbf{M} whose rows are the η vectors in B , has rank η . By row reduction, \mathbf{M} can be reduced to Hermite Normal form \mathbf{M}' , in which, to the (column) position of the first non-zero entry of each of the η row vectors, there corresponds a zero entry in all the other rows. Since row reduction is equivalent to taking linear combinations of the kernel eigenvectors, the rows of \mathbf{M}' are also kernel eigenvectors of G . Deleting any vertex, v , affects just one of the row vectors so that the remaining $\eta - 1$ rows of \mathbf{M}' , restricted to $G - v$, are kernel eigenvectors of $G - v$. Moreover, there are no more kernel eigenvectors linearly independent of these $\eta - 1$ row vectors as otherwise the nullity of G would be more than η . \square

The following result follows from Proposition 12.

Corollary 13. *If a core vertex v is deleted from a graph G , of nullity η , then the nullity of $G - v$ is $\eta - 1$.*

The following result is also proved in [12], utilizing the adjugate of \mathbf{A} .

¹For the eigenvalue zero, the graph $G - X$ is said to be a *star complement* of G and the set X a *star set*. See, for instance, [7].

Corollary 14. *If a core vertex v is deleted from a singular graph G of nullity one, then $G - v$ is non-singular.*

Corollary 15. *If any vertex v is deleted from a nut graph Y , then $Y - v$ is non-singular.*

Proof. This follows since Y has nullity one and every vertex of Y is a core vertex. □

Corollary 16. *If $\eta(G - v) < \eta(G)$ for all $v \in \mathcal{V}_G$, then G is a core graph.*

Proof. This follows since a basis for the nullspace of $\mathbf{A}(G)$ can be taken to be the row vectors of M' as constructed in the proof of Proposition 12. □

Proposition 17. *A star set for the eigenvalue zero is contained in CV.*

Proof. For the nullity to decrease on deleting a vertex i , there needs to be a kernel eigenvector in M' with its first non-zero entry at position i . These positions form a star set and are in CV by definition. □

Proposition 18. *If the graph G' is obtained by coalescing a nut graph Y with a singular graph G , at a vertex v_F of a core F of G , then the nullity remains unchanged.*

Proof. Let $\eta(G) = \eta$. Now by Corollaries 13 and 15, $\eta(G - v_F) = \eta - 1$ and $\eta(Y - v) = 0$. Thus $\eta(G') \leq \eta$ by interlacing.

From Equation (i) of Theorem 11, the characteristic polynomial $\phi(G')$ of the coalescence $G.Y$ is given by $\phi(G') = \phi(G - v_F, \lambda)\phi(Y, \lambda) + \phi(G, \lambda)\phi(Y - v_F, \lambda) - \lambda\phi(G - v_F, \lambda)\phi(Y - v_F, \lambda)$. Each term on the right hand side of the equation is divisible by λ^η , so that $\eta(G') \geq \eta$. This completes the proof. □

The construction of Proposition 18 may be done iteratively, running through all the core vertices, to produce successively larger graphs of the same nullity.

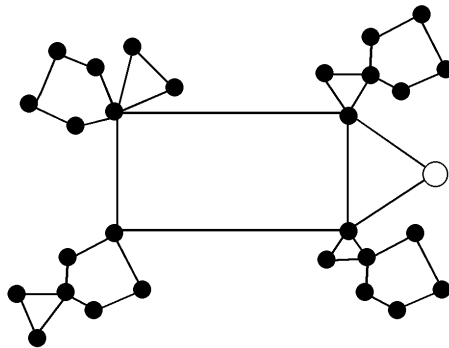


Figure 3: An enlarged MC

Figure 3 shows the graph G' , an enlargement of the five vertex MC, H (made up of C_4 and C_3 with a common edge). The smallest nut graph is the seven vertex, eight edge graph Y of Figure 1, formed by coalescing C_5 with C_3 . If Y is coalesced, at each of the four core vertices of H , a graph G' is produced. By Proposition 18, $\eta(H) = \eta(G')$.

Proposition 19. *Let N be a MC with core F . If nut graphs are coalesced with F at distinct vertices of F , then a MC is produced.*

Proof. Let G' be constructed by coalescing nut graphs with F at distinct vertices of F . At a vertex of F where no nut graph is coalesced, we say that K_1 (the trivial nut graph) is coalesced with N . If $\mathbf{N} = \begin{pmatrix} \mathbf{F} & \mathbf{B} \\ \mathbf{B}^t & \mathbf{0} \end{pmatrix}$ represents the adjacency matrix of N , then, one way to produce the adjacency matrix of G' , is to replace the diagonal entries of \mathbf{F} in \mathbf{N} by block matrices $\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_{|F|}$, where Y_i is the nut graph (or K_1) coalesced at vertex i for $1 \leq i \leq |F|$, leave the principal submatrix for the F -vertices unchanged and insert zero matrices in the remaining blocks. Let $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_{|F|}$ be the eigenvectors of $Y_1, Y_2, \dots, Y_{|F|}$, scaled so that the first entry of each u_i is one. For $Y_i = K_1$, $\mathbf{Y}_i = (0)$ and $\mathbf{u}_i = (1)$. If $\mathbf{N}\mathbf{y} = \mathbf{0}$ and $\mathbf{y} = (y_1, y_2, \dots, y_{|F|}, 0, \dots, 0)^t$, then $\mathbf{G}'\mathbf{z} = \mathbf{0}$, where $\mathbf{z} = (y_1\mathbf{u}_1^t, y_2\mathbf{u}_2^t, \dots, y_{|F|}\mathbf{u}_{|F|}^t, 0, \dots, 0)^t$. Thus G' is singular with a core F' , which is the coalescence of F with $Y_1, Y_2, \dots, Y_{|F|}$.

To show that G is a MC, there remains to show that the three conditions of Theorem 9 are satisfied. Indeed, by Proposition 18, iterative coalescence at core vertices of N preserves the nullity at the value one, so that condition (i) is satisfied. The periphery $\mathcal{P}' = \mathcal{V}(G') \setminus \mathcal{V}(F')$ is the same independent set as $\mathcal{P}F = \mathcal{V}(G) \setminus \mathcal{V}(F)$, satisfying condition (ii). Also, by Proposition 18, $\eta(F') = \eta(F)$. Thus, deleting all the vertices of the periphery in turn from G' has the same effect on the nullity of G' as deleting the corresponding vertices of \mathcal{P} in G , so that the nullity increases at each stage, as required for condition (iii). Hence G' is also a MC. \square

Remark 20. Since the construction in Proposition 19 does not affect the vertices in the periphery, the following result is immediate.

Corollary 21. *Let Y_1 and Y_2 be nut graphs. The coalescence $Y_1.Y_2$ is a nut graph.*

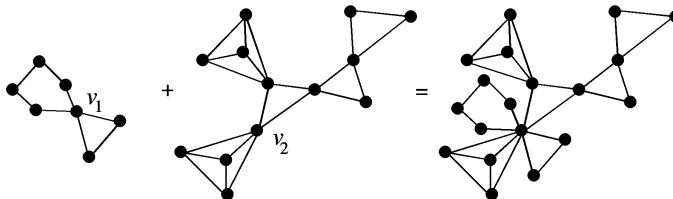


Figure 4: The coalescence of two nut graphs.

In Figure 4, the nut graph on 7 vertices is coalesced with the nut graph on 15 vertices, at arbitrary vertices v_1 and v_2 , to produce a larger nut graph.

4.2 Singular Graphs with a Nut Graph Embedding

Duplicate vertices are independent vertices having the same neighbours. They correspond to identical rows (and columns) in \mathbf{A} . A set of ℓ duplicate vertices contributes $\ell - 1$ to the nullity of a graph. A kernel eigenvector corresponding to a core graph consisting of a pair of duplicate vertices has two non-zero entries only. A vertex can always be added to form a duplicate pair with any vertex of a graph, thus increasing the nullity indefinitely. Following

Lepović, we call a graph **canonical**, if it has no duplicate vertices [5]. The kernel eigenvectors of a singular canonical graph have three or more non-zero entries.

The Reconstruction Theorem [6, 7] applied to the eigenvalue zero states that a finite number, k , of vertices are added to a zero-star complement to produce a *canonical* supergraph of maximal nullity k . By Corollary 15, a vertex-deleted subgraph of a nut graph is a zero-star complement.

Proposition 22. *If a singular graph G of nullity η is obtained by adding $\eta - 1$ vertices to a nut graph Y , then G is a core graph.*

Proof. Let B_1 be the basis containing only the nullspace generator of Y . Assume that $j - 1$ vertices have been added to Y to produce G_j with nullity j , $j \geq 1$ and the basis B_j , containing j vectors, generates the nullspace of G_j . If a vertex v can be added to increase the nullity by one, a kernel eigenvector \mathbf{x}_{j+1} , linearly independent of the ones in B_j , is included to produce B_{j+1} . We can proceed inductively to produce a larger singular graph G_η with a basis B_η , by adding to B_1 , vectors having a non-zero entry in positions $|Y| + j - 1$ corresponding to the additional vertices in turn, for $0 \leq j \leq \eta - 1$. Note that an entry of \mathbf{x}_{j+1} in the position corresponding to v is necessarily non-zero. Thus the graph G_η is a core graph. \square

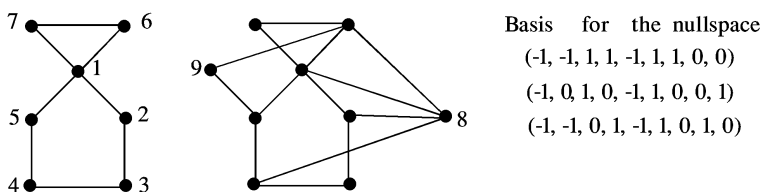


Figure 5: A core graph of nullity three with a nut graph embedded.

In Figure 5, to the nut graph on 7 vertices, two vertices can be added to produce a singular canonical graph of nullity three. The two graphs produced in the process are core graphs.

5 Nut Fullerenes

We conclude with a reference to the significance of nut graphs in chemistry, presenting ways of transforming nut regular polyhedra to larger core graphs. The Hückel Molecular Orbital (HMO) model describes the distribution of the π -electrons in unsaturated organic molecules and is an approximation to the solution of the Schrödinger Equation [4]. The molecular graph G of a Carbon (C) structure has the C-atoms as vertices and the C-C σ bonds as edges. The energy levels λ_i of the π -electrons, in the C-structure, are given by $\mathbf{Ax}_i = \lambda_i \mathbf{x}_i$, where \mathbf{x}_i describes the molecular orbital for the energy λ_i and \mathbf{A} is the adjacency matrix of G . For singular molecular graphs, $\mathbf{Ax} = \mathbf{0}$, \mathbf{A} has zero eigenvalues, and the C-structure has non-bonding molecular orbitals (NBMOs) described by $\mathbf{x}(\neq \mathbf{0})$ [4].

If G is a nut graph, then the NBMO \mathbf{x} of the π -electron occupying this orbital has non-zero entries. In chemistry, this is significant. In the radical molecule that would have the NBO as partially occupied HOMO, all centres carry non-zero spin density. The charge, spin and bond-order densities of a π -electron, occupying the NBMO, are distributed over

the whole structure and not on some substructure. Thus all C-centres are likely to be involved in reactions. [18, 20, 21].

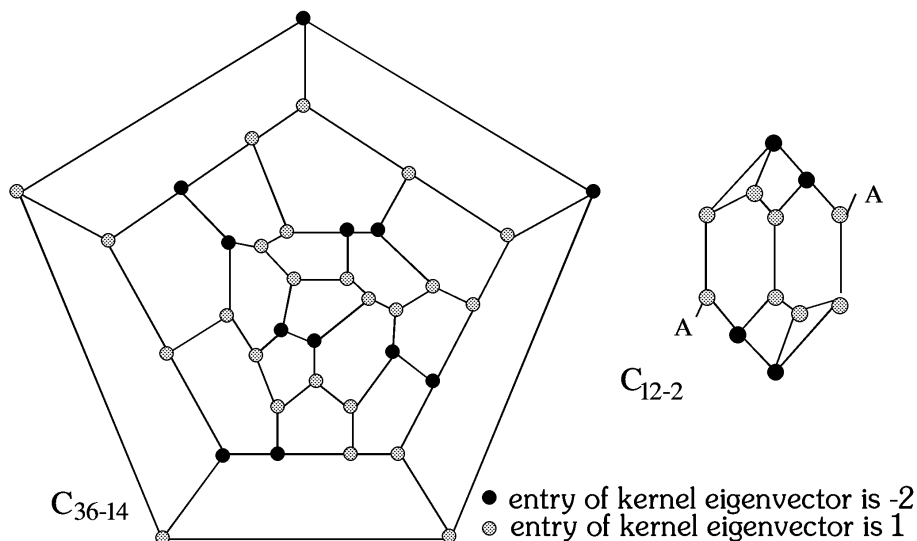


Figure 6: $C_{36} : 14$ and $C_{12} : 2$

There are 10, 190, 782 fullerene isomers on up to 120 vertices and only 41 are nut graphs. In all hypothetical nut fullerenes found so far, occupation of the NBMO requires that the fullerene carries at least five negative charges. All physically realizable fullerenes, known to date, have isolated pentagons and none of these is a nut graph.

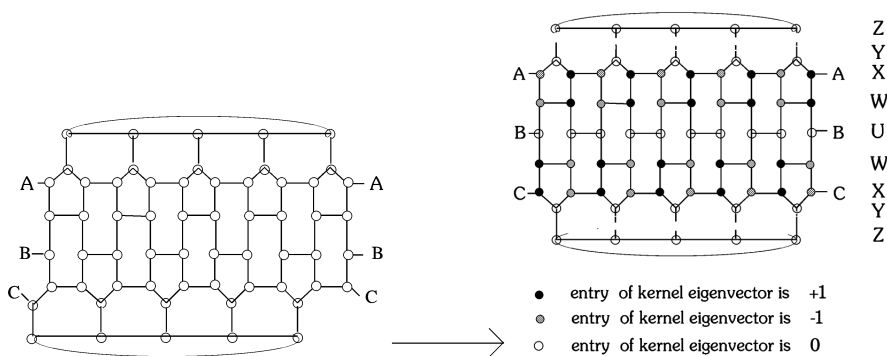


Figure 7: C_{60} and C_{70}

The smallest nut fullerene is $C_{36} : 14$ [3] and the smallest nut trivalent polyhedron is $C_{12} : 2$, both shown in Figure 6. Symmetry studies of polyhedra yield powerful mathematical results that can be immediately translated into chemical properties [18, 20]. For highly

symmetric vertex transitive or one-orbit graphs, the eigenvector entries for a simple eigenvalue, have the same non-zero absolute value. This implies equidistributivity of charge from the single NBMO of a molecule. However $\mathbf{Ax} = \mathbf{0}$, with each entry of \mathbf{x} being ± 1 , demands an even number of bonds for each C-centre which is not the case in tri-valent polyhedra. Thus vertex transitive nut fullerenes are ruled out. Several trivalent $(+1, -1, 0)$ molecules with a NBMO are possible. One is C_{70} which can be seen as the Buckminster fullerene C_{60} with an additional ten C-atoms, contributing an equatorial ring of five extra hexagons, as shown in Figure 7. Such a singular trivalent structure cannot be a MC, since every C-centre (even if it corresponds to a zero entry of the kernel eigenvector) has an adjacent atom with no charge from the NBMO. This forces two peripheral vertices to be adjacent, a configuration which is not allowed in MCs.

The two nut trivalent polyhedra $C_{36} : 14$ and $C_{12} : 2$ mentioned above have a $(-2, +1, +1)$ NBMO, that is a kernel eigenvector with $-2, +1$ as its only entries. Such graphs are said to be *uniform nut graphs*. Considering orbits, since every C-centre is adjacent to three atoms corresponding to entries $-2, +1$ and $+1$, one can deduce that the number of C atoms in uniform-nut fullerenes is a multiple of six [18, 20, 21].

Inspection of the pictures and spiral codes of the early nut fullerenes suggests some recurring patterns. We now investigate ways in which nut chemical graphs can be expanded, while the original part of the nullspace generator remains in the new nullspace.

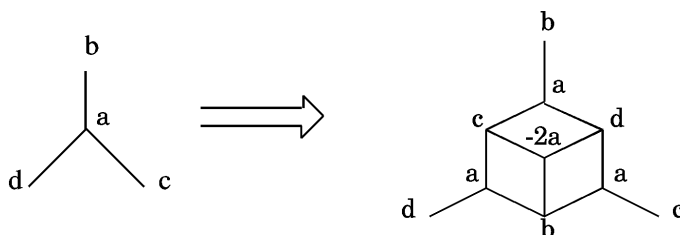


Figure 8: Local enlargement in regular chemical graphs

To preserve the regularity of a trivalent graph, coalescence cannot be employed. Instead an expansion of cubic graphs that preserves the null eigenvector can be considered. The following construction was suggested by P. W. Fowler. In a kernel eigenvector, the central vertex carries entry a and by applying the *zero-sum rule* (or eigenvector equation for the zero eigenvalue) the entries on its neighbours total $b+c+d = 0$. Expansion of the central vertex to a half-cube, as shown in Figure 8, can be achieved without disruption of the null eigenvector, if new eigenvector entries are assigned as shown. Clearly, if the parent graph is a uniform nut graph and $a = +1$, the derived vector is uniform, but if $a = (-2)^{r-1}$, $r \geq 3$, then the entries of the derived vector are in $\{(-2)^{r-1}, r \geq 1\}$.

As the vertex count increases, cylindrical nut fullerenes occur, and can be grouped into families according to their six-pentagon caps. In [21], it is shown that there exists a family of tubular fullerenes, each with a cap of six pentagons and two hexagons, circumscribed by successive rings of six hexagons and ending with the same cap, which have a kernel eigenvector with entries in $\{1, -2\}$. The pattern of coefficients is compatible with insertion of any number of extra layers of six hexagons in the starting C_{48} structure, so that we have an infi-

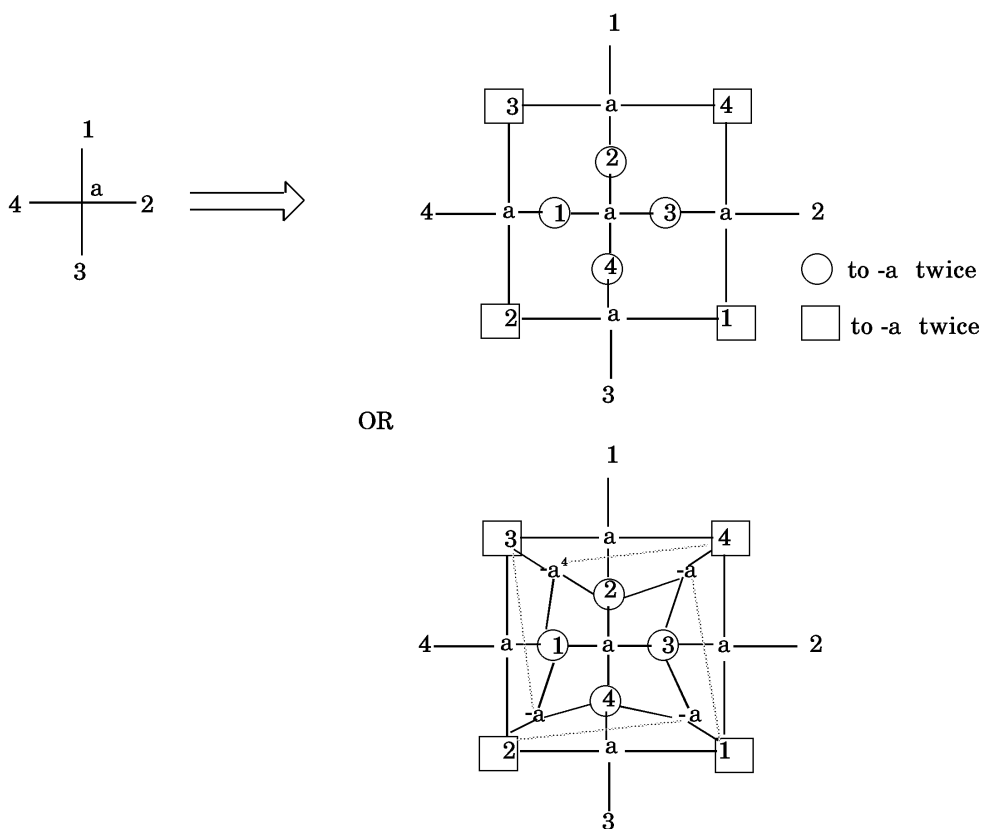


Figure 9: Local enlargement in trivalent chemical graph.

nite series of singular fullerenes, with predictable spiral codes. All members of the series are cores. Although we have no formal proof that the multiplicity of the zero eigenvector remains at the value one after each stage of the expansion, the null eigenvector in each member of the series is found to remain unique at least for all $n \leq 1000$, and it appears plausible that we have an infinite family of not only core fullerenes but also uniform-nut fullerenes.

We propose two similar expansions of tetravalent molecules where, in a kernel eigenvector, the central vertex carries entry a and the zero-sum rule necessitates that the addition of the four neighbouring entries be zero. The bonds (edges) for the added atoms (vertices) are shown in Figure 9. Note that in the first construction, two additional vertices, each carrying charge $-a$, one above and one below the plane of the diagram, are required to produce a four-valent molecule which is a core graph. In the second construction all the edges are shown.

References

- [1] D. Cvetković and I. Gutman, Algebraic Multiplicity of Zero in the Spectrum of Bipartite Graphs, *Mat. Vesnik (Beograd)* **9** (1972), 141–150.

- [2] D. M. Cvetković, P. Rowlinson and S. Simić Eigenspaces of Graphs, *Encyclopedia of Mathematics and its Applications* **66**, Cambridge University Press, Cambridge, 1997.
- [3] P. W. Fowler, P. W. Manolopoulos, An Atlas of Fullerenes, Clarendon Press, 1995.
- [4] E. Hüchel, Zur modernen Theorie ungesättigter und aromatischer Verbindungen, *Z. Elektrochem.* **61** (1957), 866–890.
- [5] M. Lepović, On Canonical Graphs and Eigenvectors of Graphs, *Utilitas Mathematica* **54** (1998), 257–272.
- [6] P. Rowlinson, Star Sets and Star Complements in Finite Graphs – A Spectral Construction Technique, *Publications de L'Istitut Mathématique, Nouvelle Série* **76 (90)** (2004), 25–30.
- [7] P. Rowlinson, Star Complements in Finite Graphs – A Survey, *Rendiconti del Seminario Matematico di Messina Ser II Supplemento al n.* **8** (2002), 145–162.
- [8] H. Sachs, Beziehungen Zwischen den in Einem Graphen Enthaltenen Kriesen und Seinem Charakteristischen Polynom, *Publ. Maths. Debrecen* **11** (1964), 261–274.
- [9] A. J. Schwenk, Computing the Characteristic Polynomial of a Graph, in: R. A. Bari and F. Harary, eds., *Graphs and Combinatorics* **406**, Springer-Verlag, 1975, 153–172.
- [10] I. Sciriha and I. Gutman, Nut Graphs – Maximally Extending Cores, *Utilitas Mathematica* **54** (1998), 257–272.
- [11] I. Sciriha, On the Construction of Graphs of Nullity One, *Discrete Math.* **181** (1998), 193–211.
- [12] I. Sciriha, On the Coefficient of λ in the Characteristic Polynomial of Singular Graphs, *Utilitas Mathematica* **52** (1997), 97–111.
- [13] I. Sciriha, On the Rank of Graphs, in eds. Y. Alavi et al., *The Eighth Quadrennial International Conference on Graph Theory, Combinatorics, Algorithms and Applications*, Springer-Verlag, 1998, 769–778.
- [14] I. Sciriha, On some Aspects of Graph Spectra, Ph.D. Thesis, University of Reading, UK, British Library, November 1998.
- [15] I. Sciriha, S. Fiorini and J. Lauri, A Minimal Basis for a Vector Space, *Graph Theory Notes of New York XXXI* 1996, 21–24.
- [16] I. Sciriha and I. Gutman, Minimal Configurations and Interlacing, *Graph Theory Notes of New York XLIX* (2005), 38–40.
- [17] I. Sciriha, A Characterization of Singular Graphs, *Electronic Journal of Algebra* **16** (2007) 451–462.
- [18] I. Sciriha and P. W. Fowler, A Spectral View of Fullerenes, *Mathematica Balkanica* **18**, Fasc. 1–2, (2004), 183–192.
- [19] I. Sciriha and I. Gutman, Minimal Configurations Trees, *Linear and Multilinear Algebra*, **54-2** (2006), 141–145.
- [20] I. Sciriha and P. W. Fowler, Nuts, Cores and Symmetry in Fullerenes, *Discrete Math.* **308** (2008), 267–276.
- [21] I. Sciriha and P. W. Fowler, Non-bonding Orbitals in Fullerenes: Nuts and Cores in Singular Polyhedral Graphs, *Journal of Chemical Information and Modeling, J. Chem. Inf. Model* **47** (2007), 1763–1775.