

EXISTENCE OF REGULAR NUT GRAPHS AND THE FOWLER CONSTRUCTION

*John Baptist Gauci**, *Tomaž Pisanski* and *Irene Sciriha*

In this paper the problem of the existence of regular nut graphs is addressed. A generalization of Fowler’s Construction which is a local enlargement applied to a vertex in a graph is introduced to generate nut graphs of higher order. Let $N(\rho)$ denote the set of integers n such that there exists a regular nut graph of degree ρ and order n . It is proven that $N(3) = \{12\} \cup \{2k : k \geq 9\}$ and that $N(4) = \{8, 10, 12\} \cup \{n : n \geq 14\}$. The problem of determining $N(\rho)$ for $\rho > 4$ remains completely open.

1. INTRODUCTION

All graphs considered in this paper are simple (that is, without loops or multiple edges). The 0–1 *adjacency matrix* $\mathbf{A} = \mathbf{A}(G) = (a_{ij})$ of a labelled graph G on n vertices is a real and symmetric $n \times n$ matrix such that $a_{ij} = 1$ if there is an edge between the vertices i and j , and $a_{ij} = 0$ otherwise. A graph G is *singular* if zero is an eigenvalue of $\mathbf{A}(G)$, and the multiplicity of the eigenvalue zero in the spectrum of G is the *nullity* of G , denoted by $\eta = \eta(G)$. Thus G is singular if and only if $\eta(G) > 0$. The *eigenvectors* \mathbf{x} of $\mathbf{A}(G)$ associated with the eigenvalue λ are the nonzero vectors determined by $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$. The vectors in the nullspace $\ker(\mathbf{A})$ of \mathbf{A} are called *kernel eigenvectors*.

In G , the fact that $\mathbf{A}\mathbf{x} = \mathbf{0}$ can be interpreted as an assignment of the entries of \mathbf{x} to the vertices of G , that is, $\mathbf{x} : V(G) \rightarrow \mathbb{R}$, such that the sum of the values assigned to the neighbours of v sums up to 0 for each $v \in V(G)$, and at least one

*Corresponding author. John Baptist Gauci

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vertex $v \in V(G)$ is assigned a non-zero value $\mathbf{x}(v) \neq 0$. It is worth noting that for any integer matrix \mathbf{A} having integer eigenvalue λ , there exists an associated eigenvector \mathbf{x} with integer entries. Moreover, one may choose the entries of \mathbf{x} to have no nontrivial common divisor so that \mathbf{x} is determined up to the sign. In general, any eigenvector \mathbf{x} corresponding to the 0 eigenvalue with non-zero entries will be called *admissible*.

A vertex of G corresponding to a non-zero entry in some kernel eigenvector is a *core vertex* of G . A *core graph* is a singular graph each of whose vertices is a core vertex, whereas a *nut graph* is a core graph of nullity one. The notion of nut graphs, introduced by Gutman and Sciriha in [7], is one that emerged from pure mathematics (linear algebra and graph theory), but which provides a clear application in different areas of chemical theory. Poorly understood observations in electronic structure theory, the chemical reactivity of radicals and the theory of molecular conduction, in particular, turn out to have natural connections with nut graphs. A molecular graph is the framework of a π -system molecule where the edges coincide with the covalent bonds between the carbon atoms, which are represented by the vertices. The defining feature of nut molecular graphs is that all vertices carry a non-zero entry in the unique nullspace generating vector, and hence spin density is distributed across the whole framework and not in particular sites, which is the case for the general molecular graph. It is worth mentioning that for the source-and-sink-potential model [4, 5, 10] of ballistic molecular condition, among all molecular graphs of nullity one, nut graphs characterize the omni-conductors. This means that nut molecules are the only graphs of nullity one that conduct when a small bias voltage is applied across any pair of vertex (atom) contacts.

We remark that since in a core graph each vertex is a core vertex, then there is a kernel eigenvector with all entries being non-zero. Thus, there is a very natural interpretation of core graphs, usually referred to in the literature as the *zero sum rule* [6, 8]. A graph G is a core graph if there exists an assignment of values from $\mathbb{Z} \setminus \{0\}$ such that the sum of the values on the neighbourhood of any vertex v adds up to 0. Using our terminology, the above can be rephrased as in the following Proposition 1.

Proposition 1. *A graph G is a core graph if and only if its adjacency matrix has an admissible eigenvector.*

There are exactly three nut graphs on 7 vertices (shown in Figure 1) and none of smaller order [14]. The first two are planar; the third one is toroidal. There are 13 nut graphs on 8 vertices [1]. One of them, the antiprism graph A_4 , is shown in Figure 2. It is quartic (or 4-regular). One of the nine smallest cubic nut graphs is one of the two asymmetric cubic graphs on 12 vertices and is the well-known Frucht graph, shown in Figure 3.

A recent computer search carried out by Coolsaet, Fowler and Goedgebeur [2] shows that there exist no cubic nut graphs on 14 and 16 vertices. However, they discovered cubic nut graphs on 20, 22, 26 and 28 vertices.

The two principal results of this note can be stated as follows.

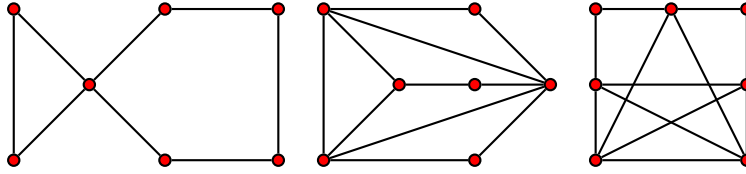
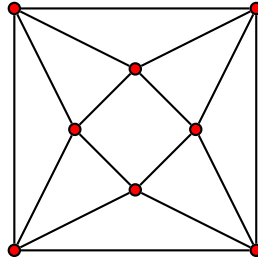


Figure 1: The three nut graphs on 7 vertices.

Figure 2: The antiprism graph A_4 on 8 vertices is the smallest quartic nut graph.

Theorem 2. *Cubic nut graphs on n vertices exist if and only if n is an even integer, $n \geq 12$ and $n \notin \{14, 16\}$.*

Theorem 3. *Quartic nut graphs on n vertices exist if and only if $n = 8, 10, 12$ or $n \geq 14$.*

These two results will be proved in Section 3. In the proof of Theorem 2 we use a “construction” so that starting from a graph G on n vertices with a vertex v of degree 3 we can generate a graph $F(G, v)$ on $n + 6$ vertices. Since this construction is due to Patrick Fowler [11, 13], we call it the *Fowler Construction*. Actually, in Section 2, we generalize it to vertices of arbitrary degree ρ in such a way that the eigenvector entries corresponding to $V(G) \setminus \{v\}$ are preserved. In general, the graph is extended by 2ρ vertices. The main result of Section 2 is that the nullity of $F(G, v)$ is the same as that of G . A direct consequence of this result that will enable us to construct an infinite family of nut graphs is that $F(G, v)$ preserves the property that G is a nut graph.

In Section 3, we first prove the existence of cubic and quartic nut graphs. We proceed to determine the forbidden orders of cubic nut graphs. Using the Fowler Construction, we prove that there is an infinite family of quartic nut graphs. The construction of this family shows that quartic nut graphs exist for all orders at least 14.

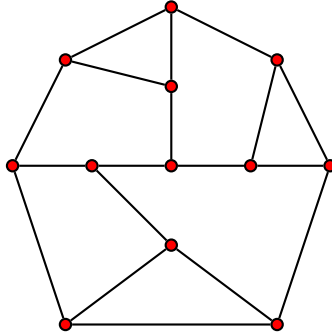


Figure 3: The Frucht graph, one of the nine smallest cubic nut graphs on 12 vertices.

2. THE FOWLER CONSTRUCTION

Let G be a graph, and v any of its vertices of degree ρ , with neighbours labelled u_1, u_2, \dots, u_ρ . We change G to produce $F(G, v)$ as follows. Add 2ρ vertices $p_1, p_2, \dots, p_\rho, q_1, q_2, \dots, q_\rho$. For each $i \in \{1, \dots, \rho\}$, remove all edges between v and u_i and insert edges between v and q_i and between each p_i and u_i . Finally, add all edges from p_i to q_j for any pair $i, j \in \{1, \dots, \rho\}, i \neq j$. The resulting graph $F(G, v)$ is called *the Fowler Construction* of G at v . This process is depicted in Figure 4.

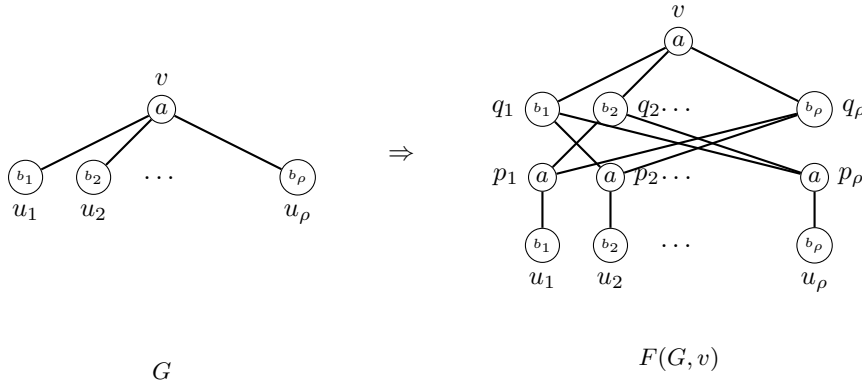


Figure 4: The Fowler Construction showing the eigenvector entries corresponding to each vertex.

From the above discussion, it is clear that the following proposition follows immediately.

Proposition 4. *If G is a ρ -regular graph then any of its Fowler constructions $F(G, v)$ is also ρ -valent.*

A simple but important lemma for the work that follows is given hereunder.

where the submatrices \mathbf{B} , \mathbf{C} and \mathbf{D} encode the adjacencies between the respective vertex-sets.

The adjacency matrix of $\mathbf{A}(F(G, v))$ can similarly be partitioned as follows:

$$\begin{array}{c|cccc|cccc|cccc}
 v & w_1 & \dots & w_{n-\rho-1} & u_1 & \dots & u_\rho & q_1 & \dots & q_\rho & p_1 & \dots & p_\rho \\
 \hline
 0 & 0 & \dots & 0 & 0 & \dots & 0 & 1 & \dots & 1 & 0 & \dots & 0 \\
 0 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 0 & & & & & & & & & & & & \\
 \hline
 0 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 0 & & & & & & & & & & & & \\
 \hline
 1 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 1 & & & & & & & & & & & & \\
 \hline
 0 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 0 & & & & & & & & & & & & \\
 \hline
 \end{array}
 \begin{array}{l}
 v \\
 w_1 \\
 \vdots \\
 w_{n-\rho-1} \\
 u_1 \\
 \vdots \\
 u_\rho \\
 q_1 \\
 \vdots \\
 q_\rho \\
 p_1 \\
 \vdots \\
 p_\rho
 \end{array}$$

where \mathbf{I} is the identity matrix and \mathbf{J} is the all-one matrix.

Elementary row and corresponding column operations which leave the rank unchanged are performed by replacing the rows and columns corresponding to v_1, \dots, v_ρ by $v_1 + q_1, \dots, v_\rho + q_\rho$, respectively, to obtain the matrix

$$\begin{array}{c|cccc|cccc|cccc}
 v & w_1 & \dots & w_{n-\rho-1} & u_1 & \dots & u_\rho & q_1 & \dots & q_\rho & p_1 & \dots & p_\rho \\
 \hline
 0 & 0 & \dots & 0 & 1 & \dots & 1 & 1 & \dots & 1 & 0 & \dots & 0 \\
 0 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 0 & & & & & & & & & & & & \\
 \hline
 1 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 1 & & & & & & & & & & & & \\
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 1 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 1 & & & & & & & & & & & & \\
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 0 & & & & & & & & & & & & \\
 \vdots & & & & & & & & & & & & \\
 0 & & & & & & & & & & & & \\
 \hline
 \end{array}
 \begin{array}{l}
 v \\
 w_1 \\
 \vdots \\
 w_{n-\rho-1} \\
 u_1 \\
 \vdots \\
 u_\rho \\
 q_1 \\
 \vdots \\
 q_\rho \\
 p_1 \\
 \vdots \\
 p_\rho
 \end{array}$$

The rank of $\mathbf{J} - \mathbf{I}$ is full. Hence, $\text{rk}(\mathbf{A}(F(G, v))) \geq \text{rk}(\mathbf{A}(G)) + 2\rho = n - 1 + 2\rho$, since the last 2ρ rows/columns are linearly independent of all the other rows/columns. Thus, $\eta(F(G, v)) \leq \eta(G)$, and by the first part of the proof, we get $\eta(F(G, v)) = \eta(G)$. \square

The result we need most is a straightforward corollary of the above theorem.

Theorem 7. *G is a nut graph if and only if its Fowler Construction $F(G, v)$ is a nut graph.*

3. THE EXISTENCE PROBLEM FOR REGULAR NUT GRAPHS

The machinery that we prepared in the previous section will be used in the following result. In the construction of $F(G, v)$, 2ρ vertices are added to G , where ρ is the degree of vertex v in G . Each of the new vertices in $F(G, v)$ acquire the degree ρ , while all other vertices retain the degree in G .

Corollary 8. *Let G be a nut graph on n vertices and let v be any of its vertices. If the degree of v is ρ , then there exists a nut graph G' on $n + 2\rho$ vertices obtained through the Fowler Construction. Moreover, if G is regular, then G' is regular.*

In the sequel, we establish the existence, or non-existence, of regular nut graphs. Before proceeding further, we recall that a **circulant matrix** is an $N \times N$ matrix $\mathbf{C} = (a_{k,j} : k, j = 1, 2, \dots, N)$ where $a_{k,j} = a_{(j-k) \bmod N}$, denoted by $\mathbf{C} = \langle a_0, a_1, \dots, a_{N-1} \rangle$. For $r \in \{0, 1, \dots, N-1\}$, the eigenvalues are given by $\lambda_r = \sum_{j=0}^{N-1} a_j \omega_r^j$, where $\omega_r = \exp(i \frac{2\pi r}{N})$ and the corresponding eigenvectors are given by $\mathbf{v}_r = (1 \ \omega_r \ \omega_r^2 \ \dots \ \omega_r^{N-1})$.

Thus, the cycle graph C_n on n vertices has eigenvalues $2 \cos \frac{2\pi r}{n}$, where $r \in \{0, 1, \dots, n-1\}$, implying that C_n is singular if and only if $n = 4k$ for $k \in \mathbb{N}$, in which case the nullity is two. This observation settles the case when $\rho = 2$, presented in the following theorem.

Theorem 9. *There are no regular nut graphs of degree two.*

The case when $\rho = 3$ is presented in Theorem 2 stated in the introduction, which we can now proceed to prove.

Proof. (Proof of Theorem 2.) For cubic graphs, n must be even. Non-existence for $n < 12$ and $n \in \{14, 16\}$ has been shown by computer search. Since a cubic nut graph exists for $n = 12$, cubic nut graphs for $n = 12 + 6 = 18$ and $n = 18 + 6 = 24$ exist as well. Using the same argument, the existence of cubic nut graphs of order n , for n divisible by 6 is guaranteed. Using the cubic nut graphs for $n = 20$ and for $n = 22$ as seeds (shown in Figure 5), the remaining cases are also covered. \square

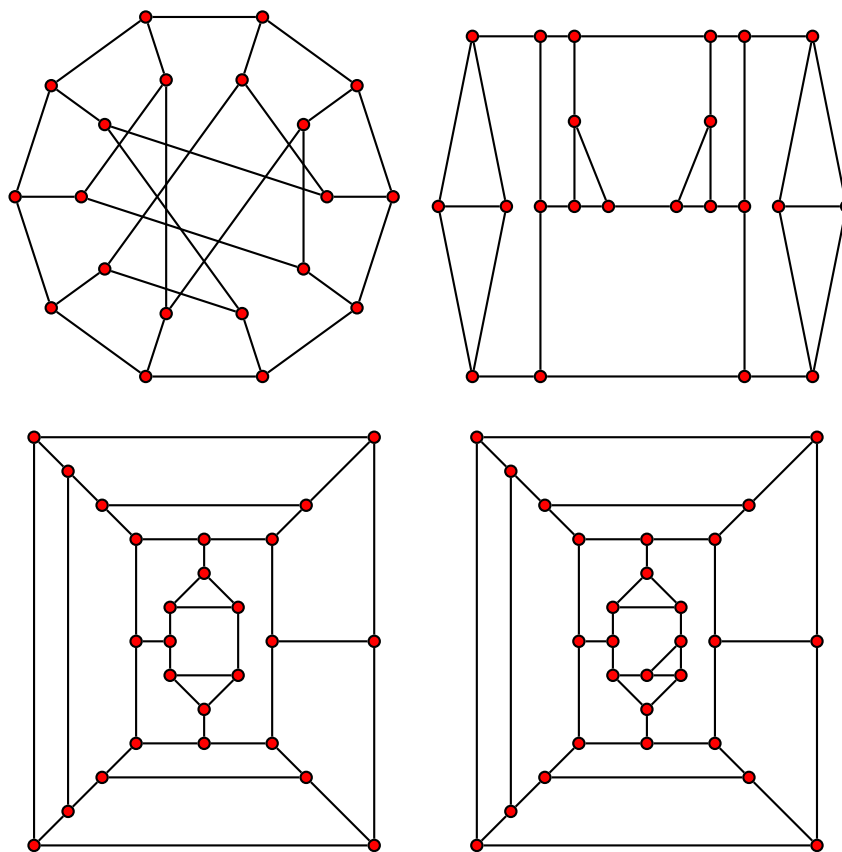


Figure 5: Cubic nut graphs of order 20, 22, 26 and 28.

We remark that a computer search was needed to verify that the graphs shown in Figure 5 are nut graphs due to the large order of these graphs. For smaller graphs, the Zero Sum Rule, long used by chemists for kernel basis calculations by hand, can be used [3]. Starting with a vertex of low degree, weights a, b, \dots are assigned to all but one neighbour, whose weight can then be determined. This is repeated for every vertex. Eventually, the number of free parameters is equal to the nullity of the graph.

The idea used in the previous proof whereby repeated Fowler constructions are used starting from a seed graph implies the next result.

Proposition 10. *If there exists a ρ -regular nut graph, then there exist infinitely many such graphs.*

We now shift our attention to the case $\rho = 4$.

Proposition 11. *The quartic antiprism graph A_n of order $2n$ is a nut graph if and only if n is not divisible by 3.*

Proof. The antiprism graph A_n is isomorphic to the circulant graph $Ci_{2n}(1, 2)$ described by the circulant matrix

$$\mathbf{C} = \langle 0 \quad 1 \quad 1 \quad \mathbf{0} \quad 0 \quad 1 \quad 1 \rangle^T,$$

where $\mathbf{0}$ is the $(2n - 6)$ -row-vector composed of zero entries.

Thus, for $r \in \{0, 1, \dots, 2n - 1\}$, $\lambda_r = \omega^r + \omega^{2r} + \omega^{(2n-2)r} + \omega^{(2n-1)r} = (\omega^r + \omega^{-r}) + (\omega^{2r} + \omega^{-2r}) = 2(2 \cos \frac{\pi r}{n} - 1)(\cos \frac{\pi r}{n} + 1)$. Hence, $\lambda_r = 0$ if and only if $\cos \frac{\pi r}{n} = \frac{1}{2}$ or $\cos \frac{\pi r}{n} = -1$, that is, if and only if $r = \pm \frac{n}{3} + 2kn$ or $r = n + 2kn$, where $k \in \mathbb{Z}$. Now, if n is divisible by 3, then $\lambda_r = 0$ if and only if $r \in \{\frac{n}{3}, n, \frac{5n}{3}\}$, whereas if n is not divisible by 3, then $\lambda_r = 0$ if and only if $r = n$. Hence in the former case, the nullity of A_n is three, whereas in the latter case, the nullity of A_n is one.

We remark that, by using the properties of circulant matrices mentioned above, it immediately follows that if the nullity is one, then the eigenvector $(1 \quad -1 \quad 1 \quad -1 \quad 1 \quad -1 \quad \dots)$ is a kernel eigenvector and thus A_n is a nut graph.

When the nullity is three, we substitute the respective values of $r \in \{\frac{n}{3}, n, \frac{5n}{3}\}$ to get three linearly independent kernel eigenvalues as follows:

$$\begin{aligned} & (1 \quad y \quad y^2 \quad -1 \quad y^4 \quad y^5 \quad \dots), \\ & (1 \quad -1 \quad 1 \quad -1 \quad 1 \quad -1 \quad \dots), \\ & (1 \quad y^5 \quad y^4 \quad -1 \quad y^2 \quad y \quad \dots), \end{aligned}$$

where $y^3 = 1$. We note that since $y + y^5 = -(y^2 + y^4) = 1$ and $y^5 - y = (y^4 - y^2) = -\sqrt{3}i$, we get the linearly independent kernel eigenvectors

$$(1) \quad \begin{aligned} & (1 \quad -1 \quad 1 \quad -1 \quad 1 \quad -1 \quad \dots), \\ & (2 \quad 1 \quad -1 \quad -2 \quad -1 \quad 1 \quad \dots), \\ & (0 \quad 1 \quad 1 \quad 0 \quad -1 \quad -1 \quad \dots), \end{aligned}$$

implying that, in this case, A_n is a core graph but not a nut graph. \square

From the proof of Proposition 11 it follows immediately that a general kernel eigenvector \mathbf{x} of the adjacency matrix \mathbf{A} of the antiprism A_n is of the form

$$(a \quad -a \quad a \quad -a \quad \dots \quad a \quad -a)^T,$$

when n is not divisible by 3, and of the form

$$(a \quad b \quad c \quad -a \quad -b \quad -c \quad \dots \quad a \quad b \quad c \quad -a \quad -b \quad -c)^T$$

otherwise. Indeed the three vectors in (1) are of the indicated form and are linearly independent.

We shall now prove the second main theorem stated in the introduction, namely Theorem 3.

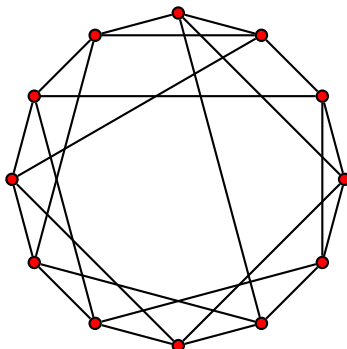


Figure 6: One of the 269 quartic nut graphs of order 12.

Proof. (Proof of Theorem 3) Starting from the antiprism graphs A_4, A_5 and A_7 implies that there exist quartic nut graphs on 8, 10 and 14 vertices, respectively. Computer search has revealed an exhaustive list of 269 quartic nut graphs on 12 vertices. This computer search was carried out using SageMath [15], which uses graph generator nauty by Brendan McKay [9]. Note that the computer search for nut graphs involves the computation of the nullity of the adjacency matrix A of a graph. Since A is integer valued, all computations can be performed using integer arithmetic and avoiding division, thereby eliminating any rounding errors. The 269 quartic nut graphs on 12 vertices are listed on [1], in the section of the “Graph meta-directory” dedicated to “Nut graphs”. One of these quartic nut graphs on 12 vertices is shown in Figure 6. Using the graphs of order 8, 10, 12 and 14 as seeds for repeated Fowler constructions takes care of all even orders at least eight.

For the odd case, an exhaustive computer search has shown that no quartic nut graphs of odd order at most 13 exist and there is only one quartic nut graph of order 15 (shown in Figure 7). Quartic nut graphs of order 17, 19 and 21 are also shown in Figure 7. Using these orders as seeds for repeated Fowler constructions proves that quartic nut graphs of odd order at least 13 exist. \square

4. AN OPEN PROBLEM

In this paper we have determined the values of n for which there exist ρ -regular nut graphs of order n for $\rho = 3, 4$. These results lead to a very natural question, namely:

Problem 12. For each degree ρ , determine the set $N(\rho)$ such that there exists a ρ -regular nut graph of order n if and only if $n \in N(\rho)$.

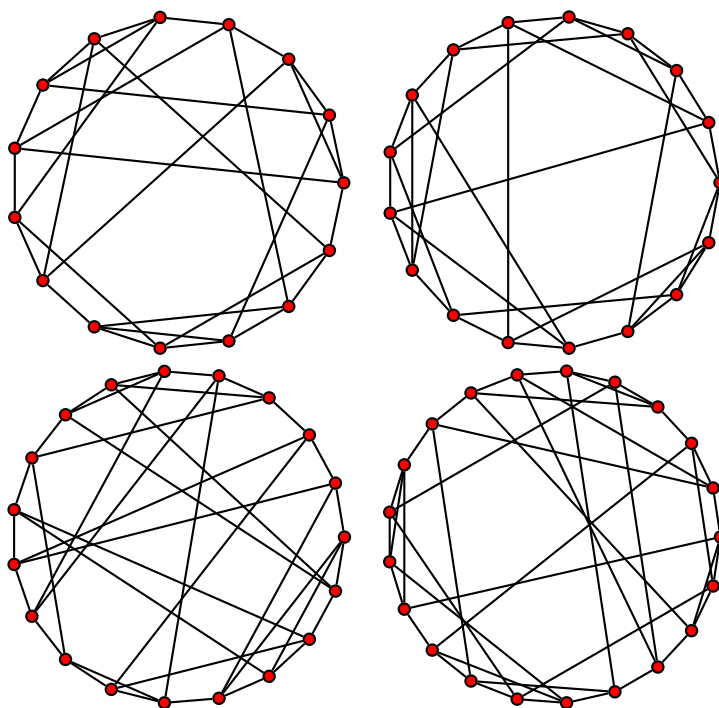


Figure 7: Quartic nut graphs of order 15, 17, 19 and 21.

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John Baptist Gauci

Department of Mathematics

Faculty of Science

University of Malta

Msida

Malta

E-mail: *john-baptist.gauci@um.edu.mt*

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Tomaž Pisanski

Department of Theoretical Computer Science, IMFM

University of Ljubljana

Ljubljana

Slovenia

&

Department of Information Sciences and Technologies

FAMNIT

University of Primorska

Koper

Slovenia

E-mail: *pisanski@upr.si***Irene Sciriha**

Department of Mathematics

Faculty of Science

University of Malta

Msida

Malta

E-mail: *irene.sciriha-aquilina@um.edu.mt*