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NULLITY OF GRAPHS: AN UPDATED SURVEY

Abstract. The nullity $\eta = \eta(G)$ of a graph G is the multiplicity of the number zero in the spectrum of G. The chemical importance of this graph-spectrum based invariant lies in the fact, that within the Hückel molecular orbital model, if $\eta(G) > 0$ for the molecular graph G, then the corresponding chemical compound is highly reactive and unstable, or nonexistent. This chapter in an updated version of the an earlier survey [B. Borovićanin, I. Gutman, *Nullity of graphs*, in: D. Cvetković, I. Gutman, Eds. *Applications of Graph Spectra*, Math. Inst., Belgrade, 2009, pp. 107–122] and outlines both the chemically relevant aspects of η (most of which were obtained in the 1970s and 1980s) and the general mathematical results on η obtained recently.

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Contents

1. Graph nullity and its chemical applications

This chapter is an updated, extended, and modified version of the survey [3] that was a part of the booklet "*Applications of Graph Spectra*". Since the completion of [3], a number of relevant results came to the authors' attention, that now are appropriately taken care of.

Let G be a graph of order n, having vertex set $V(G)$ and edge set $E(G)$. Let $A(G)$ be the adjacency matrix of G. The graph G is said to be singular (resp. non-singular) if its adjacency matrix $A(G)$ is singular (resp. non-singular). The *nullity* of G, denoted by $\eta = \eta(G)$, is the algebraic multiplicity of the number zero in the spectrum of G.[1]

In addition to its evident relevance in "pure" spectral graph theory, the nullity has a noteworthy application in chemistry. The recognition of this fact, first outlined in [8], was not only an important discovery per se, but happened to be the starting point of an unprecedented activity in theoretical and mathematical chemistry, resulting in thousands of published papers, and leading to a new field of research, nowadays referred to as *Chemical Graph Theory* [13, 19, 23, 40].

In order to explain the role of the nullity of graphs in chemistry, we need to recall a few basic facts from the quantum theory of molecules [12]. The behavior of the electrons in molecules is considered to be responsible for the majority of properties of chemical compounds. This behavior is governed by laws of quantum theory and is described by the so-called Schrödinger equation. Finding the solutions of the Schrödinger equation is one of the main tasks of quantum chemistry.

In an early stage of quantum chemistry, during the time when computers were not available, the German theoretical chemist Erich Hückel proposed an approximate method for solving the Schrödinger equation for a special (for chemistry very important) class of organic molecules, the so-called *unsaturated conjugated hydrocarbons* [28]. Nowadays, this method is known under the name *Hückel molecular orbital* (*HMO*) *theory* [5, 12, 41].

A quarter of century was needed to recognize that the mathematics on which the HMO theory is based is graph spectral theory [20, 35]. In a nutshell: The (approximate) energies $E_1, E_2, \dots$ that the electrons may possess are related to the

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[1] The symbol η for nullity was first used by I. G. in his correspondence with Dragoš Cvetković, which eventually resulted in the paper [8]. The choice for η was fully arbitrary. Yet, nowadays this symbol is used by the majority of scholars. Another notation for nullity is n_0.

eigenvalues $\lambda_1, \lambda_2, \ldots$ of a so-called "*molecular graph*" as

$$E_j = \alpha + \beta\,\lambda_j,\ j = 1, 2, \ldots, n$$

where α and β are certain constants; for more detail see [19, 23]. Because $\beta < 0$, if the graph eigenvalues are labelled in the usual non-increasing manner as

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$$

then E_1 is the lowest energy level, E_2 is the second–lowest energy level, etc.

Each energy level in a molecule can be occupied by at most two electrons. Usually, the total number of electrons to which HMO theory is applied is equal to n, and n is most frequently an even number. Usually, $E_{n/2+1} < E_{n/2}$ or, what is the same, $\lambda_{n/2} > \lambda_{n/2+1}$.

If so, then in order to achieve the lowest-energy state of the underlying molecule, it has to possess two (= the maximum possible number) of electrons with energy E_1, two (= the maximum possible number) of electrons with energy $E_2, \ldots$ and two (= the maximum possible number) of electrons with energy $E_{n/2}$. This will result in a stable arrangement of electrons; in the language of theoretical chemistry, the molecule will have a "*closed–shell electron configuration*".

If, however, $E_{n/2+1} = E_{n/2}$, then a total of four electrons could fill the two "degenerate" energy levels. Because the number of available electrons is only two, an irregular and unstable arrangement of electrons will result; in the language of theoretical chemistry, the molecule will have an "*open–shell electron configuration*".

The above described filling of the energy levels with electrons is in quantum chemistry referred to as the *Aufbau principle* (a word originating from German language). Details on this matter can be found elsewhere [33].

Molecules with an open-shell electron configuration are known to be highly reactive and in many cases are simply not capable of existence.

We now show how the nullity of the molecular graph is related to the closed/open-shell character of the underlying molecule.

Long before the above-sketched graph-spectral connections were envisaged, some important results in HMO theory were discovered. One of these is the so-called "*Pairing theorem*" [6]. According to it, for the majority of unsaturated conjugated hydrocarbons, the eigenvalues of the molecular graph are "paired", so that

$$\lambda_j = -\lambda_{n-j+1} \tag{1}$$

holds for all $j = 1, 2, \ldots, n$. In the language of HMO theory, the hydrocarbons to which the Pairing theorem applies are referred to as "*alternant*". With today's knowledge it is straightforward to recognize that an unsaturated conjugated hydrocarbon is "alternant" if and only if its molecular graph is bipartite. Indeed, the relation (1) is a well known spectral property of bipartite graphs [7].

An immediate consequence of the Pairing theorem is that a molecular graph with even number of vertices has either nullity zero (in which case $\lambda_{n/2} > 0 > \lambda_{n/2+1}$), or its nullity is an even positive integer (in which case $\lambda_{n/2} = \lambda_{n/2+1} = 0$). In HMO theory this means the following [32]:

- If the nullity of the molecular graph of an alternant unsaturated conjugated hydrocarbon is zero, then the respective molecule is predicted to have a stable, closed-shell, electron configuration and the respective compound predicted to have a low chemical reactivity and to be chemically stable.
- If the nullity of the molecular graph of an alternant unsaturated conjugated hydrocarbon is greater than zero, then the respective molecule is predicted to have an unstable, open-shell, electron configuration and the respective compound is expected to be highly reactive, chemically unstable and often not capable of existence.

Thus, the nullity of a molecular graph has a far-reaching inference on the expected stability of unsaturated conjugated hydrocarbons. This prediction of HMO theory has been experimentally verified in numerous cases. The most drastic such case is the fact that whereas there exist more than a thousand benzenoid hydrocarbons whose molecular graphs have nullity zero, not a single such hydrocarbon is nowadays known, whose molecular graph would have a non-zero nullity.

2. Elementary properties of nullity

Let $r(A(G))$ be the rank of $A(G)$. Clearly, $\eta(G) = n - r(A(G))$. The rank of a graph G is the rank of its adjacency matrix $A(G)$, denoted by $r(G)$. Then, $\eta(G) = n - r(G)$. Each of $\eta(G)$ and $r(G)$ determines the other (once n is specified).

Lemma 1. *Let G be a graph on n vertices. Then $\eta(G) = n$ if and only if G is a graph without edges* (*empty graph*).

For some classes of graphs the spectrum is known and thereby so is the nullity η. We list some examples.

Lemma 2. [7, 8, 36] (i) *The spectrum of the complete graph K_n consists of two distinct eigenvalues $n-1$ and -1, with multiplicities 1 and $n-1$, respectively. Thus, $\eta(K_n) = 1$ for $n = 1$ and $\eta(K_n) = 0$ for $n > 1$.*

(ii) *The eigenvalues of the path P_n are of the form $2\cos\frac{\pi r}{n+1}$, $r = 1, 2, \ldots, n$. According to this,*

$$\eta(P_n) = \begin{cases} 1, & \text{if } n \text{ is odd} \\ 0, & \text{if } n \text{ is even.} \end{cases}$$

(iii) *The eigenvalues of the cycle C_n are $2\cos\frac{2\pi r}{n}$, $r = 0, 1, \ldots, n-1$. Therefore,*

$$\eta(C_n) = \begin{cases} 2, & \text{if } n \equiv 0 \pmod 4, \\ 0, & \text{otherwise.} \end{cases}$$

Lemma 3. (i) *Let H be an induced subgraph of G. Then $r(H) \leqslant r(G)$.*

(ii) *Let $G = G_1 \cup G_2 \cup \cdots \cup G_t$, where $G_1, G_2, \ldots, G_t$ are connected components of G. Then $r(G) = \sum_{i=1}^{t} r(G_i)$, i.e., $\eta(G) = \sum_{i=1}^{t} \eta(G_i)$.*

In the sequel we give some simple inequalities concerning $\eta(G)$ that are direct consequences of Lemmas 2 and 3.

Recall that the path P is a graph with $V(P) = \{v_1, v_2, \ldots, v_k\}$ and $E(P) = \{v_1v_2, v_2v_3, \ldots, v_{k-1}v_k\}$, where the vertices $v_1, v_2, \ldots, v_k$ are all distinct. We say that P is a path from v_1 to v_k, or a (v_1, v_k)-path. It can be denoted by P_k, where k is its *length*. The *distance* $d(x, y)$ in G of two vertices x, y is the length of a shortest (x, y)-path in G; if no such path exists, we define $d(x, y)$ to be infinite. The greatest distance between any two vertices in G is the *diameter* of G, denoted by $\operatorname{diam}(G)$.

Lemma 4. [11] *Let G be a simple graph on n vertices, and let the complete graph K_p be a subgraph of G, where $2 \leqslant p \leqslant n$. Then $\eta(G) \leqslant n - p$.*

A *clique* of a simple graph G is a complete subgraph of G. A clique S is maximum if G has no clique S' with $|V(S')| > |V(S)|$. The number of vertices in a maximum clique of G is called the clique number of G and is denoted by $\omega(G)$.

The following inequality is clear from the previous result.

Corollary 1. [11] *Let G be a simple non-empty graph on n vertices. Then $\eta(G) + \omega(G) \leqslant n$.*

From Lemma 3 and Lemma 2(iii) we arrive at:

Lemma 5. [11] *Let G be a simple graph on n vertices and let the cycle C_p be an induced subgraph of G, where $3 \leqslant p \leqslant n$. Then*

$$\eta(G) \leqslant \begin{cases} n - p + 2, & \text{if } p \equiv 0 \pmod 4, \\ n - p, & \text{otherwise.} \end{cases}$$

The length of the shortest cycle in a graph G is the *girth* of G, denoted by $\operatorname{gir}(G)$. A relation between $\eta(G)$ and $\operatorname{gir}(G)$ is given by:

Corollary 2. [11] *If G is a simple graph on n vertices, and G has at least one cycle, then*

$$\eta(G) \leqslant \begin{cases} n - \operatorname{gir}(G) + 2, & \text{if } \operatorname{gir}(G) \equiv 0 \pmod 4, \\ n - \operatorname{gir}(G), & \text{otherwise.} \end{cases}$$

If we bear in mind Lemma 2(ii) and Lemma 3, the following result is obvious.

Lemma 6. [11] *Let G be a simple graph on n vertices and let the path P_k be an induced subgraph of G, where $2 \leqslant k \leqslant n$. Then*

$$\eta(G) \leqslant \begin{cases} n - k + 1, & \text{if } k \text{ is odd}, \\ n - k, & \text{otherwise.} \end{cases}$$

Corollary 3. [11] *Suppose that x and y are two vertices in G and that there exists an (x, y)-path in G. Then*

$$\eta(G) \leqslant \begin{cases} n - d(x, y), & \text{if } d(x, y) \text{ is even}, \\ n - d(x, y) - 1, & \text{otherwise.} \end{cases}$$

Corollary 4. [11] *Suppose G is a simple connected graph on n vertices. Then*

$$\eta(G) \leqslant \begin{cases} n - \operatorname{diam}(G), & \textit{if } \operatorname{diam}(G) \textit{ is even}, \\ n - \operatorname{diam}(G) - 1, & \textit{otherwise}. \end{cases}$$

3. Relations between nullity and graph structure

In the general case, the problem of finding connections between the structure of a graph G and its nullity seems to be difficult. For example, $\eta(G)$ is not determined by the set of vertex degrees of G (see Fig. 1)

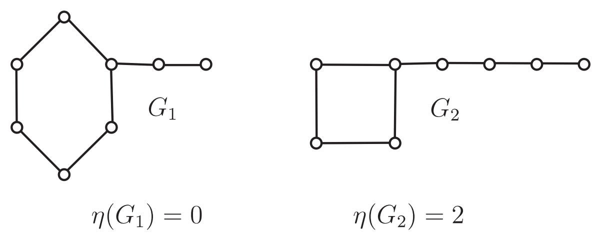

FIGURE 1

In what follows we consider mostly bipartite graphs, although some of the theorems stated below can be extended to non-bipartite graphs (see [9]).

Before proceeding we need some definitions. A matching of G is a collection of independent (mutually non-adjacent) edges of G. A maximum matching is a matching with the maximum possible number of edges. The size of a maximum matching of G, i.e., the maximum number of independent edges of G, is denoted by $m = m(G)$.

Denote by $P_G(\lambda)$ the characteristic polynomial of G. Let

$$P_G(\lambda) = |\lambda I - A| = \lambda^n + a_1 \lambda^{n-1} + \cdots + a_n$$

Then [7]

$$a_i = \sum_U (-1)^{p(U)}\, 2^{c(U)} \quad (i = 1, 2, \ldots, n), \tag{2}$$

where the sum is over all subgraphs U of G consisting of disjoint edges and cycles and having exactly i vertices (called "basic figures"). If U is such a subgraph, then $p(U)$ is the number of its components, of which $c(U)$ components are cycles.

For some special classes of bipartite graphs it is possible to find relatively easily the relation between the structure of G and $\eta(G)$. The problem is solved for trees by the following theorem [8].

Theorem 1. [8] *Let T be a tree on $n \geqslant 1$ vertices and let m be the size of its maximum matching. Then its nullity is equal to $\eta(T) = n - 2m$.*

This theorem is an immediate consequence of the statement concerning the coefficients of the characteristic polynomial of the adjacency matrix of a tree (which can be easily deduced from eq. (2)).

Theorem 1 is a special case of one more general theorem that will be formulate in the following.

Theorem 2. [10] *If a bipartite graph G with $n \geqslant 1$ vertices does not contain any cycle of length $4s$ ($s = 1, 2, \ldots$), then $\eta(G) = n - 2m$, where m is the size of its maximum matching.*

Proof. According to the assumption, a bipartite graph G does not contain any basic figure (with an arbitrary number of vertices) with cycles of lengths $4s$ ($s = 1, 2, \ldots$). For a particular basic figure U it holds that $p(U)$ is equal to the total number of cycles of lengths $4s + 2$ ($s = 1, 2, \ldots$) and of graphs K_2. Let $4t_i + 2$ ($i = 1, 2, \ldots, p(U)$) be the numbers of vertices contained in these cycles or graphs K_2. If U is a basic figure with $2q$ ($2q \leqslant n$) vertices we get

$$\sum_{i=1}^{p(U)} (4t_i + 2) = 2q \qquad \text{and} \qquad 2\sum_{i=1}^{p(U)} t_i + p(U) = q.$$

Hence, $p(U) \equiv q \pmod 2$ and all terms (summands) in the expression for the coefficient a_{2q} of the characteristic polynomial have the same sign. Because of this, $a_{2q} \neq 0$ if and only if there is at least one basic figure with $2q$ vertices. Since m is the size of maximum matching of G the statement of the theorem now follows immediately. □

The formula $\eta(G) = n - 2m$ was shown to hold also for all benzenoid graphs (which may contain cycles of the size $4s$) [22]. As a curiosity, we mention that almost twenty years later, Fajtlowicz (using his famous computer system *Grafitty*) conjectured the precisely same result. Although being informed about the existence of the proof of this "conjecture" [22], Sachs and John produced an independent paper on this "discovery" and (together with Fajtlowicz) published it [15].

The problem concerning the relation between the structure of a bipartite graph and its nullity can be reduced to another problem which can be solved in certain special cases. The vertices of a bipartite graph may be numbered so that the adjacency matrix has the following form:

$$A = \begin{pmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{pmatrix}.$$

The matrix B is the "incidence matrix" between the two sets X and Y of vertices of the bipartite graph $G = (X, Y, U)$ (U is the set of edges).

Theorem 3. [32] *For the bipartite graph G with n vertices and incidence matrix B, $\eta(G) = n - 2\,r(B)$, where $r(B)$ is the rank of B.*

Since for $G = (X, Y, U)$, we have $r(B) \leqslant \min(|X|, |Y|)$ and Theorem 3 yields the following:

Corollary 5. [8] *$\eta(G) \geqslant \max(|X|, |Y|) - \min(|X|, |Y|)$.*

If the number of vertices is odd, then $|X| \neq |Y|$ and $\eta(G) > 0$. Thus a necessary condition to have no zeros in the spectrum of a bipartite graph is that the number of vertices is even (what is also in accordance with Theorem 2).

The following three theorems ([8], [10]) enable, in special cases, the reduction of the problem of determining $\eta(G)$ for some graphs to the same problem for simpler graphs.

Theorem 4. [8] *Let $G_1 = (X_1, Y_1, U_1)$ and $G_2 = (X_2, Y_2, U_2)$, where $|X_1| = n_1$, $|Y_1| = n_2$, $n_1 \leqslant n_2$, and $\eta(G_1) = n_2 - n_1$. If the graph G is obtained from G_1 and G_2 by joining (any) vertices from X_1 to vertices in Y_2 (or X_2), then the relation $\eta(G) = \eta(G_1) + \eta(G_2)$ holds.*

Proof. Let B_1, B_2, B be the incidence matrices of the graphs G_1, G_2, G. We may assume that

$$B = \begin{pmatrix} B_1 & M \\ \mathbf{0} & B_2 \end{pmatrix}$$

where B_1 is an $n_1 \times n_2$ matrix, $\mathbf{0}$ is a zero matrix, and M is an arbitrary matrix with entries from the set $\{0, 1\}$.

From $\eta(G_1) = n_2 - n_1$ we have $r(B_1) = n_1$. Thus B_1 contains n_1 linearly independent columns. Consequently, each column of the matrix M can be expressed as a linear combination of the aforementioned columns of B_1. Hence, the matrix B can be reduced by operations not changing the rank to the form

$$B' = \begin{pmatrix} B_1 & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix}.$$

whence $r(B) = r(B_1) + r(B_2)$. Theorem 3 gives $\eta(G) = \eta(G_1) + \eta(G_2)$. □

Corollary 6. [8] *If the bipartite graph G contains a pendent vertex, and if the induced subgraph H of G is obtained by deleting this vertex together with the vertex adjacent to it, then $\eta(G) = \eta(H)$.*

This corollary of Theorem 4 is proved in the following way: we take the complete graph with two vertices as G_1 and the graph H as G_2.

Corollary 7. [8] *Let G_1 and G_2 be bipartite graphs. If $\eta(G_1) = 0$, and if the graph G is obtained by joining an arbitrary vertex of G_1 by an edge to an arbitrary vertex of G_2, then $\eta(G) = \eta(G_2)$.*

Example 1. See Fig. 2.

Theorem 5. [10] *A path with four vertices of degree 2 in a bipartite graph G can be replaced by an edge* (see Fig. 3) *without changing the value of $\eta(G)$.*

Theorem 6. [10] *Two vertices and the four edges of a cycle of length 4, which are positioned in a bipartite graph G as shown in Fig. 4, can be removed without changing the value of $\eta(G)$.*

Remark. Corollary 6 of Theorem 4, as well as Theorems 5 and 6 hold also in the case when the graph G is non-bipartite [9].

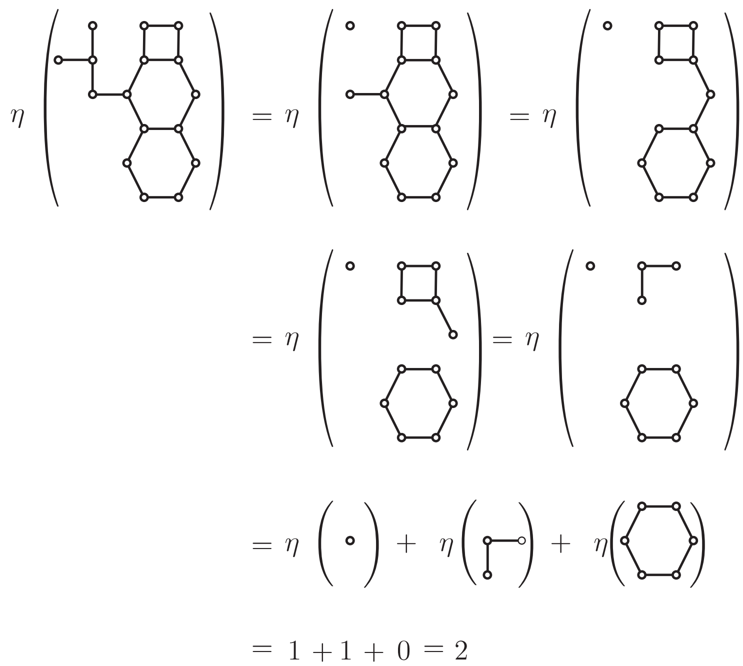

FIGURE 2

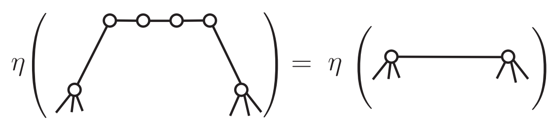

FIGURE 3

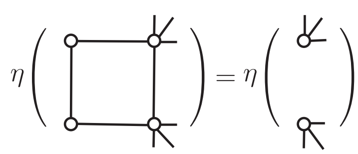

FIGURE 4

Example 2. See Fig. 5.

4. Graphs with maximum nullity

If we bear in mind Lemmas 1 and 4, it is obvious that $0 \leqslant \eta(G) \leqslant n-2$ if G is a simple non-empty graph on n vertices.

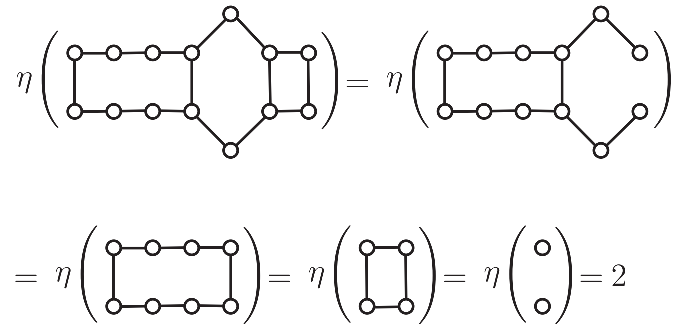

FIGURE 5

A natural problem is to characterize the extremal graphs whose nullities attain the upper bound $n-2$ and the second upper bound $n-3$.

Theorem 7. [11] *Suppose that G is a simple graph on n vertices and G has no isolated vertices. Then*

(i) $\eta(G) = n-2$ *if and only if G is isomorphic to a complete bipartite graph K_{n_1,n_2}, where $n_1+n_2=n$, $n_1,n_2>0$.*

(ii) $\eta(G) = n-3$ *if and only if G is isomorphic to a complete tripartite graph K_{n_1,n_2,n_3}, where $n_1+n_2+n_3=n$, $n_1,n_2,n_3>0$.*

Several results on the graphs satisfying $\eta = n-t$ for some fixed value t, $t>3$ were obtained. Before stating them we give some necessary definitions.

Let $\mathcal{G}_n$ be the set of all n-vertex graphs, and let $[0,n] = \{0,1,\dots,n\}$. A subset N of $[0,n]$ is said to be the *nullity set* of $\mathcal{G}_n$ provided that for any $k \in N$, there exists at least one graph $G \in \mathcal{G}_n$ such that $\eta(G)=k$.

A connected simple graph on n vertices is said to be *unicyclic* if it has n edges and *bicyclic* if it has $n+1$ edges. Denote by $\mathcal{U}_n$ and $\mathcal{B}_n$ the set of all n-vertex unicyclic and bicyclic graphs, respectively. For convenience, let $\mathcal{T}_n$ denote the set of n-vertex trees.

First we determine all graphs with pendent vertices that attain the third-maximum nullity $n-4$ and the fourth-maximum nullity $n-5$, using the results of Li [30]. Then we proceed recursively, as in [30], to construct all graphs having pendent vertices with $\eta(G)>0$.

Let G_1^* be an n-vertex graph obtained from a complete bipartite graph $K_{r,s}$ and a star $K_{1,t}$ by identifying a vertex of $K_{r,s}$ with the center of $K_{1,t}$, where $r,s,t \geqslant 1$ and $r+s+t=n$. Let $K_{1,l,m}$ be a complete tripartite graph with the maximum-degree vertex v, where $l,m>0$. Then let G_2 be the n-vertex graph created from $K_{1,l,m}$ and a star $K_{1,p}$ by identifying the vertex v with the center of $K_{1,p}$, where $l,m,p \geqslant 1$ and $l+m+p+1=n$.

Theorem 8. [30] *Let G be a connected n-vertex graph with pendent vertices. Then $\eta(G) = n-4$ if and only if G is isomorphic to the graph G_1^* or G_2^*, where G_1^* is* *depicted in Fig. 6, and G_2^* is a connected spanning subgraph of G_2 (see Fig. 6) and contains $K_{l,m}$ as its subgraph.*

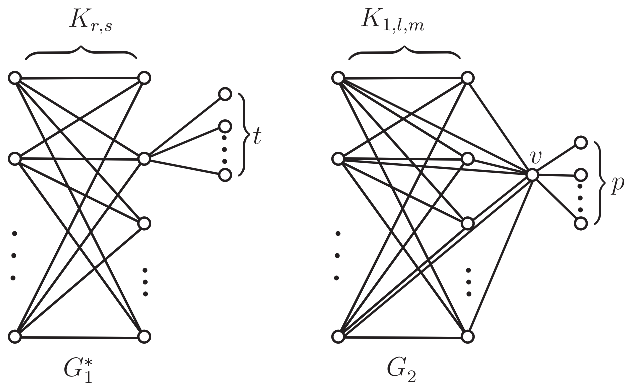

FIGURE 6

Let G_3^* be an n-vertex graph obtained from a complete tripartite graph $K_{r,s,t}$ and a star $K_{1,q}$ by identifying a vertex of $K_{r,s,t}$ with the center of $K_{1,q}$, where $r, s, t, q > 0$ and $r + s + t + q = n$. Let $K_{1,l,m,p}$ be a tetrapartite graph with the maximum-degree vertex v, where $l, m, p > 0$. Then let G_4 be the n-vertex graph created from $K_{1,l,m,p}$ and a star $K_{1,d}$ by identifying the vertex v and the center of $K_{1,d}$, where $l, m, p, d > 0$ and $l + m + p + d + 1 = n$.

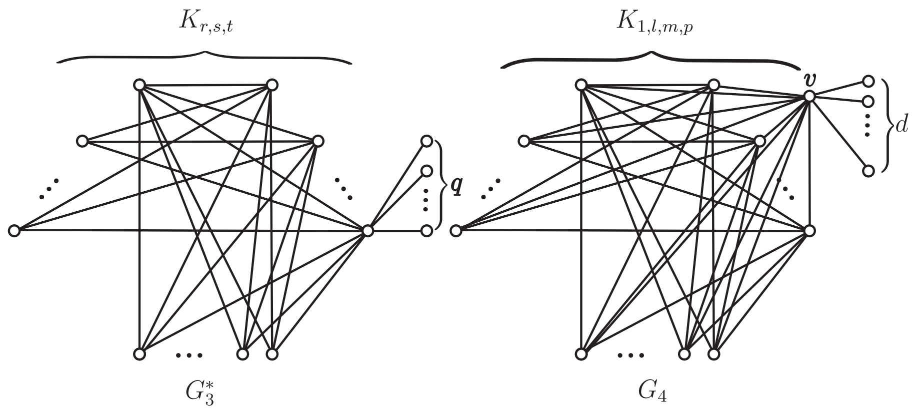

FIGURE 7

Theorem 9. [30] *Let G be a connected graph on n vertices and assume that G has no isolated vertex. Then $\eta(G) = n-5$ if and only if G is isomorphic to the graph G_3^* or G_4^*, where G_3^* is depicted in Fig. 7, G_4^* is a connected spanning subgraph of G_4 (see e.g. Fig. 7) and contains $K_{l,m,p}$ as its subgraph.*

Using similar reasoning as in Theorems 8 and 9, we may proceed recursively to construct all n-vertex graphs having pendent vertices with $\eta(G) = n-6$, $n-7$, $n-8$, and so on. In that way, all n-vertex graphs with pendent vertices satisfying $\eta(G) > 0$ can be determined [30]. Recently, also graphs with pendent trees were examined with regard to their nullity [18].

In the sequel we formulate some results on the extremal nullity of trees, unicyclic and bicyclic graphs. We also give the characterization of their nullity sets.

For an n-vertex tree, if it is a complete bipartite graph, then the tree should be the star. Since any complete tripartite graph is cyclic, there does not exist a tree that is a complete tripartite graph. Therefore, the following result is a direct consequence of Theorems 7, 8, and 9.

Theorem 10. [14, 30] *Let $\mathcal{T}_n$ be the set of all n-vertex trees.*

(i) *Let $T \in \mathcal{T}_n$. Then $\eta(T) \leqslant n-2$, and the equality holds if and only if $T \cong S_n$* [14].

(ii) *Let $T \in \mathcal{T}_n \setminus \{S_n\}$. Then $\eta(T) \leqslant n-4$, and the equality holds if and only if $T \cong T_1$ or $T \cong T_2$, where T_1 and T_2 are depicted in Fig.* 8 [30].

(iii) *Let $T \in \mathcal{T}_n \setminus \{S_n, T_1, T_2\}$. Then $\eta(T) \leqslant n-6$, and the equality holds if and only if $T \cong T_3$ or $T \cong T_4$ or $T \cong T_5$, where trees T_3, T_4, T_5 are shown in Fig.* 8 [30].

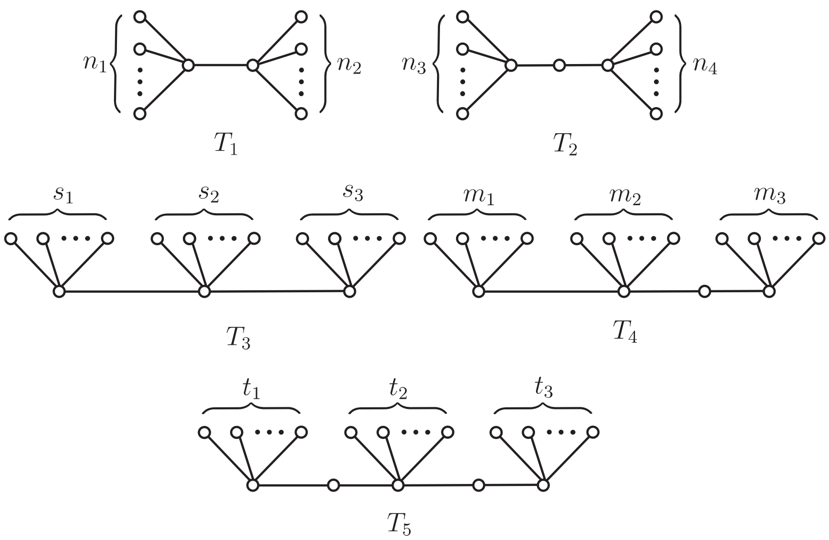

FIGURE 8

Just as in Theorem 10, we can use graphs in $\mathcal{T}_n$ (see [30]) whose nullity is $n-6$ to determine n-vertex trees whose nullity is $n-8$, and so on. This implies:

Corollary 8. [30] *The nullity set of $\mathcal{T}_n$ is $\{0, 2, 4, \ldots, n-4, n-2\}$ if n is even and $\{1, 3, 5, \ldots, n-4, n-2\}$, otherwise.*

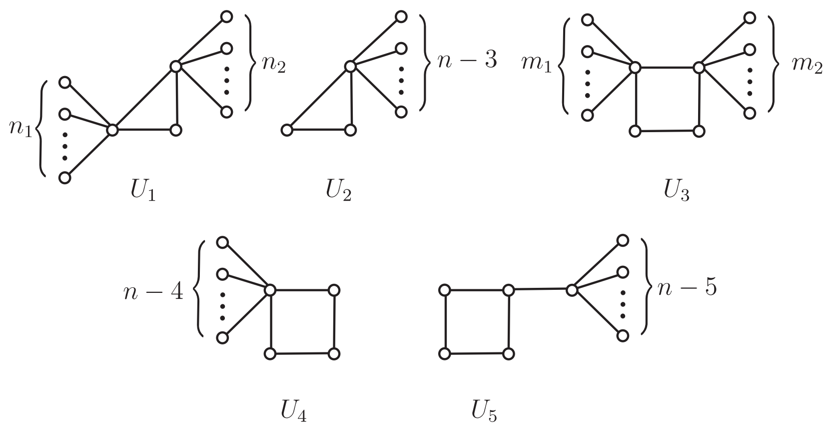

FIGURE 9

As already mentioned, for the cycle C_n, if $n \equiv 0 \pmod 4$, then $\eta(C_n) = 2$ and $\eta(C_n) = 0$, otherwise. Therefore, unicyclic graphs with maximum nullity must contain pendent vertices. On the other hand, the cycle C_4 is the only cycle which is also a complete bipartite graph and the cycle C_3 is the only cycle which is also a complete tripartite graph. So, for the unicyclic graphs with maximum nullity Tan and Liu obtained:

Theorem 11. [39] *Let $U \in \mathcal{U}_n$ $(n \geqslant 5)$. Then $\eta(U) \leqslant n-4$ and the equality holds if and only if G is isomorphic to some of the graphs U_1, U_2, U_3, U_4 and U_5, depicted in Fig.* 9.

The nullity set of unicyclic graphs was also determined in [39].

Theorem 12. [39] *The nullity set of $\mathcal{U}_n$ $(n \geqslant 5)$ is $[0, n-4]$.*

Recently, Guo, Yan, and Yeh [21] have somewhat extended the results of [39] by characterizing unicyclic graphs for which $\eta = n - 5$. They also proved:

Theorem 13. [21] *Let $G \in \mathcal{U}_n$. Let m be the size of a maximum matching of G. Then $\eta(G) = n - 2m - 1$ or $\eta(G) = n - 2m$ or $\eta(G) = n - 2m + 2$.*

In [21] the structure of the graphs belonging to each of the three cases in Theorem 13 was fully determined.

In [39] the characterization of unicyclic graphs for which $\eta = 0$ remained as an open problem. In [21] the following was shown:

Theorem 14. *Let $G \in \mathcal{U}_n$ and let C_ℓ be the unique cycle of G. Then $\eta(G) = 0$ holds if and only if either G has a unique perfect matching, or ℓ is odd and $G - C_\ell$ has a perfect matching, or $\ell \not\equiv 0 \pmod 4$ and G has two perfect matchings.*

In the set of bicyclic graphs, the graph $K_{2,3}$ is the only complete bipartite graph and the graph $K_4 - e$ is the only complete tripartite graph [26, 29]. Thus, the following results are proved.

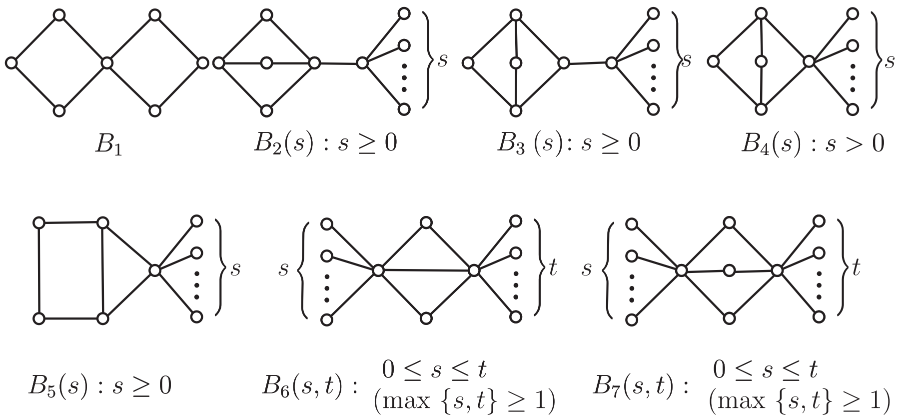

FIGURE 10

Theorem 15. [26, 29] *Let $B \in \mathcal{B}_n$. Then*

(i) *$\eta(B) = n - 2$ if and only if $B \cong K_{2,3}$.*
(ii) *$\eta(B) = n - 3$ if and only if $B \cong K_4 - e$.*
(iii) *If $B \in \mathcal{B}_n \setminus \{K_{2,3}, K_4 - e\}$, then $\eta(B) \leqslant n - 4$ and the equality holds if and only if $B \cong B_i$ $(1 \leqslant i \leqslant 7)$* (Fig. 10)

Theorem 16. [26, 29] *The nullity set of $\mathcal{B}_n$ is $[0, n-2]$.*

From previous considerations it is clear that the problem of finding trees with maximum nullity is easily solved. In the sequel we are concerned with a related problem: namely, determining the greatest nullity among n-vertex trees in which no vertex has degree greater than a fixed value Δ [17].

Let Δ be a positive integer. Denote by $\mathcal{T}(n, \Delta)$ the set of all n-vertex trees in which all vertex degrees are less than or equal to Δ. Furthermore, let $\mathcal{T}(\Delta) = \bigcup_{n \geqslant 1} \mathcal{T}(n, \Delta)$.

For $\Delta = 1$ and $n \geqslant 3$, $\mathcal{T}(n, \Delta) = \emptyset$. For $\Delta = 2$ and $n \geqslant 3$, each set $\mathcal{T}(n, \Delta)$ consists of a single element (the n-vertex path P_n for which $\eta(P_n) \leqslant 1$). Therefore in what follows we assume that $\Delta \geqslant 3$.

Theorem 17. [17] *For all $n \geqslant 1$ and $\Delta \geqslant 3$, if $T \in \mathcal{T}(n, \Delta)$, then $\eta(T) \leqslant n - 2\lceil (n-1)/\Delta \rceil$. For all $n \geqslant 1$ and $\Delta \geqslant 3$ there exist trees $T \in \mathcal{T}(n, \Delta)$ such that $\eta(T) = n - 2\lceil (n-1)/\Delta \rceil$.*

Let $\mathcal{T}(n, \Delta, \max)$ be the set of trees from $\mathcal{T}(n, \Delta)$ with maximum nullity (equal to $n - 2\lceil (n-1)/\Delta \rceil$).

In [17] a method for constructing the trees in $\mathcal{T}(n, \Delta, max)$ was given, and it is conjectured that these trees are all of maximum nullity. Li and Chang [31] gave a counter-example, showing that there exist additional trees with maximum nullity. Furthermore, they slightly modified way in which the elements of $\mathcal{T}(n, \Delta, max)$ are constructed.

Before presenting the Li–Chang method, we need some preparation.

An edge belonging to a matching of a graph G is said to cover its two end vertices. A vertex is said to be perfectly covered (PC) if it is covered in all maximum matchings of G. Obviously, any vertex adjacent to a pendent vertex is a PC-vertex, and there is at most one vertex between any consecutive PC-vertices. However, there may exist PC-vertices that are not adjacent to pendent vertices.

A subset of $\mathcal{T}(n, \Delta, \max)$, denoted by $\mathcal{T}_1^*(n, \Delta, \max)$ is constructed as follows. For $n = 1, 2, \ldots, \Delta$, the unique element of $\mathcal{T}_1^*(n, \Delta, \max)$ is the n-vertex star. For $n = k\Delta + i$, $k \geqslant 1$, $i = 1, 2, \ldots, \Delta$, any tree in $\mathcal{T}_1^*(n, \Delta, \max)$ is obtained from tree $T' \in \mathcal{T}_1^*(n - \Delta, \Delta, \max) \cup \mathcal{T}_2^*(n - \Delta, \Delta, \max)$ and a copy of a Δ-vertex star, by joining one vertex of T' with degree less than Δ to the center of S_Δ, where $\mathcal{T}_2^*(n - \Delta, \Delta, \max)$ is obtained by moving (one-by-one) some pendent vertices of $T \in \mathcal{T}_1^*(n - \Delta, \Delta, \max)$ to some other PC-vertices, taking care that

(i) the vertex degrees do not exceed Δ, and that

(ii) in each step the vertex to which a pendent vertex is added is PC.

Theorem 18. [31] $\mathcal{T}(n, \Delta, \max) = \mathcal{T}_1^*(n, \Delta, \max) \cup \mathcal{T}_2^*(n, \Delta, \max)$.

A result analogous to Theorem 17 has recently been proved for bipartite graphs:

Theorem 19. [34] *Let G be a bipartite graph with $n \geqslant 1$ vertices, e edges and maximum vertex degree Δ. If G does not have as subgraph any cycle whose size is divisible by 4, then $\eta(G) \leqslant n - 2\lceil e/\Delta \rceil$.*

For bipartite graphs Fan and Qian [16] obtained the following results. Let Bip_n be the set of all bipartite graphs on n vertices.

Theorem 20. [16] *The nullity set of* Bip_n *is* $\{n - 2k \mid k = 0, 1, 2, \ldots, \lfloor n/2 \rfloor\}$.

In order to formulate the next two theorems, we need to define the concepts of *extended path* and *extended cycle*.

Let for $n \geqslant 2$, $P_n := v_1 v_2 \cdots v_n$ be a path on vertices $v_1, v_2, \ldots, v_n$ with edges $(v_i, v_{i+1}$ for $i = 1, 2, \ldots, n-1$. Let O_p denote the p-vertex graph without edges, an empty graph. Replace each vertex v_i of P_n by an empty graph O_{p_i} for $i = 1, 2, \ldots, n$, and add edges between each vertex of O_{p_i} and each of $O_{p_{i+1}}$ for $i = 1, 2, \ldots, n-1$. The graph thus obtained is of order $N = p_1 + p_2 + \cdots + p_n$ and will be referred to as an *extended path* of length n. In an analogous manner we construct an *extended cycle* of length n, $n \geqslant 3$, by additionally joining all vertices of O_{p_1} with all vertices of O_{p_n}.

At this point we note that the nullity of an extended path of length n, $n \geqslant 2$, and of order N is equal to $N - n$ if n is even, and is equal to $N - n + 1$ if n is odd [16].

Theorem 21. [16] *Let $G \in \mathrm{Bip}_n$, $n \geqslant 4$. Then $\eta(G) = n - 4$ if and only if G is isomorphic to a graph H to which possibly some isolated vertices are added, where H is either the union of two extended paths of length* 2*, or an extended path of length* 4*, or an extended path of length* 5.

Theorem 22. [16] *Let $G \in \mathrm{Bip}_n$, $n \geqslant 6$. Then $\eta(G) = n - 6$ if and only if G is isomorphic to a graph H to which possibly some isolated vertices are added, where*

H is either the union of three extended paths of length 2, or an extended cycle of length 6, or an extended cycle of length 8, and in any of these graphs the number of all extended vertices (i.e., the p_i-values) are mutually equal.

Finally, we mention another family of graphs where the nullity problem has been solved [25]. It is the class of line graphs of trees.

We first observe that the nullity of line graphs may assume any positive integer value. A trivial example for this is $L(pK_2)$, whose nullity is p (see Fig. 11).

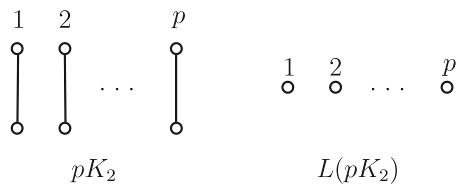

FIGURE 11

If we restrict ourselves to connected graphs then the nullity of the line graph may still be any positive integer. For instance [25], for the graph G_r depicted in Fig. 12, $\eta(L(G_r)) = r + 1$.

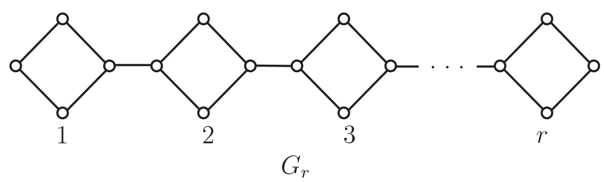

FIGURE 12

With the line graphs of trees the situation is different:

Theorem 23. [25] *If T is a tree, then $L(T)$ is either non-singular or has nullity one.*

Remark. It is easy to find examples of trees with $\eta(L(T))=0$ and with $\eta(L(T))=1$. For instance, $\eta(L(P_n)) = 0$ and $\eta(L(P_n)) = 1$ for, respectively, odd and even value of n.

More results on graphs whose nullity is one can be found in the papers [37, 38].

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