Chapter 19 Nullity of Graphs

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Abstract The nullity of a graph is defined as the multiplicity of the eigenvalue zero of graph *G* which is named the nullity of *G* denoted by $\eta(G)$. In this chapter we investigate the nullity of some family of graphs.

19.1 Introduction

Let G = (V, E) be a graph and $e \in E(G)$. Then denoted by $G \setminus e$ is the subgraph of G obtained by removing the edge e from G. Denoted by $G \setminus \{v_1, \ldots, v_k\}$ means a graph obtained by removing the vertices v_1, \ldots, v_k from G and all edges incident to any of them.

The adjacency matrix A(G) of graph G with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ is the $n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i and v_j are adjacent and 0, otherwise. The characteristic polynomial of graph G is

$$\chi_G(\lambda) = \chi_\lambda(G) = \det(A(G) - \lambda I),$$

The roots of the characteristic polynomial are the eigenvalues of graph *G* and form the spectrum of this graph. The number of zero eigenvalues in the spectrum of the graph *G* is called the nullity of G which is denoted by $\eta(G)$. Suppose r(A(G)) is the rank of A(G); it is a well-known fact that $\eta(G) = n - r(A(G))$.

A null graph is a graph in which all vertices are isolated. In other words, a graph has no edges, only vertices called the null graph. It is clear that $\eta(G) = n$ if and only if *G* is a null graph; see Cvetković et al. (1980).

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Main Results 19.2

In this section, we study the properties of graph nullity with applications in chemistry. Throughout this chapter, all notations are standard and mainly taken from Biggs (1993) and Cvetković and Gutman (2009). Throughout this chapter, all notations are standard and mainly taken from Cvetković et al. (1975), Godsil and McKay (1978), Biggs (1993), Li and Shiu (2007) and Cvetković and Gutman (2009).

Theorem 19.2.1 Suppose that G is a simple graph on n vertices and $n \ge 2$. Then $\eta(G) = n - 2$ if and only if A(G) is permutation similar to matrix $O_{n1:n1} \bigoplus O_{n2:n2} \bigoplus O_{k:k}$, where $n_1 + n_2 + k = n$, n_1 ; $n_2 > 0$, and $k \ge 0$.

Theorem 19.2.2 (Cheng and Liu 2007) Suppose that G is a simple graph on *n* vertices. Then n(G) = n - 3 if and only if A(G) is permutation similar to matrix $O_{n1:n1} \bigoplus O_{n2:n2} \bigoplus O_{n3:n3} \bigoplus O_{k:k}$, where $n_1 + n_2 + n_3 + k = n$, $n_1; n_2; n_3 > 0$ and k > 0.

Lemma 19.2.3 (Cvetković et al. 1980)

- (i) The adjacency matrix of the complete graph K_n , $A(K_n)$ has 2 distinct eigenvalues n - 1, -1 with multiplicities 1, n - 1, respectively, where n > 1.
- (ii) The eigenvalues of C_n are $\lambda_r = \frac{2 \cos 2r}{n}$, where $r = 0, \ldots, n-1$. (iii) The eigenvalues of P_n are $\lambda_r = \frac{2 \cos 2r}{n+1}$, where $r = 1, 2, \ldots, n$.

Lemma 19.2.4

- (i) Let *H* be an induced subgraph of *G*. Then r(H) < r(G).
- (ii) Let $G = G_1 + G_2$, then $r(G) = r(G_1) + r(G_2)$, i.e., $\eta(G) = \eta(G_1) + \eta(G_2)$.

Proposition 19.2.5 Let $= G_1 \cup G_2 \cup \ldots \cup G_t$, where G_1, G_2, \ldots, G_t are connected components of G. Then

$$\eta(G) = \sum_{i=1}^t \eta(G_i).$$

Proposition 19.2.6 (Cheng and Liu 2007) Let G be a simple graph on n vertices and K_p be a subgraph of G, where $2 \le p \le n$. Then $\eta(G) \le n - p$.

A clique of a simple graph G is a subset S of V(G) such that G[S] is complete. A clique S is maximum if G has no clique S'with |S'| > |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 resulted from Proposition 19.2.6.

Corollary 19.2.7 (Cheng and Liu 2007)

- (i) Let G be a simple graph on n vertices and G is not isomorphic to nK_1 . Then $\eta(G) + \omega(G) \le n$.
- (ii) Let G be a simple graph on n vertices and let C_p be an induced subgraph of G, where $3 \le p \le n$. Then

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

The length of the shortest cycle in a graph G is the girth of G. denoted by gir(G).A relation between gir(G) and $\eta(G)$ is as follows:

If G is simple graph on n vertices and G has at least one cycle, then

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

Corollary 19.2.8 (Cheng and Liu 2007) Suppose x and y are two vertices in G and there exists an(x; y)- path in G. Then

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

Corollary 19.2.9 (Cheng and Liu 2007) Suppose G is simple connected graph on n vertices. Then

$$\eta(G) \leq \begin{cases} n - \operatorname{diam}(G) & \text{if } \operatorname{diam}(G) \text{ is even}; \\ n - \operatorname{diam}(G) - 1; & \text{otherwise.} \end{cases}$$

Proposition 19.2.10 Denote by $\chi_G(\lambda)$ the characteristic polynomial of *G*. Let $\chi_G(\lambda) = |\lambda I - A| = \lambda_n + a_1 \lambda_{n-1} + \ldots + a_n$. Then

$$a_i = \sum_U (-1)^{p(U)} 2^{c(U)} (i = 1, 2, ..., n),$$
(19.1)

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.

Example 19.2.11 In Fig. 19.1, the graph G and its basic figures H_1 , H_2 , and H_3 are shown.

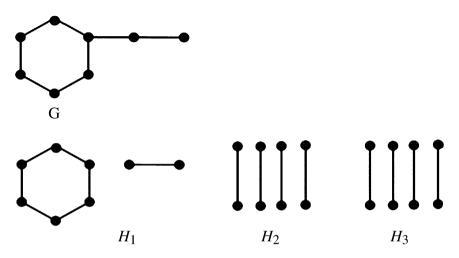


Fig. 19.1 Graph G and its basic figures H_1 , H_2 , and H_3

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

Theorem 19.2.12 (Cvetković and Gutman 1972; Li et al. 2007) Let *T* be a tree on $n \ge 1$ 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 with the coefficients of the characteristic polynomial of the adjacency matrix of a tree (which can be easily deduced from Eq. (19.1)). Theorem 19.2.12 is a special case of one more general theorem that will be formulated in the following.

Recall that a set M of edges of G is a matching if every vertex of G is incident with at most one edge in M; it is a perfect matching if every vertex of G is incident with exactly one edge in M. 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).

Theorem 19.2.13 (Cvetković et al. 1972) If a bipartite graph *G* with $n \ge 1$ vertices does not contain any cycle of length 4s (s = 1, 2, ...), then $\eta(G) = n - 2m$, where *m* is the size of its maximum matching.

Theorem 19.2.14 (Longuet–Higgins 1950) For the bipartite graph *G* with *n* vertices and incidence matrix, $\eta(G) = n - 2r(B)$, where r(B) is the rank of *B*.

Since for G = (X, Y, U), we have $r(B) \le \min(|X|, |Y|)$ and Theorem 19.2.14 yields the following:

Corollary 19.2.15 (Cvetković and Gutman 1972) $\eta(G) \ge \max(|X|, |Y|) - \min(|X|, |Y|)$.

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

Theorem 19.2.16 (Cvetković and Gutman 1972) Let $G_1 = (X_1, Y_1, U_1)$ and $G_2 = (X_2, Y_2, U_2)$, where $|X_1| = n_1, |Y_1| = n_2, n_1 \le n_2$, 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.

Corollary 19.2.17 (Cvetković et al. 1972) 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

$$\eta(G) = \eta(H)$$

Corollary 19.2.18 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 $\eta(G) = \eta(G_2)$.

Theorem 19.2.19 (Cvetković et al. 1972)

- (i) A path with four vertices of degree 2 in a bipartite graph G can be replaced by an edge without changing the value of $\eta(G)$.
- (ii) Two vertices and the four edges of a cycle of length 4, which are positioned in a bipartite graph *G*, can be removed without changing the value of $\eta(G)$.

Theorem 19.2.20 (Gutman and Sciriha 2001) If T is a tree, then L(T) is either nonsingular or has nullity one.

Proposition 19.2.21 Let $H = K_{p,q}$ be a complete bipartite graph on p + q = n vertices. Then

$$\chi_{\lambda}(H) = \frac{n\lambda + 2pq}{\lambda^2 - pq}.$$

Definition 19.2.22 Let *H* be a labeled graph on *n* vertices. Let *G* be a sequence of *n* rooted graphs *G*, G_1, \ldots, G_n . Then by H(G) we denote the graph obtained by identifying the root of G_i with the *i*-th vertex of *H*. We call H(G) the *rooted product* of *H* by *G*.

Figure 19.2 illustrates this construction with H the path on three vertices and G consisting of three copies of the rooted path on two vertices.

Definition 19.2.23 Given a labeled graph *H* on *n* vertices and a sequence *G* of *n* rooted graphs, we define the matrix $A_{\lambda}(H, G)$ as follows:

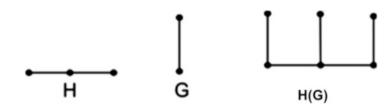


Fig. 19.2 Rooted product P_3 with P_2

$$A_{\lambda}(H, G) = (a_{ij})$$

Where

$$a_{ij} = \begin{cases} G_i(\lambda) &, & i = j \\ -h_{ij}G_i^{\prime(\lambda)} &, & i \neq j \end{cases}$$

and $A(H) = (h_{ij})$ is the adjacency matrix of H.

If, for example, *H* and *G* are represented in Fig. 19.2, then $A_{\lambda}(H, G) = (a_{ij})$ is the matrix

$$\begin{pmatrix} \lambda^2-1 & -\lambda & 0 \\ -\lambda & \lambda^2-1 & -\lambda \\ 0 & -\lambda & \lambda^2-1 \end{pmatrix}.$$

Lemma 19.2.24 (Ghorbani 2014) Let *K* and *L* be rooted graphs, and let $K \cdot L$ denote the graph obtained by identifying the roots of *K* and *L*. Then

$$\chi_{K \bullet L}(\lambda) = \chi_K(\lambda)\chi_{L'}(\lambda) + \chi_{K'}(\lambda)\chi_L(\lambda) - \lambda\chi_{K'}(\lambda)\chi_{L'}(\lambda).$$

Proposition 19.2.25 (Guo et al. 2009) Let v be any vertex (which does not need to be a cut point) of a graph G with order at least 2. Then

$$\eta(G) - 1 \le \eta(G - v) \le \eta(G) + 1.$$

Theorem 19.2.26 (Guo et al. 2009) Let v be a cut point of a graph G of order n and $G_1, G_2, ..., G_s$ be all components of G - v. If there exists a component, say G_1 , among $G_1, G_2, ..., G_s$ such that $\eta(G_1) = \eta(G_1 + v) + 1$, then

$$\eta(G) = \eta(G - v) - 1 = \sum_{i=1}^{s} \eta(G_i) - 1.$$

Theorem 19.2.27 (Guo et al. 2009) Let v be a cut-point of a graph G of order n and G_1 be a component of G - v. If $\eta(G_1) = \eta(G_1 + v) - 1$, then

$$\eta(G) = \eta(G_1) + \eta(G - G_1).$$

Theorem 19.2.28 (Guo et al. 2009) Suppose *G* and *H* are two graphs with eigenvalues λ_i $(1 \le i \le n)$ and μ_j $(1 \le j \le m)$. Then the eigenvalues of Cartesian product $G \times H$ are $\lambda_i + \mu_j$.

As a corollary of Theorem 19.2.28, we compute the nullity of the hypercube $H_n = K_2 \times \underbrace{\dots}_{n \text{ times}} \times K_2$. It is a well-known fact that the spectrum of K_n is as follows:

$$\operatorname{Spec}(K_n) = \begin{pmatrix} -1 & n-1 \\ n-1 & 1 \end{pmatrix}.$$

So, the eigenvalues of H are ± 1 with multiplicity 1. According to Theorem 19.2.28,

$$\operatorname{Spec}(K_2 \times K_2) = \begin{pmatrix} -2 & 0 & 2\\ 1 & 2 & 1 \end{pmatrix}.$$

By continuing this method, one can see that the spectrum of $K_2 \times \cdots \times K_2$ is:

$$Spec(K_{2} \times \dots \times K_{2}) = \begin{cases} \begin{pmatrix} -n & \cdots & -2 & 0 & 2 & \cdots & n \\ 1 & \cdots & \binom{n}{(n-2)/2} & \binom{n}{n/2} & \binom{n}{(n+2)/2} & \cdots & 1 \end{pmatrix} & 2|n \\ \begin{pmatrix} -n & 2-n & \cdots & -1 & 1 & \cdots & n-2 & n \\ 1 & \binom{n}{1} & \cdots & \binom{n}{(n-2)/2} & \binom{n}{n/2} & \cdots & \binom{n}{n-1} & 1 \end{pmatrix} & 2|n \end{cases}$$

This implies the nullity of K_n is as follows:

$$\eta(K_n) = \begin{cases} \binom{n}{n/2} & 2|n\\ 0 & 2|n \end{cases}.$$

Example 19.2.29 Consider graph G_r , with *r* hexagons depicted in Fig. 19.3a. By using Theorem 19.2.19, it is easy to see that $\eta(G_r) = \eta(G_{r-1})$ (r = 1, 2, ...). By induction on *r*, it is clear that $\eta(G_r) = 0$. Now consider graph H_r (Fig. 19.3b). Since this graph has a pendent vertex, so by Corollary 19.2.15, $\eta(H_r) = \eta(T_{r-1})$. Again

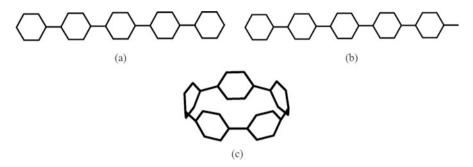


Fig. 19.3 (a) Graph G_r , (b). Graph H_r , (c). Graph T_{r-1}

use Theorem 19.2.27 and then we have $\eta(T_{r-1}) = \eta(H_{r-1})$. By continuing this method we see that $\eta(H_r) = \eta(H_1).H_1$, has a pendent vertex joined to a hexagon. Theorem 19.2.28 implies that $\eta(H_1) = \eta(P_5)$. Corollary 19.2.18 results that $\eta(H_r) = \eta(P_5) = 1$.

Here, by using Theorem 19.2.13, we compute the nullity of triangular benzenoid graph G[n], depicted in Fig. 19.4. The maximum matching of G[n] is depicted in Fig. 19.5. In other words, to obtain the maximum matching at first we color the boundary edges, they are exactly $3 \times n$ edges. The number of colored vertical edges in the k-th row is k - 1. Hence, the number of colored vertical edges is $1 + 2 + \ldots + n - 2 = (n - 1) (n - 2) / 2$. By summation of these values, one can see that the number of colored edges are $3n + (n - 1) (n - 2)/2 = (n^2 + 3n + 2)/2$ which is equal to the size of maximum matching. This graph has $n^2 + 4n + 1$ vertex, $3(n^2 + 3n)/2$ edges and by using Theorem 19.2.13, $\eta(G[n]) = n^2 + 4n + 1 - (n^2 + 3n + 2) = n - 1$, thus we proved the following Theorem.

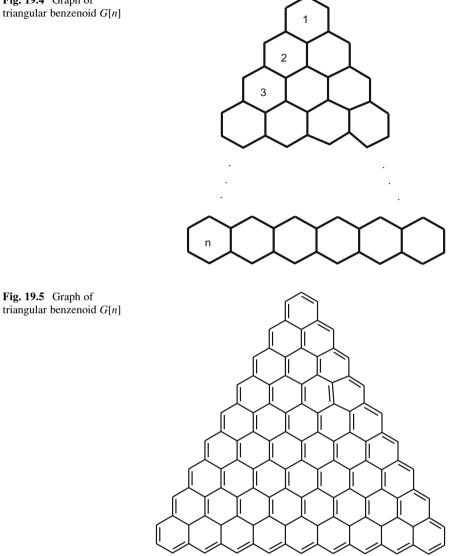
Theorem 19.2.30 $\eta(G[n]) = n - 1$.

Definition 19.2.31 Let G_1 be a graph containing a vertex u, and let G_2 be a graph of order n that is disjoint from G_1 . For $1 \le k \le n$, the k-joining graph of G_1 and G_2 with respect to u, denoted by $G_1(u) \bigotimes^k G_2$, is obtained from $G_1 \cup G_2$ by joining u and arbitrary k vertices of G_2 . Note that in above definition, the graph $G_1(u) \bigotimes^k G_2$ is indefinite in some extent, and there are $\binom{n}{k}$ such graphs. In addition, if G_1 is a tree, then G_1 is called a pendant tree of $\ldots G_1(u) \bigotimes^k G_2$ and $G_1(u) \bigotimes^k G_2$ is said a graph with pendant tree. Let $= G_1 \bigoplus G_2 \bigoplus \ldots \bigoplus G_t$. Then $\eta(G) = \sum_{i=1}^n \eta(G_i)$.

Lemma 19.2.32 (Guo et al. 2009) Let T be a tree containing a vertex v. The following are equivalent:

v is mismatched in *T*.
 μ(*T* - *v*) = μ(*T*);.
 η(*T* - *v*) = η(*T*) - 1.

Fig. 19.4 Graph of triangular benzenoid G[n]



Lemma 19.2.33 (Guo et al. 2009) If v is a quasi-pendant vertex of a tree T, then v is matched in T.

Lemma 19.2.34 (Guo et al. 2009) If v is a mismatched vertex of a tree T, then for any neighbor u of v, u is matched in T and is also matched in the component of T - v that contains u.

19.2.1 Nullity of Graphs with Pendant Trees

Theorem 19.2.1.1 (Guo et al. 2009) Let *T* be a tree with a matched vertex *u* and let *G* be a graph of order *n*. Then for each integer $k(1 \le k \le n)$,

$$\eta \left(T(u) \bigotimes G \right) = \eta(T) + \eta(G).$$

Corollary 19.2.1.2 (Guo et al. 2009) Let *T* be a *PM*-tree and *G* be a graph of order *n*. Then for each integer *k* ($1 \le k \le n$) and for every vertex $u \in T$, $\eta(T(u) \bigotimes^k G) = \eta(G)$.

Theorem 19.2.1.3 Let *T* be a tree with a mismatched vertex *u* and let *G* be a graph of order *n*. Then for each integer $k(1 \le k \le n)$,

$$\eta\left(T(u)\bigotimes^{k}G\right) = \eta(T-u) + \eta(G+u) = \eta(T) + \eta(G+u) - 1.$$

In the following Theorem denoted by H means a reduced form of bicyclic graphs. In other words, in H all paths of length 4 are replaced by an edge.

Theorem 19.2.1.4 Let G be a bicyclic graph as depicted in Fig. 19.6, then $\eta(G) = \begin{cases} ||T|| - 2\mu(T) + \alpha v \text{ is matched} \\ ||T|| - 2\mu(T) - 1 + \beta v \text{ is mismatched } \end{cases}$

where

$$\alpha = \begin{cases} 0 & 2|n,m\\ 1 & 2|n,2|m & \text{and} & \beta = \begin{cases} 0H \cong G_1, G_8\\ 3H \cong G_2\\ 1H \cong G_3, G_4, G_5, G_6, G_7, G_9 \end{cases}$$

and the number of vertices of graph G is denoted by ||G||.

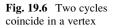
Proof According to Lemma 19.2.32, we should to consider two cases:

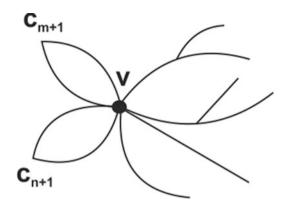
• Case 1: v is matched and

$$\alpha = \begin{cases} 0 & 2|n,m \\ 1 & 2\nmid n, 2|m \\ 2 & 2|n, 2\nmid m \end{cases}$$

In this case one can see that $G \cong T(v) \bigcirc^4 P_n \cup P_m$ and so,

$$\eta(G) = \eta(T) + \eta(P_n) + \eta(P_m) = ||T|| - 2\mu(T) + \alpha.$$





• *Case 2*: *v* is mismatched:

In this case one can see that

$$\eta(T(v) \odot^4 P_n \cup P_m) = \eta(T - v) + \eta(P_n \cup P_m + v) = ||T|| - 2\mu(T) + \eta(P_n \cup P_m + v) - 1 = ||T|| - 2\mu(T) + \eta(H) - 1 = ||T|| - 2\mu(T) + \eta(H) - 1.$$

Let $\beta = \eta(H)$. By Corollary 19.2.17 we have to compute just the nullity of graphs G_1, \ldots, G_6 reported in Table 19.1 and this completes the proof.

Suppose *G* is a unicyclic graph with *n* vertices and the length of this cycle be *l*. If *G* is a cycle C_l or a cycle C_l with pendent edges at some or all vertices of C_l , we call *G* a canonical unicyclic graph. If *G* is not canonical, *G* contains at least one pendent star H_1 such that $G_1^* = G - H_1$ is also a unicyclic graph. We call the procedure of obtaining $G - H_1$ from *G* a "deleting operator." With repeated applications of the "deleting operators," then a canonical unicyclic graph, denoted by G^* , is obtained from *G*.

Lemma 19.2.1.5 (Guo et al. 2009) Suppose *G* is a unicyclic graph with *n* vertices and the length of the cycle in *G* is *l*. Let G^* be the graph defined above. Then η $(G) = n - 2\nu(G) - 1$ if $G^* = C_l$ and *l* is odd, $\eta(G) = n - 2\nu(G) + 2$ if $G^* = C_l$ and $l = 0 \pmod{4}$, and $\eta(G) = n - 2\nu(G)$ otherwise.

Denoted by $C_{n,l,k}$ means a cycle graph with *n* vertices, *k* pendent stars, and *l* pendent vertices. We have the following Theorem.

Theorem 19.2.1.6

$$\eta(C_{n,l,k}) = \|C_{n,l,k}\| - 2k - 2\omega + \begin{cases} -1 & 2|n \\ 2 & 4|n \\ 0 & \text{otherwise} \end{cases},$$

where $\omega = \max\{[n/2], l\}$.

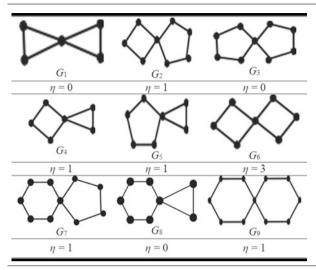


Table 19.1 The nullity of graphs G_1, \ldots, G_9

Proof By Corollary 19.2.17, one can remove the pendent vertices from *G* without changing in nullity of *G*. In other words, $\eta(G) = \eta(C_{l,n,k})$. According to Lemma 19.2.33, it is easy to see that

$$\eta(G) = (n_1 - 2) + \dots + (n_k - 2) + \eta(C_{n,l}).$$

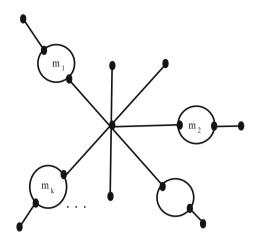
Let $\omega = \max\{ [\frac{n}{2}], l\}$, then $\eta(C_{n,l}) = n + l - 2\omega + \begin{cases} -1 & 2|n \\ 2 & 4|n \\ 0 & \text{otherwise} \end{cases}$.

This implies that

$$\eta(G) = \sum_{i=1}^{k} n_i - 2k + n + l - 2\omega + \begin{cases} -1 & 2|n \\ 2 & 4|n \\ 0 & \text{otherwise} \end{cases}$$
$$= \|G\| - 2k - 2\omega + \begin{cases} -1 & 2|n \\ 2 & 4|n \\ 0 & \text{otherwise} \end{cases}.$$

Suppose C_i is a cycle and put $C_i^* = C_i + u_i$ (a vertex u_i is added to cycle C_i). Now join to k vertices of a star graph on n vertices the graph C_i^* . We denote this graph by $S_{n,k,l}$ in which l = n - k (as depicted in Fig. 19.7). We also recall a cycle whose length is an odd number by odd cycle. In the following Theorem we can obtain a bound for the nullity of $S_{n,k,l}$.

Fig. 19.7 The graph $S_{n,k,l}$



Theorem 19.2.1.7 Let *r* be the number of odd cycles in $S_{n,k,l}$. Then

$$1 + l + 2r \le \eta(S_{n,k,l}) \le 1 + l + 4r$$

Proof Let n_i be the number of vertices of C_i^* . Remove the pendent vertices attached to *r* odd cycles. By Corollary 19.2.17 the nullity of resulted graph is the same as *G*. On the other hand, the resulted graph is bipartite and so by using Theorem 19.2.13, it is enough to compute its maximum matching as follows:

$$\mu(G) = \sum_{i=1}^{r} [n_i/2] + \sum_{i=r+1}^{k} ([n_i/2] - 1).$$

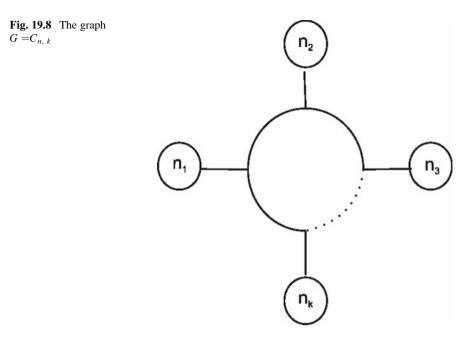
Since for every integer number $x, x - 1 \le [x] \le x$ and $\sum_{i=1}^{k} n_i + l + 1 = n$, then

$$\frac{1}{2}\sum_{i=1}^{k} n_i - \sum_{i=1}^{r} 2 \le \mu(G) \le \frac{1}{2}\sum_{i=1}^{k} n_i - \sum_{i=1}^{r} 1$$

$$\Rightarrow \frac{1}{2}(n-l-1) - r \le \mu(G) \le \frac{1}{2}(n-l-1) - r$$

$$\Rightarrow 1 + l + 2r \le \eta(G) \le 1 + l + 4r.$$

Let C_n be a cycle on *n* vertices, we recall that $\eta(C_n) = 0$ if $n \not\equiv 0 \pmod{4}$ and $\eta(C_n) = 2$ otherwise. Consider the graph *G* depicted in Fig. 19.8. If the central cycle has *n* vertices and the number of cycles of length 4s (s = 1, 2, ...) of *G* is *m*, then we show this graph by $C_{n,m}$ and the nullity of this graph is as follows.



Theorem 19.2.1.8 Let *n* is an even number, then

$$\eta(C_{m,n}) = n + 2m - 1 + \alpha,$$

where,

$$\alpha = \begin{cases} 2 & 4 \mid n \\ 0 & \text{otherwise} \end{cases}$$

Proof By Theorem 19.2.13 one can remove all cycles of length $s, s \neq 0 \pmod{4}$ and by Theorem 19.2.13, one can replace all 4s (s = 1, 2, ...) with C_4 . Thus the resulted graph is composed of a central cycle with *n* vertices together *m* cycles C_4 attached to it. Again using Lemma 19.2.3 (*vii*) results a canonical cycle graph $C_{n,m}$ together with *m* isolated vertices. Since the final graph is bipartite, apply Lemma 19.2.4 and the proof is completed.

19.2.2 Unicyclic Graphs with a Given Nullity

In this section, we deal with connected unicyclic graphs. Let *G* be a unicyclic graph and let *C* be the unique cycle of *G*. For each vertex $v \in C$, denote by $G\{v\}$ an induced

connected subgraph of *G* with maximum possible of vertices, which contains the vertex *v* and contains no other vertices of *C*. One can find that $G\{v\}$ is a tree and *G* is obtained by identifying the vertex *v* of $G\{v\}$ with the vertex *v* on *C* for all vertices $v \in C$. The unicyclic graph *G* is said to be of *Type I* if there exists a vertex *v* on the cycle such that v is matched in $G\{v\}$; otherwise, *G* is said to be of *Type II*.

Theorem 19.2.2.1 (Guo et al. 2009) Let *G* be a unicyclic graph and let *C* be the cycle of *G*. If *G* is of *Type I* and let $v \in C$ be matched in $G\{v\}$, then $\eta(G) = \eta(G\{v\}) + \eta(G - G\{v\})$. If *G* is of *Type II*, then $\eta(G) = \eta(G - C) + \eta(C)$.

Corollary 19.2.2. (Guo et al. 2009) Let *G* be a unicyclic graph with $\eta(G) = k$, and let C_l be the cycle of *G*. If *G* is of *Type I* and let $v \in C_l$ be matched in $G\{v\}$, then $\eta(G\{v\}) + \eta(G - G\{v\}) = k$. If *G* is of *Type II* and $l = 0 \pmod{4}$, then $\eta(G - C_l) = k - 2$; otherwise, $\eta(G - C_l) = k$.

Lemma 19.2.2.3 (Guo et al. 2009) Suppose *G* is a unicyclic graph with *n* vertices and the length *l* of the cycle C_l in *G* is odd. Then $\eta(G) = n - 2\mu(G) - 1$ if $\mu(G) = \frac{l-1}{2} + \mu(G - C_l)$ and $\eta(G) = n - 2\mu(G)$ otherwise.

Lemma 19.2.2.4 (Guo et al. 2009) Suppose *G* is a unicyclic graph with *n* vertices and the length *l* of the cycle C_l in *G* is even. If $\mu(G) \neq \frac{l}{2} + \mu(G - C_l)$ or $\mu(G) = \frac{l}{2} + \mu(G - C_l)$ and $l = 2 \pmod{4}$, then $\eta(G) = n - 2\mu(G)$.

Lemma 19.2.2.5 (Guo et al. 2009) Suppose *G* is a unicyclic graph with *n* vertices and cycle C_l of length $l=0 \pmod{4}$, and $\mu(G) = \frac{l}{2} + \mu(G - C_l)$. Let E_1 be the set of edges of *G* between C_l and $G - C_l$ and E_2 be a matching of *G* with $\mu(G)$ edges. Then $\eta(G) = n - 2\mu(G) + 2$ if $E_1 \cap M = \emptyset$ for all $M \in E_2$, and $\eta(G) = n - 2\mu(G)$ otherwise.

Theorem 19.2.2.6 Suppose G is a unicyclic graph with n vertices and the cycle in G is C_l . Let E_1 be the set of edges of G between C_l and $G - C_l$ and E_2 the set of matchings of G with $\mu(G)$ edges. Then

- 1. $\eta(G) = n 2\mu(G) 1$ if $\mu(G) = \frac{l-1}{2} + \mu(G C_l)$. 2. $\eta(G) = n - 2\mu(G) + 2$ if *G* satisfies properties: $\mu(G) = \frac{l}{2} + \mu(G - C_l)$ 2, $l = 0 \pmod{4}$, and $E_1 \cap M = \emptyset$ for all $M \in E_2$.
- 3. $\eta(G) = n 2\mu(G)$ otherwise.

Lemma 19.2.2.7 (Guo et al. 2009) Suppose *H* is a pendant star of a graph *G*. Then $\mu(G) = \mu(G_0) + 1$, where $G_0 = G - H$; see Fig. 19.9.

Suppose G is a unicyclic graph with n vertices. Let the length of the cycle in G be l. If G is a cycle C_l or a cycle C_l with pendant edges at some or all vertices of C_l , we call G a canonical unicyclic graph. If G is not canonical, G contains at least one pendant star H_1 such that $G_1^* = G - H_1$ is also a unicyclic graph. We call the procedure of obtaining $G - H_1$ from G a "deleting operator." With repeated

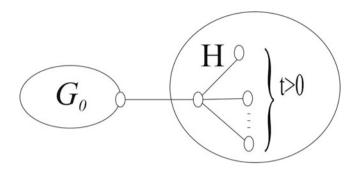


Fig. 19.9 A graph G and a pendant star H of G, where $G_0 = G - H$

applications of the "deleting operators," then a canonical unicyclic graph, denoted by G^* , is obtained from G.

Theorem 19.2.2.8 Suppose *G* is a unicyclic graph with *n* vertices and *G*^{*} is the graph defined above. Then $\eta(G) = n - 2\mu(G) - 1$ if and only if $|\eta(G^*)| = |V(G^*)| - 2\mu(G) - 1$; $\eta(G) = n - 2\mu(G)$ if and only if $|\eta(G^*)| = |V(G^*)| - 2\mu(G^*)$; and $\eta(G) = n - 2\mu(G) + 2$ if and only if $|\eta(G^*)| = |V(G^*)| - 2\mu(G) + 2$.

Corollary 19.2.2.9 (Guo et al. 2009) Suppose G is a unicyclic graph with n vertices and the length of the cycle in G is l. Let G^* be the graph defined above. Then $(G) = n - 2\mu(G) - 1$ if $G^* = C_l$ and l is odd, $\eta(G) = n - 2\mu(G) + 2$ if $G^* = C_l$, and $l = 0 \pmod{4}$ and $\eta(G) = n - 2\mu(G)$ otherwise.

19.2.3 The Unicyclic Graphs with Extremal Nullity

In this section, we use some results in the past section to characterize the unicyclic graphs *G* with $\eta(G) = 0$ and n - 5, respectively.

Theorem 19.2.3.1 (Guo et al. 2009) Let G be a unicyclic graph with n vertices ($n \ge 5$) and with $\eta(G) = n - 5$. Then G must have the form of U_4^* illustrated in Fig. 19.7 or $G = C_5$, where r > 0.

Lemma 19.2.3.2 (Guo et al. 2009) Let *G* be a unicyclic graph with *n* vertices and the length *l* of the cycle C_l in *G* be odd. Then *G* is nonsingular if and only if *G* has a perfect matching or $G - C_l$ has a perfect matching (Fig. 19.10).

Lemma 19.2.3.3 (Guo et al. 2009) Let G be a unicyclic graph with n vertices and the length l of the cycle C_l in G be even. Then G is nonsingular if and only if G contains a unique perfect matching or $l \neq 0 \pmod{4}$ and G has two perfect matching.

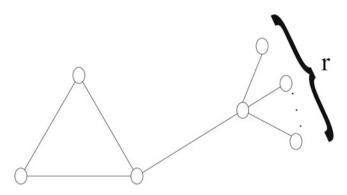


Fig. 19.10 The graph U_4^* in Lemma 19.2.3.2

Theorem 19.2.3.4 (Guo et al. 2009) Suppose *G* is a unicyclic graph and the cycle in *G* is denoted by C_l . Then *G* is nonsingular if and only if *G* satisfies one of the following properties:

- 1. *l* is odd and $G C_l$ contains a perfect matching.
- 2. G contains a unique perfect matching.
- 3. $l \neq 0 \pmod{4}$ and G contains two perfect matching.

19.2.4 On the Nullity of Bicyclic Graphs

Call a graph $\theta(p, l, q)$ (or $\infty(p, l, q)$) the base of the corresponding bicyclic graph *B* which contain it. Denote the base of *B* by ρ_B . Let $P = B - V(\rho_B)$. *P* is said to be the periphery of *B* (Fig. 19.11).

Lemma 19.2.4.1 (Cheng and Liu 2007) Let *G* be a connected graph of order *n*. Then r(G) = 2 if and only if $G = K_{r,n-r}$; r(G) = 3 if and only if $G = K_{a,b,c}$ where a + b + c = n.

Lemma 19.2.4.2 (Tan and Liu 2005) Let *B* be a bicyclic graph of order *n*. Then r(B) = 2 if and only if $B = K_{2,3}$; r(B) = 3 if and only if B = K4 - e, $e \in E(K_4)$.

Corollary 19.2.4.3 (Hu et al. 2008; Li 2008) Let $B \in B_n$ and $B \notin \{K_{2,3}, K_4 - e\}$. Then $\eta(B) \leq n - 4$.

Lemma 19.2.4.4 (Tan and Liu 2005) The bicyclic graphs with rank 4 are $\theta(1, 2, 3)$ or $\infty(4, 1, 4)$.

Theorem 19.2.4.5 (Tan and Liu 2005) Let $B \in B_n$.

- 1. $\eta(B) = n 2$ if and only if $B = K_{2,3}$;
- 2. $\eta(B) = n 3$ if and only if $B = K_{4-e}$;
- 3. $\eta(B) = n 4$ if and only if $B = B_i$ ($1 \le i \le 7$) (Fig. 19.12).

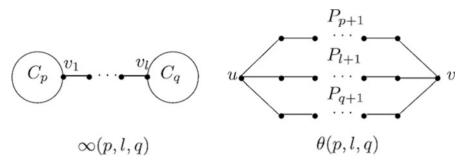


Fig. 19.11 Two bicyclic graphs

Theorem 19.2.4.6 (Hu et al. 2008; Li 2008) The nullity set of B_n is [0, n-2].

Theorem 19.2.4.7 (Hu et al. 2008; Li 2008) Let B be a bicyclic graph satisfying the following conditions:

(i) $\eta(\rho_B) = 0;$

(ii) \mathcal{P} is the union of *PM*-trees.

Then *B* is a nonsingular bicyclic graph.

Theorem 19.2.4.8 (Tan and Liu 2005) 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. 19.13, G_2^* is a connected spanning subgraph of G_2 (see, e.g., Fig. 19.13) and contains $K_{l,m}$ as its subgraph.

Theorem 19.2.4.9 (Tan and Liu 2005) Let *G* be a connected graph on *n* vertices and *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. 19.14; G_4^* is a connected spanning subgraph of G_4 (see, e.g., Fig. 19.14) and contains $K_{1,m,p}$ as its subgraph.

Theorem 19.2.4.10 (Tan and Liu 2005) Let T_n denote the set of all *n*-vertex trees.

- (i) Let $T \in \mathcal{T}_n$, then $\eta(T) \leq n-2$; the equality holds if and only if $T \cong S_n$.
- (ii) Let $T \in \mathcal{T}_n S_n$, then $\eta(T) \le n 4$, 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. 19.15.
- (iii) Let $T \in \mathcal{T}_n \{S_n, T_1, T_2\}$, then $\eta(T) \le n 6$; the equality holds if and only if $T \cong T_3$ or $T \cong T_4$ or $T \cong T_5$, where T_3, T_4, T_5 are shown in Fig. 19.15.

Corollary 19.2.4.11 (Tan and Liu 2005) The nullity set of \mathcal{T}_n is $\{0, 2, 4, ..., n-4, n-2\}$ if *n* is even, otherwise is $\{1, 3, 5, ..., n-4, n-2\}$.

Let \mathcal{U}_n denote the set of all *n*-vertex unicyclic graphs.

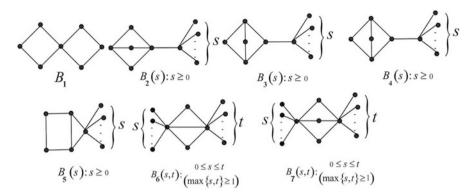
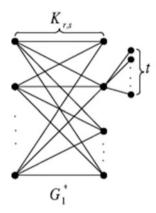


Fig. 19.12 Graphs B1–B7 in Theorem 19.2.4.5



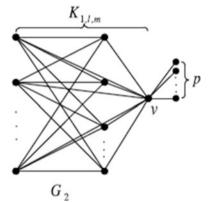
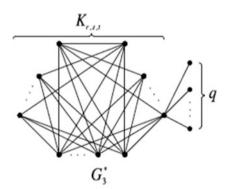


Fig. 19.13 Graphs G_1^* and G_2



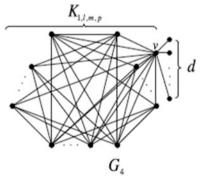


Fig. 19.14 Graphs G_3^* and G_4

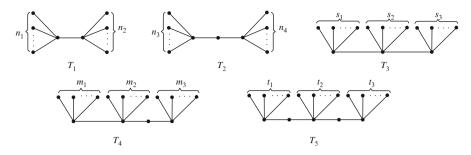


Fig. 19.15 Graphs T_1 , T_2 , T_3 , T_4 and T_5

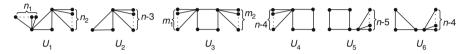


Fig. 19.16 Graphs U_1, U_2, U_3, U_4, U_5 and U_6

Theorem 19.2.4.12 Let $U_n(n-5)$ be the set of unicyclic graphs on n vertices. Let $U \in U_n$, then $\eta(U) \le n-4$; the equality holds if and only if

$$G \cong U_1$$
 or $G \cong U_2$ or $G \cong U_3$ or $G \cong U_4$ or $G \cong U_5$,

where U_1, U_2, U_3, U_4 , and U_5 are depicted in Fig. 19.16.

Corollary 19.2.4.13 (Tan and Liu 2005) The nullity set of $U_n (n \le 5)$ is $\{0, 1, 2, ..., n-4\}$.

Here, we compute the eigenvalues of a bridge graph. To do this, let G and H be two connected graphs, $u \in V(G)$ and $v \in V(H)$, respectively. By connecting the vertices u and v, we obtain a bridge graph denoted by GuvH

Theorem 19.2.4.14

$$\eta(GuvH) = \min\{\eta(G), \eta(G-u)\} + \min\{\eta(H), \eta(H-v)\}.$$

Proof It is easy to see that the characteristic polynomial of *G* can be written as follows:

$$\chi_x(G) = x^{\eta(G)} f(x),$$

where f(x) is a polynomial of degree of rank(G). It follows that

$$\chi_x(H) = x^{\eta(H)}g(x), \ \chi_x(G-u) = x^{\eta(G-u)}h(x) \text{ and } \chi_x(H-v) = x^{\eta(H-v)}k(x)$$

for some polynomials g(x), h(x), and k(x), respectively. On the other hand, by Lemma 19.2.3.4, we have

$$\chi_x(GuvH) = \chi_x(G)\chi_x(H) - \chi_x(G-u)\chi_x(H-v).$$

This leads us to conclude that

$$\chi_{x}(GuvH) = x^{\eta(G) + \eta(H)} f_{1}(x) + x^{\eta(G-u) + \eta(H-v)} f_{2}(x)$$

for some polynomials $f_1(x)$ and $f_2(x)$ and this completes the proof.

Corollary 19.2.4.15 In Theorem 19.2.4.13, suppose u and v are cut vertices, G_1 , G_2, \ldots, G_k and H_1, H_2, \ldots, H_k be respectively the components of G-u and H-v in which

$$\eta(G_1) = \eta(G_1 + u) + 1$$
 and $\eta(H_2) = \eta(H_2 + v) + 1$

Then

$$\eta(GuvH) = \eta(G) + \eta(H).$$

Let $G \bullet H$ be a graph obtained by coinciding vertex u of G by vertex v of H. Then we have:

Corollary 19.2.4.16

$$\eta(G \bullet H) = \eta(G) + \eta(H) + 1.$$

Proof By Lemma 19.2.3.4, it is easy to see that

$$\begin{split} \chi_{x}(G \cdot H) &= \chi_{x}(G)\chi_{x}(H - v) + \chi_{x}(G - u)\chi_{x}(H) \\ &- x\chi_{x}(G - u)\chi_{x}(H - v) = x^{\eta(G) + \eta(H - v)}p_{1}(x) \\ &+ x^{\eta(G - u) + \eta(H)}p_{2}(x) - x^{\eta(G - u) + \eta(H - v) + 1}p_{3}(x), \end{split}$$

where $p_1(x)$, $p_2(x)$, and $p_3(x)$ are some polynomials. Clearly we have

$$\begin{split} \eta(G \cdot H) &= \min\{\eta(G) + \eta(H - v), \eta(G - u) + \eta(H), \eta(G - u) + \eta(H - v) + 1\} \\ &= \min\{\eta(G) + \eta(H) + 1, \eta(G) + \eta(H) + 3\} \\ &= \eta(G) + \eta(H) + 1. \end{split}$$

19.2.5 Some Bounds of Nullity of Graphs

Suppose $\chi(G)$, $\alpha(G)$, and $\omega(G)$ are the chromatic number, independence number, and clique number of graph *G*, respectively. Let K_p be an induced subgraph of *G*.

Clearly, $\operatorname{rank}(G) \ge p$, and so $\eta(G) \le n - \omega(G)$. In Theorem 19.2.5.1, we compute an upper bound for the nullity of graph G with respect to its chromatic number.

Lemma 19.2.5.1 (Chartrand and Zhang 2008)

$$\omega(G) \ge 2\chi(G) + \alpha(G) - n - 1.$$

Theorem 19.2.5.2

$$\eta(G) \leq 2n - 2\chi(G) - \alpha(G) + 1.$$

Proof Since $\eta(G) \le n - \omega(G)$, by using Lemma 19.2.5.1 the proof is completed.

It is easy to see that the edge set E(G) of G can be partitioned to disjoint independent sets. Let $E(G) = \bigcup_{i=1}^{s} E_i$ be a partition of disjoint elements of E(G), where r_i is the number of parts of size $e_i = |E_i|$, i = 1, 2, ..., s.

Lemma 19.2.5.3 Let G be a bipartite graph with $n \ge 1$ vertices and m edges without any cycle of length 4s(s=1, 2, ...), then

$$n - 2\frac{m - (s - 1)r_1e_1}{r_s} \le \eta(G) \le n - 2\frac{m + (s - 1)r_1}{r_s + (s - 1)r_1}$$

Proof Since e_s is the size of maximum matching of $G, e_s = \mu(G)$ and then

$$m = |E(G)| = r_1 e_1 + r_2 e_2 + \dots + r_s \mu(G)$$

$$\leq r_s \mu(G) + \sum_{i=1}^{s-1} r_i (\mu(G) - 1) \leq r_s \mu(G) + (\mu(G) - 1)(s - 1)r_1.$$

This implies that

$$\mu(G) \ge \frac{m + (s - 1)r_1}{r_s + (s - 1)r}.$$

For computing the lower bound, it follows that

$$m = \sum_{i=1}^{s} r_i e_i \ge (s-1)r_1 e_1 + r_s \mu(G).$$

Hence,

$$\mu(G) \le \frac{m - (s - 1)r_1e_1}{r_s}$$

and the proof is completed.

Recall that a vertex in graph G is well connected if it is adjacent with other vertices of G.

Lemma 19.2.5.4 Let v be a well-connected vertex so that $G - \{v\}$ is a connected regular graph on n vertices. Then

$$\eta(G) = \eta(G - \{v\}).$$

Proof It is easy to see that $G = G - \{v\} + K_1$. Since $G - \{v\}$ is regular, so by Cvetković et al. (1980), rank $(G) = rank(G - \{v\}) + rank(K_1)$. This implies that

$$\eta(G) = n + 1 - \operatorname{rank}(G) = n + 1 - [\operatorname{rank}(G - \{v\}) + 1] = \eta(G - \{v\}).$$

Corollary 19.2.5.5 If G satisfies in conditions of Lemma 19.2.5.4, then

$$\eta(\overline{G}) = 1 + \eta(G - \{v\}).$$

Theorem 19.2.5.6 Let *G* be connected graph and *w* be a vertex of *G* in which *N* $(w) = N(u) \cup N(v)$ and $N(u) \cap N(v) = \phi$ for some vertices *u* and *v*. Then

$$\eta(G) = \eta(G - \{\mathbf{w}\}).$$

Proof Let G satisfy in the above conditions and A be adjacency matrix of G. Clearly, the sum of u-th and v-th rows is equal with w-th row of A, and this completes the proof.

Corollary 19.2.5.7 Let *G* be connected graph and *w* be a vertex of *G* in which *N* $(w) = \bigcup_{i=1}^{n} N(u_i)$ so that $N(u_i) \cap N(u_j) = \phi$ $(1 \le i, j \le n)$. Then

$$\eta(G) = \eta(G - \{\mathbf{w}\}).$$

19.3 Some Classes of Dendrimers

The aim of this section is computing the nullity of some bipartite graphs. Polymer chemistry and technology have traditionally focused on linear polymers, which are widely in use. Linear macromolecules only occasionally contain some smaller or longer branches. In the recent past, it has been found that the properties of highly branched macromolecules can be very different from conventional polymers. The structure of these materials has also a great impact on their applications. First discovered in the early 1980s by Donald Tomalia and coworkers, these hyperbranched molecules were called dendrimers. The term originates from "dendron," meaning a tree in Greek. At the same time, Newkome's group independently reported synthesis of similar macromolecules. They called them arborols from the Latin word "arbor" also meaning a tree. The term cascade molecule is also used, but "dendrimer" is the best established one.

Example 19.3.1 (Ghorbani and Songhori 2011) Consider the graph *C* depicted in Fig. 19.17. By using Corollary 19.2.18, $\eta(C) = \eta(C_1)$, and by Corollary 19.2.17 $\eta(C_1) = \eta(C_2)$. By continuing this method, one can see that $\eta(C) = \eta(C_5) = 1$.

By using above method we can prove the following Theorem.

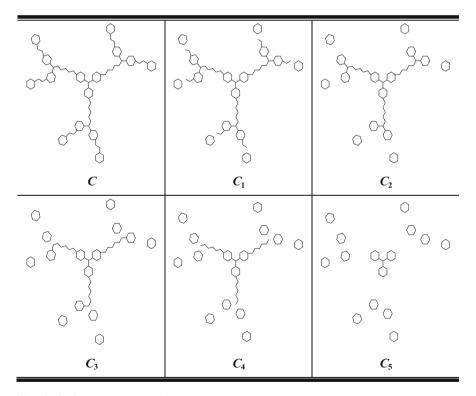


Fig. 19.17 2-D graph of dendrimer C

Fig. 19.18 2–*D* Graph of *S* [*n*]

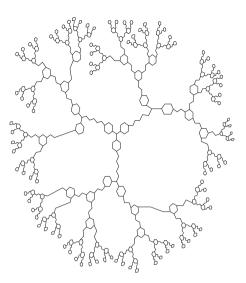
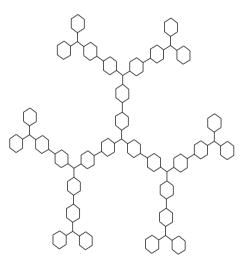


Fig. 19.19 2-D Graph of D[n], for n = 3



Theorem 19.3.2 (Ghorbani and Songhori 2011) Consider dendrimer graph S[n] depicted in Fig. 19.18. Then $\eta(S[n]) = 1$.

Theorem 19.3.3 (Ghorbani 2014) Consider nanostar dendrimer D[n], then (Figs. 19.19 and 19.20) $\eta(D[n]) = 2^{n-1}, n = 1, 2, ...$

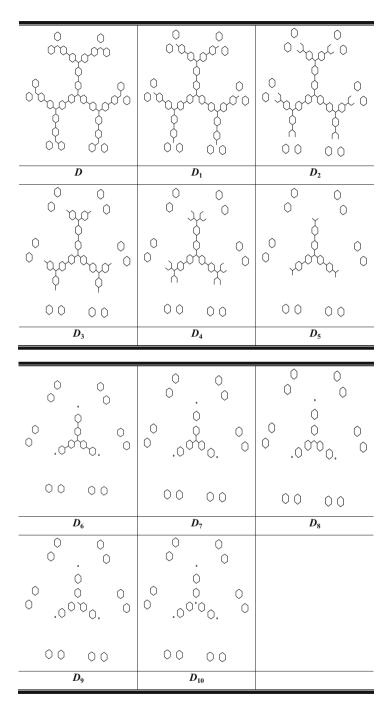


Fig. 19.20 Computing nullity of D[n], for n = 3

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