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# On the nullity and the matching number of unicyclic graphs

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#### ABSTRACT

Let *G* be a graph with *n* vertices and  $\nu(G)$  be the matching number of *G*. Let  $\eta(G)$  denote the nullity of *G* (the multiplicity of the eigenvalue zero of *G*). It is well known that if *G* is a tree, then  $\eta(G) = n - 2\nu(G)$ . Tan and Liu [X. Tan, B. Liu, On the nullity of unicyclic graphs, Linear Alg. Appl. 408 (2005) 212–220] proved that the nullity set of all unicyclic graphs with *n* vertices is  $\{0, 1, ..., n - 4\}$  and characterized the unicyclic graphs with  $\eta(G) = n - 4$ . In this paper, we characterize the unicyclic graphs with  $\eta(G) = n - 5$ , and we prove that if *G* is a unicyclic graph, then  $\eta(G)$  equals  $n - 2\nu(G) - 1$ ,  $n - 2\nu(G)$ , or  $n - 2\nu(G) + 2$ . We also give a characterization of these three types of graphs. Furthermore, we determine the unicyclic graphs *G* with  $\eta(G) = 0$ , which answers affirmatively an open problem by Tan and Liu.

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# 1. Introduction

Let G = (V(G), E(G)) be a simple graph with vertex set  $V(G) = \{v_1, v_2, ..., v_n\}$  and edge set E(G). A set M of edges in 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. We denote by m(G, i)the number of matchings of G with i edges and by v(G) the matching number of G (i.e., the number of edges of a maximum matching in G). A subgraph  $\Lambda$  of G is an elementary subgraph if each component of  $\Lambda$  is a single edge or a cycle. We use  $r(\Lambda)$  (resp.  $s(\Lambda)$ ) to denote the number of even components

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(resp. the number of cycles) in an elementary subgraph  $\Lambda$ . A unicyclic graph is a connected graph with equal number of vertices and edges. Obviously, there exists exactly one cycle in a unicyclic graph. Denote by  $K_n$ ,  $C_n$ ,  $P_n$ , and  $S_n$  the complete graph, the cycle, the path, and the star  $K_{1,n-1}$  with n vertices, respectively.

The adjacency matrix of a graph *G* with *n* vertices, denoted by  $A(G) = (a_{ij})_{n \times n}$ , is the  $n \times n$  symmetric matrix such that  $a_{ij} = 1$  if vertices  $v_i$  and  $v_j$  are adjacent and 0 otherwise. The characteristic polynomial of *G*, denoted by  $\phi(G, x)$ , is defined as det $(xI_n - A(G))$ , where  $I_n$  is a unit matrix of order *n*. A graph *G* is said to be singular (resp. nonsingular) if  $\phi(G, 0) = 0$  (resp.  $\phi(G, 0) \neq 0$ )). The roots of  $\phi(G, x)$  are called the eigenvalues of *G*. The multiplicity of the eigenvalue zero of *G* is called the nullity of *G*, which is denoted by  $\eta(G)$ .

The following result, which will play a key role in the proofs of our main results, is well known and useful ([1,2,15–18]):

**Proposition 1.1** [4]. Suppose *G* is a graph with *n* vertices. Then the coefficients of the characteristic polynomial  $\phi(G, x) = \sum_{i=0}^{n} a_i x^{n-i}$  of *G* is given by

$$(-1)^i a_i = \sum (-1)^{r(\Lambda)} 2^{\mathfrak{s}(\Lambda)},$$

where the summation ranges over all elementary subgraphs  $\Lambda$  of G with i vertices.

Collatz and Sinogowitz [3] and Schwenk and Wilson [7] posed the problem of characterizing all singular or nonsingular graphs. This problem is very difficult. At present, only some particular cases are known [4–6,8–12,14]. On the other hand, this problem is very interesting in chemistry, because, as has been shown in Longuet-Higgins [6], the occurrence of a zero eigenvalue of a bipartite graph (corresponding to an alternant hydrocarbon) indicates the chemical instability of the molecule which such a graph represents. The question is of interest also for non-alternant hydrocarbons (non-bipartite graph), but a direct connection with the chemical stability in these cases is not so straightforward. The following result gives a concise formula for the nullity of a tree T in terms of the matching number of T:

**Proposition 1.2** [4]. Suppose *T* is a tree with *n* vertices and the matching number of *T* is v(T). Then

$$\eta(T) = n - 2\nu(T).$$

Recently, Tan and Liu [13] investigated the nullity of the unicyclic graphs and proved the following interesting results:

**Proposition 1.3** [13]. The nullity set of all unicyclic graphs with n vertices  $(n \ge 5)$  is  $\{0, 1, 2, ..., n - 4\}$ .

**Proposition 1.4** [13]. Let *G* be a unicyclic graph with *n* vertices  $(n \ge 5)$ . Then  $\eta(G) = n - 4$  if and only if  $G \cong U_1^*, U_2^*$  or  $U_3^*$ , where  $U_i^*$  are illustrated in Fig. 1 for  $1 \le i \le 3$ , where  $S_{n_i}$  is the star  $K_{1,n_i-1}$ .

In order to investigate the unicyclic graphs with  $\eta(G) = 0$ , Tan and Liu [13] introduced the definition of the elementary unicyclic graphs as follows. A unicyclic graph *G* is called an elementary unicyclic graph if *G* is a cycle of length *l* and  $l \neq 0 \pmod{4}$ , or *G* is obtained from a cycle  $C_l$  and *t* isolated vertices (where  $0 < t \le l$  and  $l = t \pmod{2}$ ) by the rule: first select *t* vertices from  $C_l$  such that there are an even number (which may be 0) of vertices between any two consecutive such vertices. Then join an edge from each of the *t* vertices chosen in  $C_l$  to an isolated vertex. Tan and Liu [13] proved the following:

**Proposition 1.5** [13]. If U is an elementary unicyclic graph, or a graph obtained by joining a vertex of an elementary unicyclic graph with an arbitrary vertex of a tree with a perfect matching, then U is a nonsingular unicyclic graph.



**Fig. 1.** Three graphs  $U_1^*$ ,  $U_2^*$  and  $U_3^*$  in Proposition 1.4, where  $n_1 \ge 1$  and  $n_2 \ge 2$ .

Let  $X_n$  be the set of the unicyclic graphs with n vertices and with  $\eta(G) = 0$ , and let  $Y_n$  be the set of unicyclic graphs with n vertices each of which is obtained from an arbitrary elementary unicyclic graph G' by joining a vertex of trees with a perfect matching to some or all vertices of G'. Clearly, we have  $Y_n \subseteq X_n$ . Tan and Liu [13] posed the following open problem:

# **Problem 1.1.** *Does* $X_n = Y_n$ ?

In the next section, we prove that if *G* is a unicyclic graph, then  $\eta(G)$  equals  $n - 2\nu(G) - 1$ ,  $n - 2\nu(G)$  or  $n - 2\nu(G) + 2$ . We also characterize these three types of graphs. In Section 3, we determine the unicyclic graphs *G* with  $\eta(G) = n - 5$ , and we also characterize the nonsingular unicyclic graphs, which answers affirmatively Problem 1.1.

### 2. The nullity of unicyclic graphs

For the sake of convenience, we will assume that *G* is a unicyclic graph with *n* vertices and the the cycle in *G* is denoted by  $C_l$ , where *l* is the length of the cycle. Let  $G - C_l$  denote the induced subgraph of *G* by deleting, from *G*, vertices in  $C_l$  and their incident edges. We use the symbols p = v(G) and  $q = v(G - C_l)$  if not specified.

Now we can determine the nullity of non-bipartite unicyclic graphs as follows.

**Lemma 2.1.** Suppose *G* is a unicyclic graph with *n* vertices and the length *l* of the cycle *C*<sub>*l*</sub> in *G* is odd. Then  $\eta(G) = n - 2\nu(G) - 1$  if  $\nu(G) = \frac{l-1}{2} + \nu(G - C_l)$ , and  $\eta(G) = n - 2\nu(G)$  otherwise.

**Proof.** Let  $\nu(G) = p$  and  $\nu(G - C_l) = q$ . Suppose the characteristic polynomial of *G* is given by

$$\phi(G, x) = \sum_{i=0}^{n} a_i x^{n-i}.$$
(1)

By Proposition 1.1, we have

$$(-1)^{i}a_{i} = \sum (-1)^{r(\Lambda)} 2^{s(\Lambda)},$$
(2)

where the summation ranges over all elementary subgraphs  $\Lambda$  of G with i vertices.

Note that  $p \ge \frac{l-1}{2} + q$ , that is,  $2p \ge l - 1 + 2q$ . Hence, if  $i > 2p + 1 \ge l + 2q$ , then *G* contains no elementary subgraphs with *i* vertices, which implies that if i > 2p + 1 we have  $a_i = 0$ . Since  $x^{n-2p-1}$  is a factor of  $\phi(G, x)$ ,  $\eta(G) \ge n - 2p - 1$ .

If 
$$p = \frac{l-1}{2} + q$$
, by (2) we have  
 $(-1)^{2p+1}a_{2p+1} = \sum (-1)^{r(\Lambda)} 2^{s(\Lambda)}$ ,

where the summation ranges over all elementary subgraphs  $\Lambda$  of G with 2p + 1 vertices. Note that the set of the unions of the cycle  $C_l$  of G and every matching of  $G - C_l$  with q edges equals exactly the set of elementary subgraphs of G with 2p + 1 vertices. Hence

$$a_{2p+1} = 2(-1)^{q+1}m(G - C_l, q) \neq 0,$$

where  $m(G - C_l, q)$  is the number of matchings of  $G - C_l$  with q edges. So we have proved that if  $p = \frac{l-1}{2} + q$  then  $\eta(G) = n - 2\nu(G) - 1$ .

If  $p \neq \frac{l-1}{2} + q$ , then 2p + 1 > l + 2q. Hence *G* contains no elementary subgraphs with 2p + 1 vertices, which shows that  $\eta(G) \ge n - 2p$ . By a similar discussion, we have

$$a_{2p} = (-1)^p m(G, p) \neq 0,$$

which implies  $\eta(G) = n - 2p$  and the lemma follows.  $\Box$ 

In Lemma 2.1 we have characterized the nullity of non-bipartite unicyclic graphs. Now we start to consider the case in which *G* is a bipartite unicyclic graph.

**Lemma 2.2.** Suppose *G* is a unicyclic graph with *n* vertices and the length *l* of the cycle  $C_l$  in *G* is even. If  $\nu(G) \neq \frac{l}{2} + \nu(G - C_l)$ , or  $\nu(G) = \frac{l}{2} + \nu(G - C_l)$  and  $l = 2 \pmod{4}$ , then  $\eta(G) = n - 2\nu(G)$ .

**Proof.** Let  $\nu(G) = p$  and  $\nu(G - C_l) = q$ . Note that *G* is a bipartite graph. Hence the characteristic polynomial of *G* can be expressed by

$$\phi(G, x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_i x^{n-2i}.$$
(3)

By Proposition 1.1, we have

$$b_i = \sum (-1)^{r(\Lambda)} 2^{s(\Lambda)},$$
(4)

where the summation ranges over all elementary subgraphs  $\Lambda$  of G with 2i vertices.

By a similar discussion as in the proof of Lemma 2.1, we can prove the following results:

(i)  $\eta(G) \ge n - 2p$ ;

(ii) 
$$b_p = (-1)^p m(G, p) \neq 0$$
 if  $p \neq \frac{1}{2} + q$ ;

(iii)  $b_p = (-1)^p m(G, p) - 2(-1)^q \tilde{m}(G - C_l, q)$  if  $p = \frac{l}{2} + q$ .

Hence, by (i) and (ii), if  $p \neq \frac{1}{2} + q$  then  $\eta(G) = n - 2p$ . Note that, if  $p = \frac{1}{2} + q$  and  $l \neq 0 \pmod{4}$ , then  $p \neq q \pmod{2}$ . So by (iii) we have  $b_p = (-1)^p m(G, p) - 2(-1)^q m(G - C_l, q) \neq 0$ , which also implies that  $\eta(G) = n - 2p$ .

The lemma thus follows.  $\Box$ 

**Lemma 2.3.** Suppose *G* is a unicyclic graph with *n* vertices and cycle  $C_l$  of length  $l = 0 \pmod{4}$ , and  $\nu(G) = \frac{l}{2} + \nu(G - C_l)$ . 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  $\nu(G)$  edges. Then,  $\eta(G) = n - 2\nu(G) + 2ifE_1 \cap M = \emptyset$  for all  $M \in E_2$ , and  $\eta(G) = n - 2\nu(G)$  otherwise.

**Proof.** We use the notation in the proof of Lemma 2.2. Note that, by the proof of Lemma 2.2, we have shown that  $\eta(G) \ge n - 2p$ .

First we prove that  $\eta(G) \leq n - 2p + 2$ . We only need to show that  $b_{p-1} \neq 0$ . Let

 $M_1$  = the set of matchings of *G* with p - 1 edges;

 $\mathcal{M}'_1$  = the set of matchings of  $G - C_l$  with q - 1 edges;

 $\mathcal{M}_2 = \{ \Lambda | \Lambda = C_l \cup M, M \in \mathcal{M}'_1 \}.$ 

Obviously, the set of elementary subgraphs of *G* with 2p - 2 vertices equals exactly  $M_1 \cup M_2$ . Hence, by (4), we have

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$$b_{p-1} = \sum_{\Lambda_1 \in \mathcal{M}_1} (-1)^{r(\Lambda_1)} + 2 \sum_{\Lambda_2 \in \mathcal{M}_2} (-1)^{r(\Lambda_2)} = (-1)^{p-1} m(G, p-1) - 2(-1)^{q-1} m(G - C_l, q-1).$$

In order to prove that  $b_{p-1} \neq 0$ , we only need to show that  $m(G, p-1) > 2m(G - C_l, q-1)$ , i.e.,  $|\mathcal{M}_1| > 2|\mathcal{M}_2|$ .

Note that  $C_l$  contains exactly two perfect matchings, denoted by  $M_1$  and  $M_2$ . It is obvious that

$$\mathcal{M}^* = \{M_1 \cup M | M \in \mathcal{M}'_1\} \cup \{M_2 \cup M | M \in \mathcal{M}'_1\} \subseteq \mathcal{M}_1.$$

Hence  $|\mathcal{M}_1| \ge |\mathcal{M}^*| = 2|\mathcal{M}'_1| = 2|\mathcal{M}_2|$ . Let  $M_3$  be a matching of  $G - C_l$  with q edges and  $M_4$  a matching of  $C_l$  with  $\frac{l}{2} - 1$  edges, then  $M_3 \cup M_4$  is a matching of G with  $\frac{l}{2} - 1 + q = p - 1$  edges. So  $M_3 \cup M_4 \in \mathcal{M}_1$ . Note that  $M_3 \cup M_4 \notin \mathcal{M}^*$ . Hence  $|\mathcal{M}_1| \ge |\mathcal{M}^*| + 1 = 2|\mathcal{M}_2| + 1 > 2|\mathcal{M}_2|$ .

Then the lemma follows from the following claim:

**Claim** we have  $b_p = 0$  if  $E_1 \cap M = \emptyset$  for an arbitrary  $M \in E_2$  and  $b_p \neq 0$  otherwise.

Let  $\mathcal{M}_3$  be the set of matchings of  $G - C_l$  with  $\nu(G - C_l)$  edges. Let  $\mathcal{M}_4$  be the set of matchings of G with  $\nu(G)$  edges, each of which has at least one edge in  $E_1$ . Hence  $\mathcal{M}_4 = \emptyset$  if  $E_1 \cap M = \emptyset$  for an arbitrary  $M \in E_2$  and  $\mathcal{M}_4 \neq \emptyset$  otherwise. Note that we have

$$b_p = -2 \sum_{\Lambda_1 \in \mathcal{M}_3} (-1)^{r(\Lambda_1)} + \sum_{\Lambda_2 \in E_2} (-1)^{r(\Lambda_2)}$$

For the case  $M_4 = \emptyset$ , i.e.,  $E_1 \cap M = \emptyset$  for an arbitrary  $M \in E_2$ , since  $C_l$  have exactly two perfect matchings  $M_1$  and  $M_2$ , we have  $E_2 = \{M_1 \cup M | M \in M_3\} \cup \{M_2 \cup M | M \in M_3\}$ . Hence

$$\sum_{\Lambda_2 \in E_2} (-1)^{r(\Lambda_2)} = (-1)^{|M_1|} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} + (-1)^{|M_2|} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} = 2(-1)^{\frac{l}{2}} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} + (-1)^{|M_2|} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} = 2(-1)^{\frac{l}{2}} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} + (-1)^{|M_2|} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} = 2(-1)^{\frac{l}{2}} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} + (-1)^{\frac{l}{2}} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} = 2(-1)^{\frac{l}{2}} \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} + (-1)^{\frac{l}{2}} \sum_{\Lambda \in \mathcal{M}_3} (-$$

Since  $l = 0 \pmod{4}$ , we have

$$b_p = -2 \sum_{\Lambda_1 \in \mathcal{M}_3} (-1)^{r(\Lambda_1)} + 2 \sum_{\Lambda \in \mathcal{M}_3} (-1)^{r(\Lambda)} = 0$$

For the case  $\mathcal{M}_4 \neq \emptyset$ , we have  $E_2 = \{M_1 \cup M | M \in \mathcal{M}_3\} \cup \{M_2 \cup M | M \in \mathcal{M}_3\} \cup \mathcal{M}_4$ . Hence

$$\sum_{A_2 \in E_2} (-1)^{r(A_2)} = (-1)^{|M_1|} \sum_{A \in \mathcal{M}_3} (-1)^{r(A)} + (-1)^{|M_2|} \sum_{A \in \mathcal{M}_3} (-1)^{r(A)} + \sum_{A \in \mathcal{M}_4} (-1)^{r(A)}$$
$$= 2 \sum_{A_2 \in \mathcal{M}_3} (-1)^{r(A_2)} + \sum_{A \in \mathcal{M}_4} (-1)^{r(A)},$$

which implies that  $b_p = \sum_{\Lambda \in \mathcal{M}_4} (-1)^{r(\Lambda)} \neq 0$ . Thus the claim follows.  $\Box$ 

By Lemmas 2.1–2.3, we have the following:

**Theorem 2.1.** Suppose *G* is a unicyclic graph with *n* vertices and the cycle in *G* is  $C_1$ . Let  $E_1$  be the set of edges of *G* between  $C_1$  and  $G - C_1$  and  $E_2$  the set of matchings of *G* with  $\nu(G)$  edges. Then

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

**Remark 2.1.** Let *G* be a unicyclic graph with *n* vertices and  $C_l$  the cycle in *G*. If  $\eta(G) = n - 2\nu(G) - 1$ , then, by (1) in Theorem 2.1, *l* is odd and hence *G* is a non-bipartite graph.

**Remark 2.2.** Let *G* be a unicyclic graph with  $n \ge 4$  vertices. Obviously,  $\nu(G) \ge 2$ . Hence, by Theorem 2.1,  $\eta(G) \le n - 4$ . Let *G* be a unicyclic graph with *n* vertices and with  $\eta(G) = n - 4$ , and let the length of the cycle in *G* be *l*. If *l* is odd, by Lemma 2.1,  $\eta(G) = n - 2\nu(G) - 1$ , or  $\eta(G) = n - 2\nu(G)$ . Then we have  $\nu(G) = 2$  and *G* must satisfy:  $\nu(G) > \frac{l-1}{2} + \nu(G - C_l, q)$ , i.e.,  $\nu(G) = 2$ , l = 3 and  $\nu(G - C_l) = 0$ .



**Fig. 2.** A graph *G* and a pendant star *H* of *G*, where  $G_0 = G - H$ .

Hence *G* must have the form of  $U_1^*$  shown in Fig. 1. Similarly, if *l* is even, then, by Lemmas 2.2 and 2.3, we can show that *G* must have the form of  $U_2^*$  or  $U_3^*$  illustrated in Fig. 1. Hence, Proposition 1.4, which was proved by Tan and Liu [13], can be obtained from Theorem 2.1. In Section 3, we will characterize the unicyclic graph *G* with *n* vertices and with  $\eta(G) = 0$  and n - 5, respectively.

A vertex-induced subgraph H of a graph G is called a pendant star of G if H is a star with at least two vertices and all pendant vertices of H are also pendant vertices in G. A graph G and a pendant star H of G are illustrated in Fig. 2, where  $G_0$  is the graph G - H. The following result is immediate from the definition of the pendant star:

**Lemma 2.4.** Suppose H is a pendant star of a graph G. Then  $\nu(G) = \nu(G_0) + 1$ , where  $G_0 = G - H$ .

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

**Theorem 2.2.** Suppose *G* is a unicyclic graph with *n* vertices and *G*<sup>\*</sup> is the graph defined above. Then  $\eta(G) = n - 2\nu(G) - 1$  if and only if  $\eta(G^*) = |V(G^*)| - 2\nu(G^*) - 1$ ;  $\eta(G) = n - 2\nu(G)$  if and only if  $\eta(G^*) = |V(G^*)| - 2\nu(G^*)$ ; and  $\eta(G) = n - 2\nu(G) + 2$  if and only if  $\eta(G^*) = |V(G^*)| - 2\nu(G^*) + 2$ .

**Proof.** If *G* is a canonical unicyclic graph, then  $G = G^*$  and the theorem holds. Hence we may assume that  $G \neq G^*$ . Then *G* has a pendant star *H* such that G - H is a unicyclic graph. The theorem follows from the the following claims:

1.  $\eta(G) = n - 2\nu(G) - 1$  if and only if  $\eta(G - H) = n - |V(H)| - 2\nu(G - H) - 1$ ; 2.  $\eta(G) = n - 2\nu(G)$  if and only if  $\eta(G - H) = n - |V(H)| - 2\nu(G - H)$ ; 3.  $\eta(G) = n - 2\nu(G) + 2$  if and only if  $\eta(G - H) = n - |V(H)| - 2\nu(G - H) + 2$ .

We prove that the second statement holds. Suppose that  $\eta(G) = n - 2\nu(G)$ . Note that, if G' is a graph obtained from G by deleting a pendant edge, then  $\eta(G) = \eta(G')$ , a result in [4]. Hence  $\eta(G) = |V(H)| - 2 + \eta(G - H)$ , which implies that  $\eta(G - H) = n - |V(H)| + 2 - 2\nu(G)$ . By Lemma 2.4, we have  $\eta(G - H) = n - |V(H)| + 2 - 2(\nu(G - H) + 1) = n - |V(H)| - 2\nu(G - H)$ . Similarly, we can show that if  $\eta(G - H) = n - |V(H)| - 2\nu(G - H)$  then  $\eta(G) = n - 2\nu(G)$ . By a similar discussion, we can prove the first and the third statements.  $\Box$ 

The following corollary, which can be obtained from Theorems 2.1 and 2.2, characterizes the unicyclic graphs *G* with  $\eta(G) = |V(G)| - 2\nu(G) - 1$ ,  $|V(G)| - 2\nu(G)$  and  $|V(G)| - \nu(G) + 2$ , respectively.



**Fig. 3.** The graph  $U_4^*$  in Theorem 3.3.

**Corollary 2.1.** Suppose G is a unicyclic graph with n vertices and the length of the cycle in G is 1. Let  $G^*$  be the graph defined above. Then  $\eta(G) = n - 2\nu(G) - 1$  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  $n(G) = n - 2\nu(G)$  otherwise.

# 3. The unicyclic graphs with extremal nullity

In this section, we use some results in Section 2 to characterize the unicyclic graphs G with  $\eta(G) = 0$ and n-5, respectively.

**Theorem 3.3.** 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. 3 or  $G = C_5$ , where r > 0.

**Proof.** Suppose the length of the cycle in G is l. Note that, by Theorem 2.1,  $\eta(G) = n - 2\nu(G) - 1$ ,  $n - 2\nu(G)$  or  $n - 2\nu(G) + 2$ . Hence if  $\eta(G) = n - 5$  then G must satisfy:

(i) l is odd;

(*ii*)  $\eta(G) = n - 2\nu(G) - 1$ ;

(iii)  $\nu(G) = \frac{l-1}{2} + \nu(G - C_l)$ . By (i), (ii) and (iii), we have:  $\nu(G) = 2$ , and l = 3 or l = 5. If l = 5 then  $\nu(G - C_l) = 0$ . Note that  $\nu(G) = 2$ . Hence if l = 5 then  $G = C_5$ . If l = 3, it is trivial to show that G must have the form of  $U_4^{*}$ illustrated in Fig. 3. The theorem has thus been proved.  $\Box$ 

Now we start to characterize the nonsingular unicyclic graphs. First we consider the case in which *G* is not bipartite.

**Lemma 3.5.** 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.

**Proof.** " $\Leftarrow$ ". If *G* has a perfect matching, then  $n = 2\nu(G)$ . If  $\nu(G) = \frac{l-1}{2} + \nu(G - C_l)$ , then, by Lemma 2.1, we have  $\eta(G) = n - 2\nu(G) - 1 = -1$ , a contradiction. Hence, by Lemma 2.1,  $\eta(G) = n - 2\nu(G) = 1$ 0. If  $G - C_l$  contains a perfect matching, then  $\nu(G) = \frac{l-1}{2} + \nu(G - C_l)$  and  $n = 2\nu(G) + 1$ . Hence, by Lemma 2.1, we have  $\eta(G) = n - 2\nu(G) - 1 = 0$ . Hence we have proved that sufficiency holds.

" $\Rightarrow$ ". Let G be nonsingular (i.e.,  $\eta(G) = 0$ ). By Lemma 2.1, either we have  $n = 2\nu(G)$  and  $\nu(G) > 0$  $\frac{l-1}{2} + \nu(G - C_l)$  or we have  $n = 2\nu(G) + 1$  and  $\nu(G) = \frac{l-1}{2} + \nu(G - C_l)$ , which implies that *G* has a perfect matching or  $G - C_l$  has a perfect matching.

The lemma thus follows.  $\Box$ 

For the bipartite unicyclic graphs *G* with  $\eta(G) = 0$ , we have the following:

**Lemma 3.6.** 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 matchings.

**Proof.** Since *G* is a bipartite graph with *n* vertices, the characteristic polynomial of *G* can be expressed by

$$\phi(G, x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_i x^{n-2i}.$$

" $\Leftarrow$ ". If *G* contains a unique perfect matching, by Proposition 1.1 we have  $b_{\frac{n}{2}} = (-1)^{\frac{n}{2}}$ . If *G* contains two perfect matchings,  $G - C_l$  contains a (unique) perfect matching. By Proposition 1.1, we have  $b_{\frac{n}{2}} = 2(-1)^{\frac{n}{2}} + 2(-1)^{\frac{n-l}{2}+1}$ . Note that  $l \neq 0 \pmod{4}$ . Hence we have  $b_{\frac{n}{2}} = 4(-1)^{\frac{n}{2}}$ . So we have shown that if *G* contains a unique perfect matching or  $l \neq 0 \pmod{4}$  and *G* has two perfect matchings then  $\eta(G) \neq 0$ . Sufficiency thus follows.

" $\Rightarrow$ ". We assume that *G* is nonsingular. Hence  $\eta(G) = 0$ . By Lemmas 2.2 and 2.3,  $\eta(G) = n - 2p$  or  $\eta(G) = n - 2p + 2$ , where  $p = \nu(G)$ . Hence n = 2p or n = 2p - 2. Note that  $n \ge 2p$ , thus it is impossible that n = 2p - 2. So n = 2p, which shows that *G* contains perfect matchings. Note that *G* contains at most two perfect matchings. Thus either  $l = 0 \pmod{4}$ ,  $E_1 \cap M \neq \emptyset$  for arbitrary  $M \in E_2$ , n = 2p or  $l = 2 \pmod{4}$ , n = 2p. Hence we only need to prove that if *G* contains two perfect matchings then  $l \neq 0 \pmod{4}$ . We prove this by contradiction. If  $l = 0 \pmod{4}$ , by a similar way as in the proof of Lemma 2.2, we have

$$b_{\frac{n}{2}} = (-1)^{\frac{n}{2}} m\left(G, \frac{n}{2}\right) + 2(-1)^{\frac{n-l}{2}+1} m\left(G - C_{l}, \frac{n-l}{2}\right).$$

Since *G* has two perfect matchings and  $G - C_l$  contains a unique perfect matching (a matching with  $\frac{n-l}{2}$  edges), we have

$$b_{\frac{n}{2}} = (-1)^{\frac{n}{2}} m\left(G, \frac{n}{2}\right) + 2(-1)^{\frac{n-l}{2}+1} m\left(G - C_l, \frac{n-l}{2}\right) = 0.$$

This contradicts  $\eta(G) = 0$ .

So we have finished the proof of the lemma.  $\Box$ 

The following result is immediate from Lemmas 3.5 and 3.6.

**Theorem 3.4.** Suppose *G* is a unicyclic graph and the cycle in *G* is denoted by  $C_1$ . 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 matchings.

**Corollary 3.2.** Let  $X_n$  and  $Y_n$  be as in Problem 1.1. Then  $X_n = Y_n$ .

**Proof.** Note that, by Theorem 2.2,  $Y_n \subseteq X_n$ . We only need to prove  $X_n \subseteq Y_n$ . Suppose that *G* is a non-singular unicyclic graph with *n* vertices. Let the cycle in *G* be denoted by  $C_l$  (i.e.,  $G \in X_n$ ). By Theorem 3.4, *G* must satisfy 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.

If *G* satisfies the property (1), then  $G - C_l$  is a forest with a perfect matching. By the definition of  $Y_n, G \in Y_n$ . If *G* satisfies the properties (2) or (3), then, by Theorem 2.2, either *G* is an elementary unicyclic graph or each of its pendant stars, obtained when we obtain  $G^*$  from *G* by the "deleting operators", is a  $P_2$ . Then  $G \in Y_n$ . Hence  $X_n \subseteq Y_n$  and the corollary follows.

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