Unicyclic Graphs with Nullity One

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Abstract The nullity of a graph $G$ is defined to be the multiplicity of the eigenvalue zero in its spectrum. In this paper we characterize the unicyclic graphs with nullity one in aspect of its graphical construction.

Keywords nullity of graphs; unicyclic graphs; singularity; perfectly matched vertex.

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1. Introduction

Let $G$ be a simple graph of order $n$ with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$. The adjacency matrix of $G$ is a matrix $A = A(G) = [a_{ij}]$ of order $n$ given by $a_{ij} = 1$ if $v_i$ is adjacent to $v_j$, and $a_{ij} = 0$ otherwise. The nullity of the graph $G$ is the multiplicity of the eigenvalue zero in the spectrum of $A(G)$, denoted by $\eta(G)$. When $\eta(G)=0$, the graph $G$ is called nonsingular. In 1957, Collatz and Sinogowitz [1] first proposed the problem of characterizing all graphs $G$ with $\eta(G) > 0$. This problem is of great interest in both chemistry and mathematics. For a bipartite graph $G$ which corresponds to an alternant hydrocarbon in chemistry, if $\eta(G) > 0$, it is indicated that the corresponding molecule is unstable. The nullity of a graph is also meaningful in mathematics since it is related to the singularity of adjacent matrix. The problem has not yet been solved completely. Much attention is focused on graphs with few edges, e.g. trees, unicyclic graphs, bicyclic graphs.

The nullity of a tree can be given in explicit form in terms of the matching number of the tree [10]. Tan and Liu [6] gave the nullity set of unicyclic graphs on $n$ vertices for $n \geq 5$, that is $\{0, 1, 2, \ldots, n - 4\}$. In addition, the unicyclic graphs with maximum nullity is characterized. For the unicyclic graphs with minimum nullity (or the singular unicyclic graphs), they proposed an open problem, which was at last solved by Li and Chang [7]. Hu, Liu and Tan [9] gave the nullity set of bicyclic graphs on $n$ vertices for $n \geq 6$, that is, $\{0, 1, 2, \ldots, n - 4\}$, and characterized the bicyclic graphs with extremal nullity. In addition, in paper [8], the authors presented another version of characterization for an acyclic (respectively, a unicyclic graph) to be nonsingular. Other work on nullity of graphs can be found in [4] which proved that the nullity of the line
The graph of a tree is at most one, and in [3] which provided a method of constructing singular graphs from others of smaller order, and in [2] for related topics. Cheng and Liu [5] considered general graphs on fixed number of vertices with extreme nullity, and also discussed the maximal nullity of graphs with fixed number of vertices and edges.

We notice that in the paper [3] the author considered the graphs with nullity one. In this paper we focus on the problem of characterizing the unicyclic graphs with nullity one, and give the result in aspect of the graphical construction.

2. Preliminaries

In this section, we will first give some definitions and notations, then introduce some useful results on the nullity of graphs.

Let $G = (V, E)$ be a simple graph with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G) = \{e_1, e_2, \ldots, e_m\}$. Denote by $v(G)$ and $e(G)$ the number of vertices and edges of $G$. For any $v \in V$, denote by $d_G(v)$ and $N_G(v)$, respectively, the degree and neighborhood of $v$ in $G$. A vertex $v \in V$ is called pendant if $d_G(v) = 1$, and a vertex $w \in V$ is called quasi-pendant if $w$ is adjacent to a pendant vertex. Let $W$ be a nonempty subset of $V(G)$. Denote by $G - W$ the graph obtained from $G$ by removing the vertices of $W$ together with all edges incident to them. Let $F$ be a nonempty subset of $E(G)$. Denote by $G - F$ the graph obtained from $G$ by removing the edges of $F$.

A matching of $G$ is a collection of independent edges of $G$. A maximal matching is a matching with maximum possible number of edges, whose cardinality is called the matching number of $G$ and is denoted by $m(G)$. If $m(G) = v(G)/2$, then $G$ is said to have perfect matchings, or $G$ is called a PM-graph for short. An edge belonging to a matching of a graph $G$ is said to match its two end-vertices. A vertex $v$ is said to be perfectly matched if it is matched by all maximal matchings of $G$, otherwise, $v$ is called mismatched; see Figure 1.

It is easy to see that each quasi-pendant vertex must be perfectly matched, and if $uv$ is a pendant edge of $G$, then there exists a maximal matching of $G$ which contains it. Furthermore, if $w$ is a mismatched vertex of $G$, then we can get a maximal matching of $G$ which contains $w$ and $w$ is mismatched in it. For a PM-tree $T$, let $u \in V(T)$ and $M(T)$ be one of its perfect matchings and $N_T(u) = \{v_1, v_2, \ldots, v_m\}$. Without loss of generality, suppose $v_1$ is matched by $M(T)$, then each component of $T - u - v_1$ is still a PM-tree.

![Figure 1 Perfectly matched and mismatched vertices](image)

The disjoint union of $k$ copies of a graph $G$ is written by $kG$. A graph is called null if it has no edges. As usual, the cycle and the path of order $n$ are denoted by $C_n$ and $P_n$, respectively.
An isolated vertex is sometimes denoted by $K_1$. A unicyclic graph is a simple connected graph with equal number of vertices and edges. Obviously, a unicyclic graph contains a unique cycle.

**Lemma 2.1 ([2])** For a graph $G$ containing a pendent vertex, if the induced subgraph $H$ is obtained by deleting this vertex together with the vertex adjacent to it, then $\eta(H) = \eta(G)$.

By Lemma 2.1, we can get $\eta(P_n) = 1$ if $n$ is odd and $\eta(P_n) = 0$ otherwise.

**Lemma 2.2 ([2])** Let $G = G_1 \cup G_2 \cup \cdots \cup G_n$, where $G_1, G_2, \ldots, G_n$ are disjoint connected components of $G$. Then

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

**Lemma 2.3 ([2])** A path with four vertices of degree 2 in a graph $G$ can be replaced by an edge (see Figure 2) without changing the value of $\eta(G)$.

![Figure 2 Illustration of Lemma 2.3](image)

Consequently, by Lemma 2.3, if $n \equiv 0 \pmod{4}$, then $\eta(C_n) = 2$; otherwise, $\eta(C_n) = 0$.

**Theorem 2.4 ([2])** If $T$ is a tree of order $n$, then $\eta(T) = n - 2m(T)$. Hence, $\eta(T) = 0$ if and only if $T$ is a PM-tree.

**Lemma 2.5** Let $G$ be a connected graph obtained from a connected graph (possibly being $K_1$) by attaching at a vertex $u$ a tree $T$ (i.e., identifying the vertex $u$ with some vertex of $T$). Then

(i) If $u$ is a perfectly matched vertex of $T$, $\eta(G) = \eta(G - T) + \eta(T)$;

(ii) If $u$ is a mismatched vertex of $T$, $\eta(G) = \eta(T - u) + \eta(G - (T - u))$.

**Proof** (i) Using induction principle on $e(T)$. If $e(T) = 1$, then $T = P_2$ and $u$ is a quasi-pendent vertex of $G$. By Lemma 2.1, $\eta(G) = \eta(G - T) + 0 = \eta(G - T) + \eta(T)$. Suppose the result holds for all trees $T$ with $e(T) < m$. Now we consider the case of $e(T) = m$. If $u$ is a unique quasi-pendent vertex of $T$, then $T$ is a star and by Lemmas 2.1 and 2.2, $\eta(G) = \eta(G - T) + \nu(T) - 2 = \eta(G - T) + \eta(T)$. Otherwise, let $w \in T$ ($w \neq u$) be a quasi-pendent vertex adjacent to the pendent vertex $w' \in T$. Let the components of $T - w - w'$ be $T_1, T_2, \ldots, T_s$ ($s \geq 1$), where $T_1$ contains the vertex $u$. We claim that $u$ is still perfectly matched in $T_1$. Consider a maximal matching $M$ of $T$, where $M$ contains a pendent edge $e_w$ joining $w$ and $w'$. Then $M = M_1 \cup M_2 \cup \cdots \cup M_s \cup e_w$, where $M_i = M \cap E(T_i)$ is still a maximal matching of $T_i$ for $i = 1, 2, \ldots, s$. If $u$ is not perfectly matched in $T_1$, then $T_1$ has a maximal matching such that $u$ is not matched by this matching, and in turn $T$ has a maximum matching such that $u$ is not matched by this matching, a contradiction to the
and the set of unicyclic graphs which satisfies the condition:

$$ G $$

is an elementary unicyclic graph.

Then join an edge from each of the

$$ t $$

vertices chosen in

$$ U $$

(1) Using induction principle on

$$ e(T) $$

Since

$$ u $$

is mismatched in

$$ T $$,

$$ e(T) \neq 1 $$.

Without loss of generality, let

$$ e(T) \geq 2 $$.

If

$$ e(T) = 2 $$,

$$ T = P_3 = wv $$,

by Lemma 2.1,

$$ \eta(G) = 0 + \eta(G - v - w) = \eta(T - u) + \eta(G - (T - u)). $$

Suppose the result holds for all trees

$$ T $$

with

$$ e(T) < m $$.

Now we consider the case of

$$ e(T) = m $$.

If

$$ T $$

is a star,

$$ u $$

must be a pendent vertex for it is mismatched in

$$ T $$,

by Lemmas 2.1 and 2.2,

$$ \eta(G) = \eta(G - (T - u)) + \nu(T) - 3 = \eta(G - (T - u)) + \eta(T - u). $$

Otherwise, let

$$ w \in T \ (w \neq u) $$

be a quasi-pendent vertex adjacent to the pendent vertex

$$ w' \in T $$.

Let the components of

$$ T - w - w' $$

be

$$ T_1, T_2, \ldots, T_s \ (s \geq 1) $$,

where

$$ T_1 $$

contains the vertex

$$ u $$.

We claim that

$$ u $$

is still mismatched in

$$ T_1 $$.

Consider a maximal matching

$$ M $$

of

$$ T $$,

which contains a pendent edge

$$ e_w $$

joining

$$ w $$

and

$$ w' $$,

and

$$ u $$

is mismatched in

$$ M $$.

Then

$$ M = M_1 \cup M_2 \cup \cdots \cup M_s \cup e_w $$,

where

$$ M_i = M \cap E(T_i) $$

is still a maximal matching of

$$ T_i $$

for

$$ i = 1, 2, \ldots, s $$.

If

$$ u $$

is perfectly matched in

$$ T_1 $$,

then

$$ T_1 $$

has a maximal matching such that

$$ u $$

is not matched by this matching.

Note that

$$ e(T_1) < m $$,

and then by Lemmas 2.1 and 2.2 and by induction,

$$ \eta(G) = \eta(G - w - w') = \sum_{i=2}^{s} \eta(T_i) + \eta(G - \sum_{i=2}^{s} T_i - w - w')) $$

(by Lemmas 2.1, 2.2)

$$ = \sum_{i=2}^{s} \eta(T_i) + \eta((G - \sum_{i=2}^{s} T_i - w - w')) - (T_1 - u)) + \eta(T_1 - u) $$

(by induction)

$$ = \sum_{i=2}^{s} \eta(T_i) + \eta(T_1 - u) + \eta(G - (T - u)) $$

(by Lemma 2.1).

\[ \square \]

**Corollary 2.6** Let

$$ u $$

be a mismatched vertex of a tree

$$ T $$.

Then

$$ \eta(T - u) = \eta(T) - 1. $$

We call

$$ U $$

an elementary unicyclic graph if it satisfies

(a)

$$ U $$

is the cycle

$$ C_n $$

where

$$ n \neq 0 \ (\mod 4) $$; or

(b)

$$ U $$

is obtained from

$$ C_n $$

and

$$ tK_1 $$

by the rule: First select

$$ t $$

vertices from

$$ C_n $$

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

$$ C_n $$

to an isolated vertex.

We denote by

$$ NS(\mu) $$

and

$$ U_0 $$

respectively the set of nonsingular unicyclic graph on

$$ n $$

vertices,

and the set of unicyclic graph which satisfies the condition:

$$ G \in U_0 $$

is an elementary unicyclic graph or a unicyclic graph obtained by joining a vertex of PM-trees with an arbitrary vertex of an elementary unicyclic graph.

**Theorem 2.7** ([6, 7]) Let

$$ G $$

be a unicyclic graph. Then

$$ \eta(G) = 0 $$

if and only if

$$ G \in U_0. $$
3. Unicyclic graphs with nullity one

A unicyclic graph $G$ is called a second-elementary unicyclic graph if $U$ is obtained from an even cycle by attaching a pendent edge (see Figure 3 (i)), or is obtained from an odd cycle by attaching one pendent edge at two distinct vertices respectively (see Figure 3 (ii)), or is obtained from a cycle $C_n$ by attaching one pendent edge at $t$ ($t \equiv n - 1 \pmod{2}, t > 2$) distinct vertices such that there are an odd number of vertices on the cycle lying between exactly one pair of consecutive vertices of these $t$ vertices, and there are an even number (possibly zero) of vertices on the cycle lying between any other pair of consecutive vertices (see Figure 3 (iii)). Let $G$ be a second-elementary unicyclic graph, deleting the $t$ pendent vertices together with their neighbors one by one. We get a set of separate paths and there is but one path with odd cardinality. By Lemmas 2.1 and 2.2, $\eta(G) = 1$.

Denote by $U_1$ the set of unicyclic graphs which satisfy one of the following conditions:

(i) $G$ is a second-elementary unicyclic graph;

(ii) $G$ is obtained by joining one vertex of each of several PM-trees to an arbitrary vertex of a second-elementary unicyclic graph (see Figure 4(i));

(iii) $G$ is obtained from the graph as in (ii) by the rule: First, join a mismatched vertex of a tree with nullity one to an arbitrary quasi-pendent vertex of an elementary unicyclic graph. Then join one vertex of each of several PM-trees to an arbitrary vertex of the elementary unicyclic graph (see Figure 4(ii));

(iv) $G$ is a unicyclic graph obtained by the rule: First, join a perfectly matched vertex of a tree with nullity one with an arbitrary vertex of an elementary unicyclic graph. Then join one vertex of each of several PM-trees to an arbitrary vertex of the elementary unicyclic graph (see Figure 4(iii)).
Let $G$ be a unicyclic graph with $\eta(G) = 1$. By Lemma 2.3, $G$ is not a cycle. Let $C_n$ be the cycle of $G$ and $V(C_n) = \{v_i : i = 1, 2, \ldots, n\}$, and $G - E(C_n) = T_1 \cup T_2 \cup \cdots \cup T_n$, where $T_1, T_2, \ldots, T_n$ are the set of trees in $G - E(C_n)$ containing vertices $v_1, v_2, \ldots, v_n$, respectively.

**Assertion 3.1** If for some $i$, $v_i$ is a mismatched vertex of $T_i$. By Lemma 2.5 (ii), $\eta(G) = \eta(G - (T_i - v_i)) + \eta(T_i - v_i) = 1$, thus $\eta(T_i - v_i) \leq 1$.

**Assertion 3.2** If for some $i$, $v_i$ is a perfectly matched vertex of $T_i$. By Lemma 2.5 (i), $\eta(G) = \eta(G - T_i) + \eta(T_i) = 1$, thus $\eta(T_i) \leq 1$.

For simplicity, we introduce the following notations:

- $T_{m0} = \{T \in T_i \mid v_i \text{ is a mismatched vertex of } T_i \text{ and } \eta(T_i - v_i) = 0\}$;
- $T_{m1} = \{T \in T_i \mid v_i \text{ is a mismatched vertex of } T_i \text{ and } \eta(T_i - v_i) = 1\}$;
- $T_{p0} = \{T \in T_i \mid v_i \text{ is a perfectly matched vertex of } T_i \text{ and } \eta(T_i) = 0\}$;
- $T_{p1} = \{T \in T_i \mid v_i \text{ is a perfectly matched vertex of } T_i \text{ and } \eta(T_i) = 1\}$.

**Assertion 3.3** $T_{m1} \cup T_{p0} \cup T_{p1} \neq \emptyset$.

**Proof** If for all $i$ ($1 \leq i \leq n$), $v_i$ is a mismatched vertex of $T_i$ and $\eta(T_i - v_i) = 0$, then applying Lemma 2.5 (ii) repeatedly, $\eta(G) = \eta(C_n) + \sum_{i=1}^{n} \eta(T_i - v_i) = 1$. Thus $\eta(C_n) = 1$, which is impossible. □

**Assertion 3.4** Let $U$ be an elementary unicyclic graph and $u$ be one of its pendent vertices, $N_U(u) = u_0$. Then $\eta(U + u_0v) = 1$, where $v$ is an isolated vertex.

**Proof** By Lemmas 2.1 and 2.2, $\eta(U + u_0v) = \eta(U - u_0 - u) + \eta(K_1) = \eta(U) + \eta(K_1) = 1$. □

**Theorem 3.5** Let $G$ be a unicyclic graph. Then $\eta(G) = 1$ if and only if $G \in \mathcal{U}_1$.

**Proof** ($\Rightarrow$) We carry out the proof in three cases.

**Case 1** If $T_{m1} \neq \emptyset$, then for some $i$, $v_i$ is a mismatched vertex of $T_i$, $\eta(T_i - v_i) = 1$. There is one but only one component of $T_i - v_i$ with nullity one (others zero). Let it be $T_0$ and $v_0 \in T_0$ join with $v_i$. Since $v_i$ is mismatched in $T_i$, $v_0$ must be perfectly matched in $T_0$ (or else, $\eta(T_i - v_i - v_0) = 0$ and $T_i - v_i - v_0$ is a PM-acyclic graph, we add edge $v_0v_i$ to a perfect matching of $T_i - v_i - v_0$, then we would get that $T_i$ is a PM-tree, contradiction). And in this case $G - (T_i - v_i)$ is a unicyclic graph with nullity zero. By Theorem 2.7, $G$ satisfies condition (iv).

**Case 2** If $T_{p1} \neq \emptyset$, then for some $i$, $v_i$ is a perfectly matched vertex of $T_i$ and $\eta(T_i) = 1$. Let $M(T_i)$ be one of its maximal matchings, $uv_i \in M(T_i)$. Then $\eta(T - u - v_i) = 1$ and there is one but only one component of $T_i - u - v_i$ with nullity one (others zero). Let it be $T_0$ and $v_0 \in T_0$ join with $v_i$ or $u$. If $v_0$ is adjacent to $u$, $v_0$ must be a perfectly matched vertex of $T_0$ (or else replace $uv_i$ by $uv_0$ in $M(T_i)$, we get another maximal matching of $T_i$ and $v_i$ is mismatched, contradiction). But no matter in what cases, by Lemma 2.5 (i), $\eta(G - T_0) = \eta(G) - \eta(T_0) = 0$, $G - T_0$ is a unicyclic graph with nullity zero. By Theorem 2.7, $G$ satisfies condition (iii) or (iv).
Case 3 If \( T_{m1} = \emptyset, T_{p1} = \emptyset, \) by Assertion 3.3, \( T_{p0} \neq \emptyset. \) Then \( G \) must satisfy condition (i) or (ii). By applying Lemma 2.5 repeatedly, \( \eta(G) = \eta(C_n - \bigcup_{T_i \in T_{p0}} u_i) + \sum_{T_i \in T_{m0}} \eta(T_i - u_i) + \sum_{T_i \in T_{p0}} \eta(T_i) = \eta(C_n - \bigcup_{T_i \in T_{p0}} v_i) = 1, \) and \( C_n - \bigcup_{T_i \in T_{p0}} v_i \) is composed of some paths. Then there is but one odd-path which implies that:

(a) \( C_n \) is an even cycle, when \( |T_{p0}| = 1; \)

(b) \( C_n \) is an odd cycle, when \( |T_{p0}| = 2; \)

(c) There is but one pair of consecutive vertices of \( \{v_i \in T_i | T_i \in T_{p0} \} \subseteq C_n \) with an odd number of vertices in \( C_n \) between them, when \( |T_{p0}| > 2. \)

For each \( T_i \in T_{p0}, v_i \) is a perfectly matched vertex of \( T_i \) and \( T_i \) is a PM-tree. Let \( M(T_i) \) be one of its perfect matchings, and \( u_i \in M(T_i). \) By Theorem 2.4, each component of \( T - u - v_i \) is a PM-tree, and they are joined with \( u \) or \( v_i \) by an edge.

For each \( T_i \in T_{m0}, v_i \) is a mismatched vertex of \( T_i \) (here \( T_i \neq K_1 \)). Since \( \eta(T_i - v_i) = 0, \) by Lemma 2.2 and Theorem 2.4, the nullity of each component of \( T_i - v_i \) is zero and they are all PM-trees joining with \( v_i \) by an edge.

Now we have \( G \) is a second-elementary unicyclic graph (when \( T_{m0} = \emptyset \) and for all \( T_i \in T_{p0}, T_i = P_2 \), or \( G \) is a unicyclic graph obtained by joining a vertex of \( PM \)-trees with an arbitrary vertex of a second-elementary unicyclic graph, repeatedly.

Summarizing the above, we complete the proof of the necessity.

\((\Leftarrow)\) We verify each possible cases.

If \( G \) is a unicyclic graph which satisfies condition (i), \( \eta(G) = 1. \)

If \( G \) is a unicyclic graph which satisfies condition (ii), then by applying Lemma 2.5 (i) repeatedly, we have \( \eta(G) = \eta(S) = 1, \) where \( S \) is a second-elementary unicyclic graph.

If \( G \) is a unicyclic graph satisfying condition (iii). Let \( U \) be an elementary unicyclic graph and \( u \) be one of its pendent vertices, \( N_U(u) = u_0. \) Let \( T_1 \) be a tree with nullity one, \( T_p \) be a set of disjoint \( PM \)-trees, and \( v \) be a mismatched vertex of \( T_1. \) \( G \) is obtained by joining \( v \) with \( u_0, \) and joining a vertex of \( PM \)-trees \( \subseteq T_p \) with an arbitrary vertex of \( U, \) repeatedly. Then by Corollary 2.6, \( \eta(T_1 - v) = 0. \) Using Lemma 2.5 repeatedly, we have

\[
\eta(G) = \eta(T_1 - v) + \sum_{T \in T_p} \eta(T) + \eta(U + u_0v) = \eta(U + u_0v).
\]

By Assertion 3.4, \( \eta(G) = 1. \)

If \( G \) is a unicyclic graph satisfying condition (iv), with the similar discussion as above, by applying Lemma 2.5 repeatedly, we have

\[
\eta(G) = \eta(T_1) + \sum_{T \in T_p} \eta(T) + \eta(U) = \eta(T_1) = 1.
\]

The proof of sufficiency is completed. \( \square \)

In paper [8], the author determined another necessary and sufficient condition for a graph \( G \) to be singular for acyclic and unicyclic graphs.

A pair \( V_1, V_2 \) of subsets of \( V(G) \) is said to satisfy the property (N) if \( V_1 \) and \( V_2 \) are nonempty and disjoint and \( \{N(v) | v \in V_1\} = \{N(v) | v \in V_2\}. \)
**Theorem 3.6** (see [8]) A unicyclic graph $G$ is singular if and only if there is a pair of subsets $V_1$ and $V_2$ of $V(G)$ satisfying the property (N).

Using the same method, we also have

**Theorem 3.7** Let $G$ be a unicyclic graph. Then $\eta(G) = 1$ if and only if there is a pair of subsets $V_1$ and $V_2$ of $V(G)$ satisfying the property (N), and there exists a vertex $u \in V(G)$ such that $G - u$ contains no such pair of subsets.

**Example 3.8** Consider the graphs in Figure 5.

(a) $\eta(G) > 1$, there is a pair of subsets $V_1$ and $V_2$ of $V(G)$ satisfying the property (N), and for each vertex $u \in V(G)$, $G - u$ still contains such pair of subsets;

(b) $\eta(G) = 1$, there is a pair of subsets $V_1$ and $V_2$ of $V(G)$ satisfying the property (N), and there exists a vertex $u \in V(G)$, such that $G - u$ contains no such pair of subsets;

(c) $\eta(G) = 0$, there exist no pair of subsets $V_1$ and $V_2$ of $V(G)$ satisfying the property (N).

Figure 5 Examples of Theorems 3.6 and 3.7

**References**


